

## Supporting Information

*Rec. Nat. Prod.* 17:2 (2023) 275-279

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

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Chemical Structure similarity

**REFERENCES**

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

**SUBSTANCES**

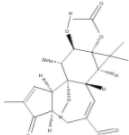
- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

**REACTIONS**

- Reaction Structure

**SUBSTANCES: CHEMICAL STRUCTURE**

Structure Editor:



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Import CXF

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<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	8
<input type="checkbox"/> 90-94	46
<input type="checkbox"/> 85-89	133
<input type="checkbox"/> 80-84	523
<input type="checkbox"/> 75-79	1732
<input type="checkbox"/> 70-74	7285
<input type="checkbox"/> 65-69	30283
<input type="checkbox"/> 0-64 (least similar)	85725

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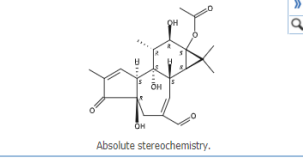
Analyze by:

- Substance Role
- Biological Study: 4
- Properties: 4
- Analytical Study: 3
- Reactant or Reagent: 3
- Uses: 3
- Preparation: 2
- Occurrence: 1
- Process: 1

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Score: 96

1. **30358-72-6**



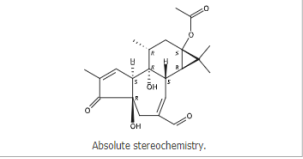
Absolute stereochemistry.

**C<sub>22</sub>H<sub>28</sub>O<sub>7</sub>**  
1*H*Cyclopropa[3,4]benz[1,2-*e*]azulene-3-carboxaldehyde, 9*a*-(acetyloxy)-1*a*,1*b*,4*a*,5*a*,7*a*,7*b*,8*a*,9*a*-decalhydro-4*a*,7*b*,9-trihydroxy-1,1,6,8-tetramethyl-5-oxo-, [1*a*]*A* (1*a*o,1*b*o,4*a*o,7*a*o,8*a*o,9*a*o): (9*CI*)

Key Physical Properties  
Spectra

Score: 96

2. **60857-09-2**



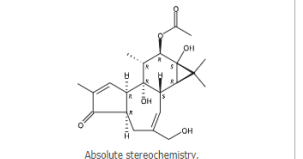
Absolute stereochemistry.

**C<sub>22</sub>H<sub>28</sub>O<sub>6</sub>**  
1*H*Cyclopropa[3,4]benz[1,2-*e*]azulene-3-carboxaldehyde, 9*a*-(acetyloxy)-1*a*,2,4,4*a*,5,7*a*,7*b*,8,9*a*-decalhydro-4*a*,7*b*-dihydroxy-1,1,6,8-tetramethyl-5-oxo-, [1*a*]*A* (1*a*o,1*b*o,5*a*o,7*a*o,7*b*o,8*a*o,8*a*o)

Key Physical Properties  
Spectra

Score: 96

3. **64181-02-8**

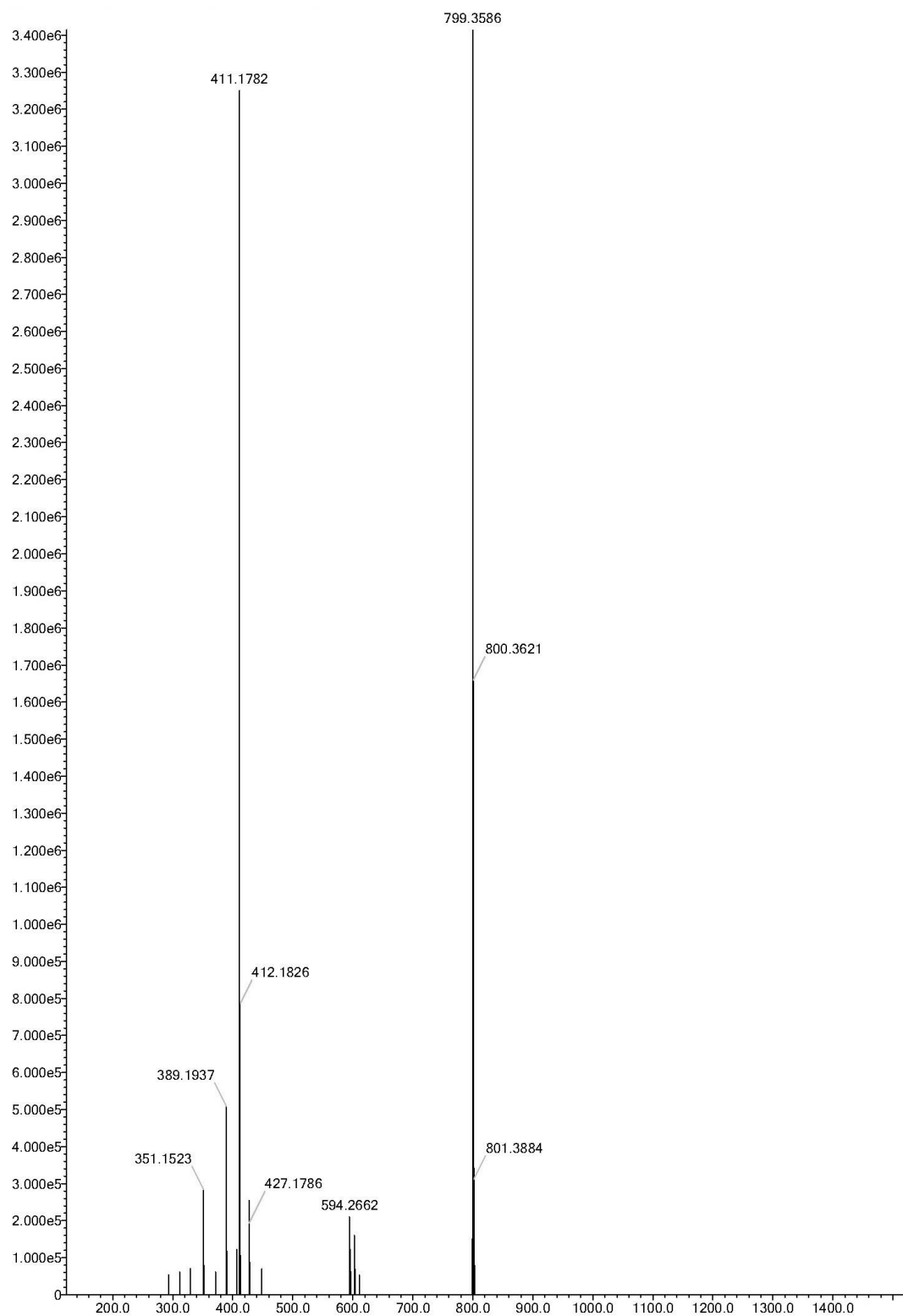


Absolute stereochemistry.

**C<sub>22</sub>H<sub>30</sub>O<sub>6</sub>**  
5*H*Cyclopropa[3,4]benz[1,2-*e*]azulene-3-one, 9-(acetyloxy)-1,1*a*,1*b*,4,4*a*,7*a*,7*b*,8,9*a*-decalhydro-7*b*,9*a*-dihydroxy-3-(hydroxymethyl)-1,1,6,8-tetramethyl-, [1*a*]*A* (1*a*o,1*b*o,4*a*o,7*a*o,7*b*o,8*a*o,9*a*o): (9*CI*)

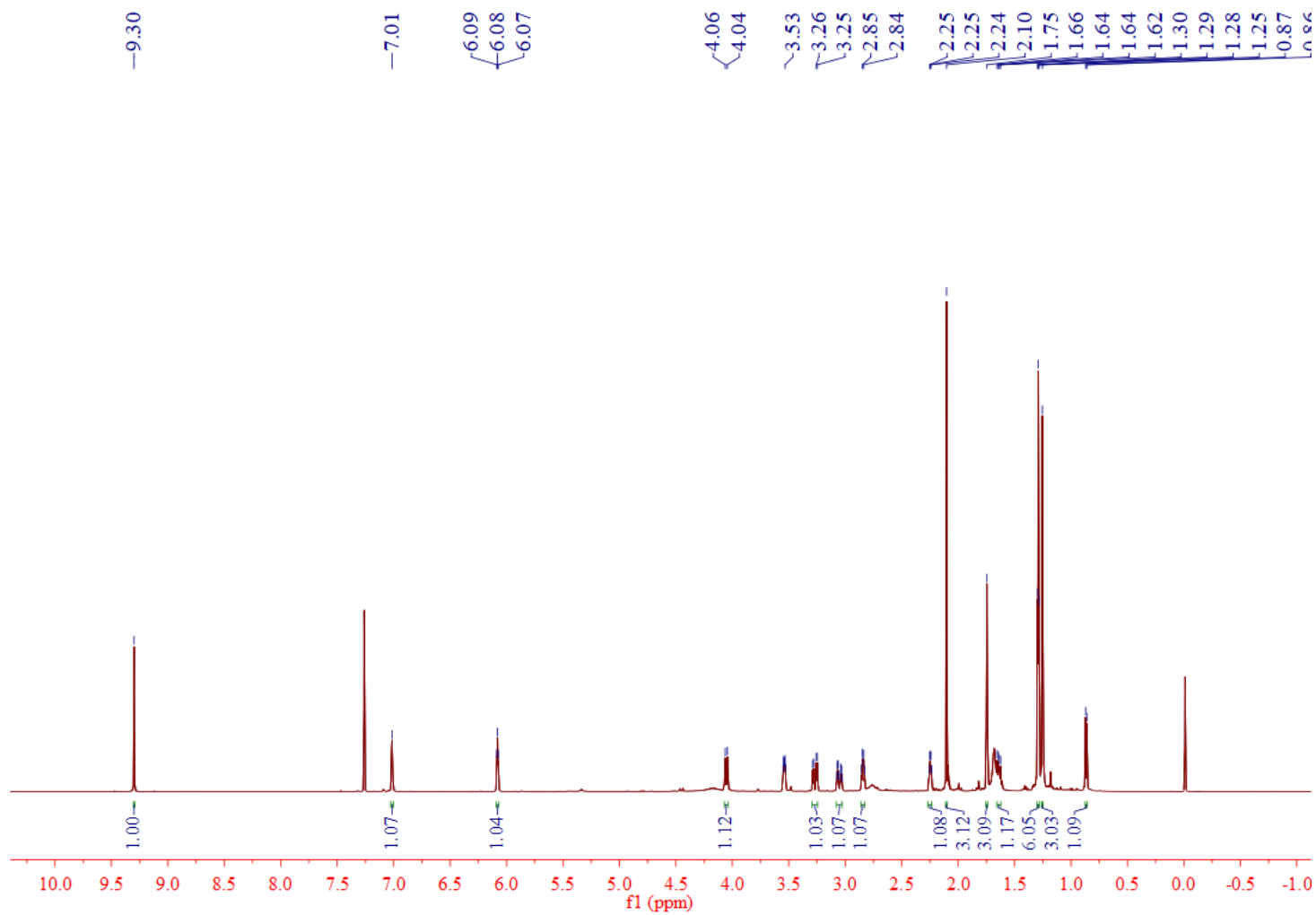
Key Physical Properties  
Spectra

**Figure S1: Scifinder search of compound 1**



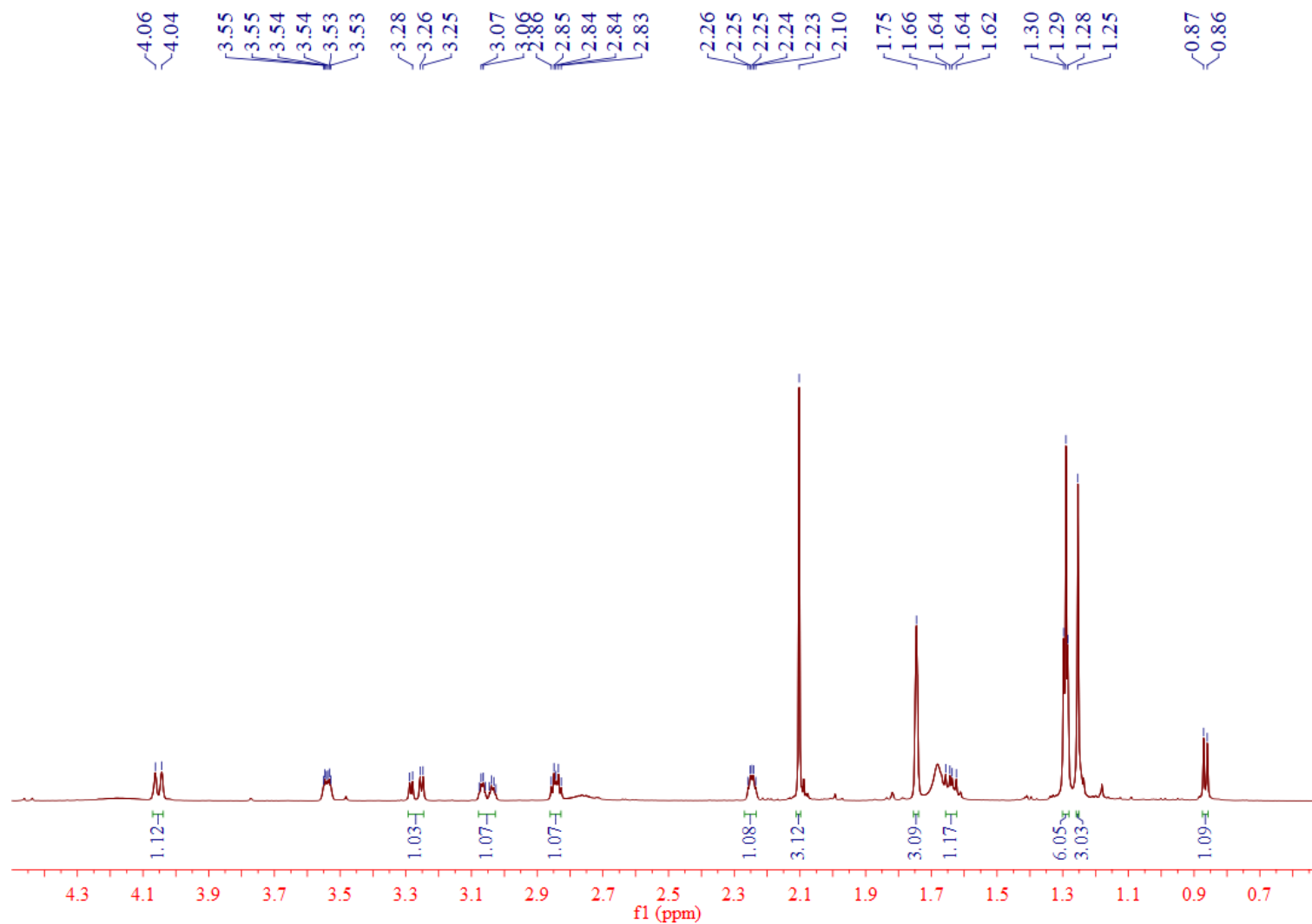
$C_{22}H_{28}O_6Na^+$ : Meas.  $m/z$  411.1782; Pred.  $m/z$  411.1778

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



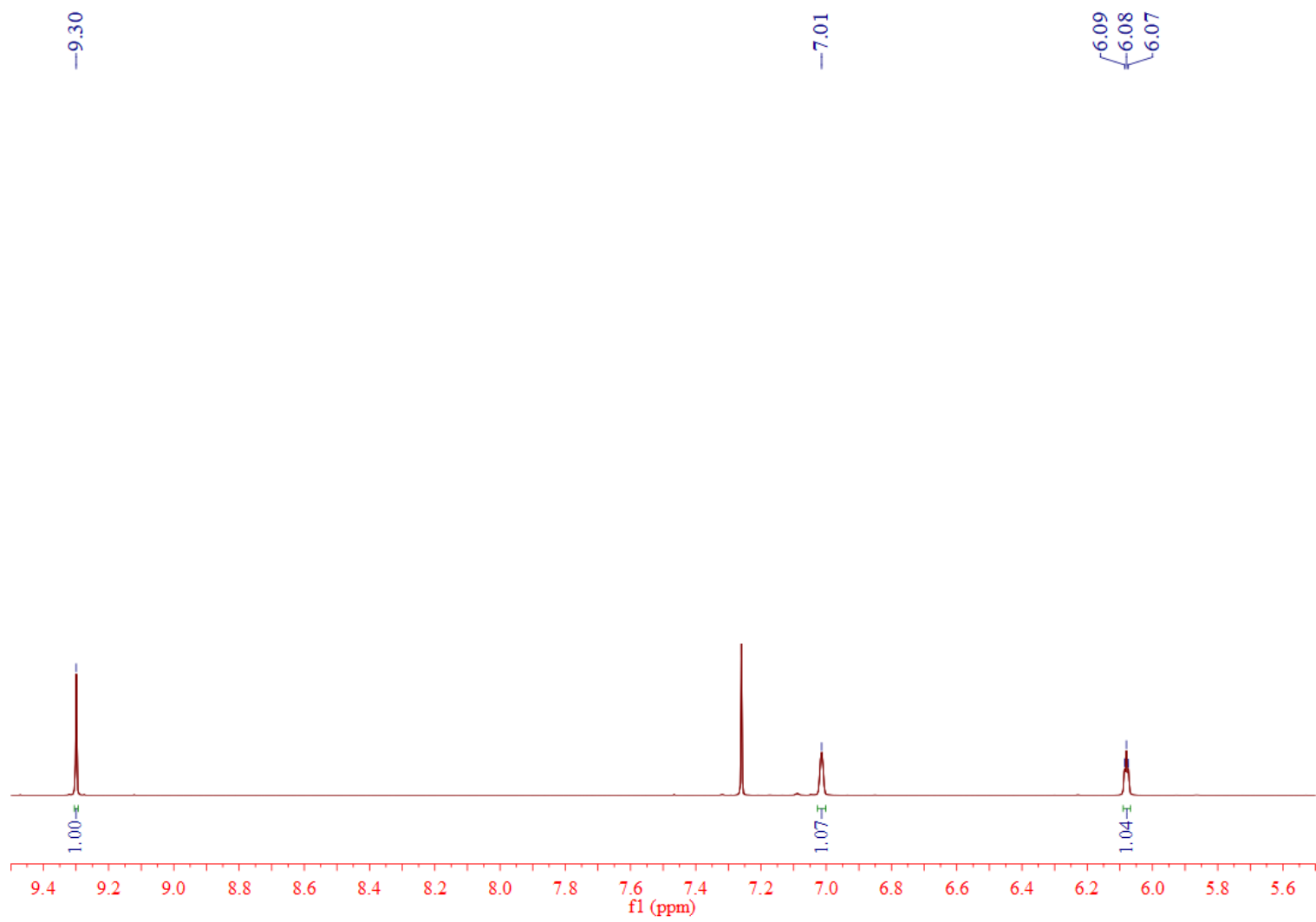
**Figure S3:** <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound **1**

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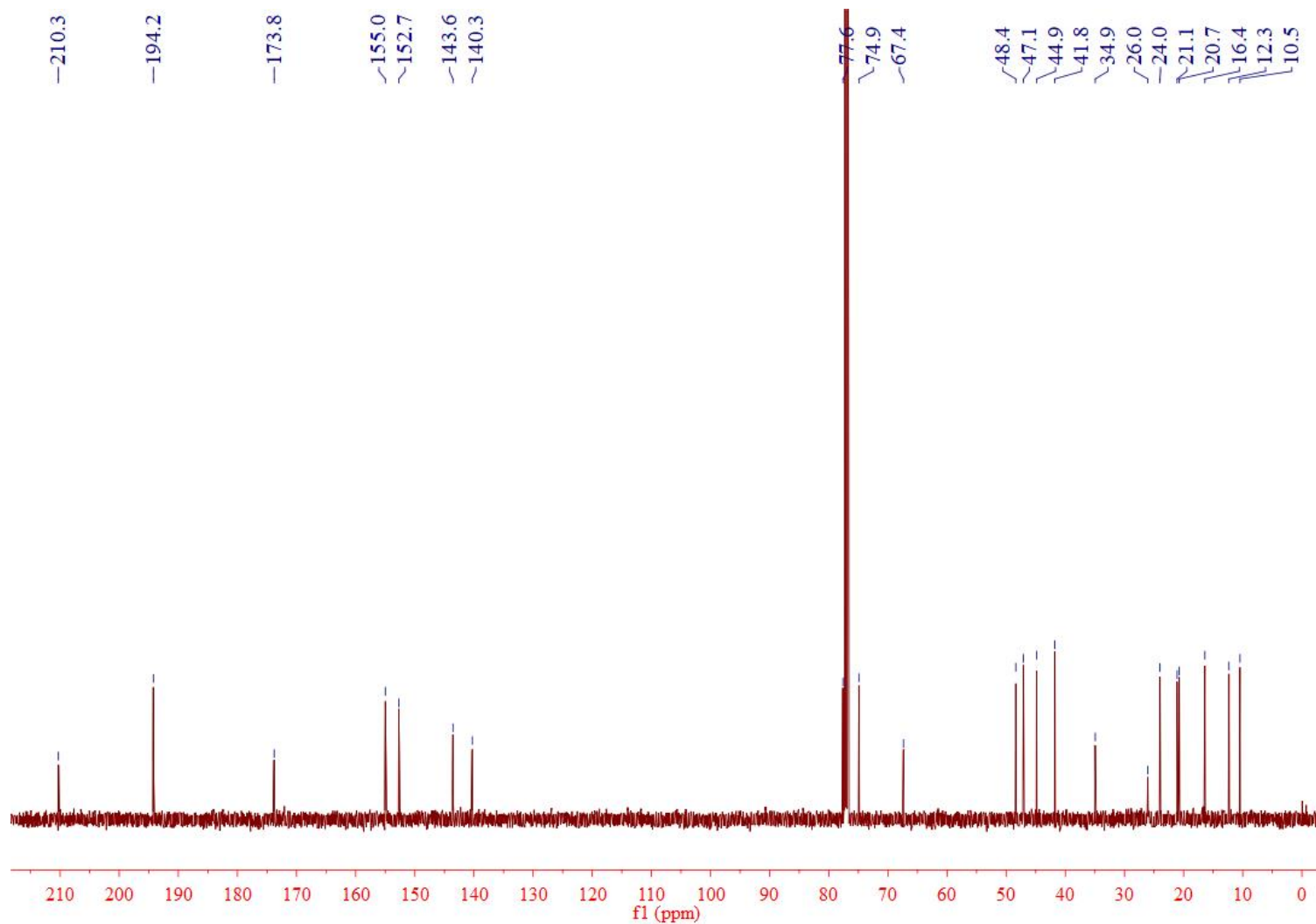
**Figure S4:** Enlarged <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound **1** ( $\delta_{\text{H}}$  0.5–4.5 ppm)

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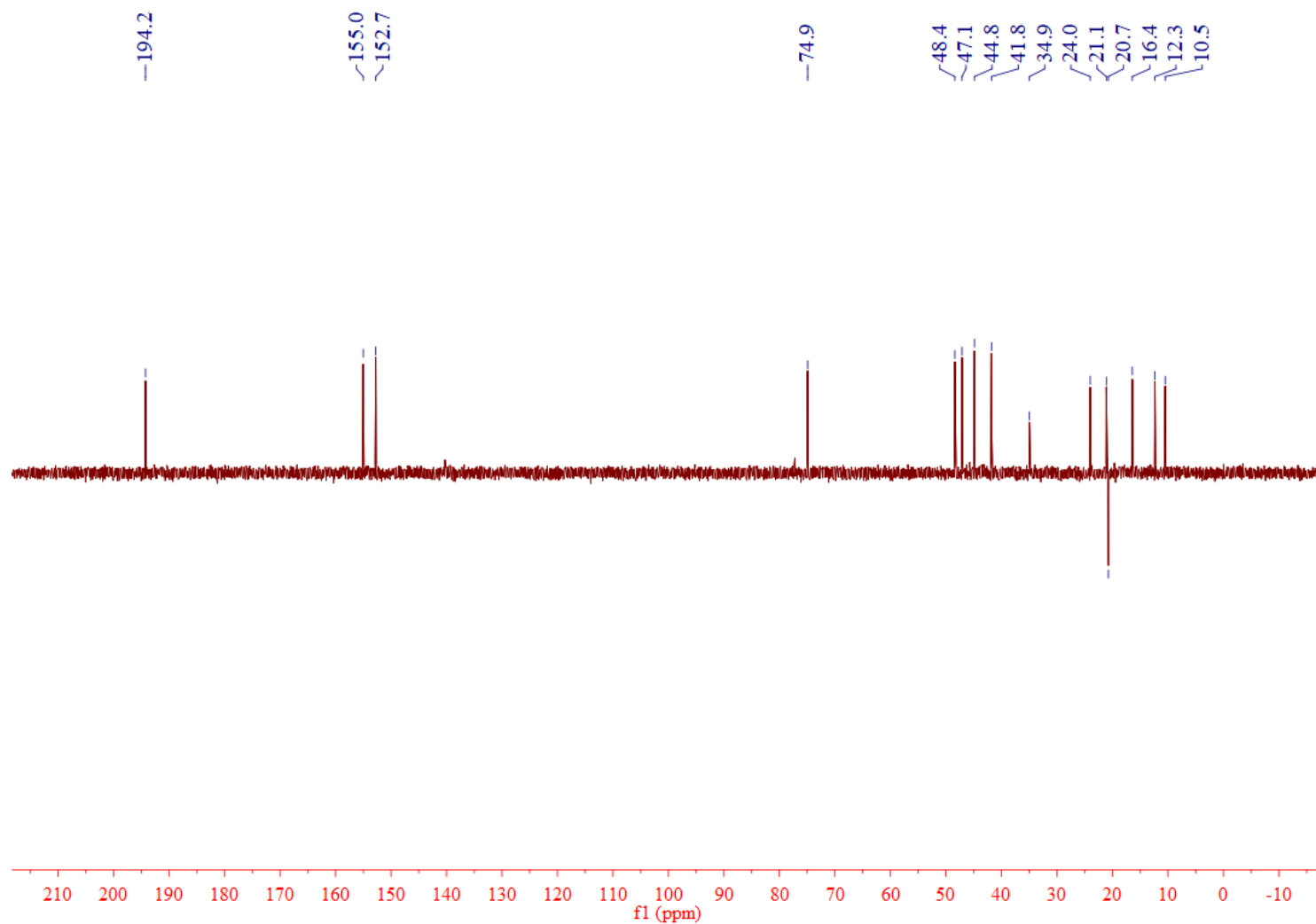
**Figure S5:** Enlarged <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound **1** ( $\delta_{\text{H}}$  5.5–9.5 ppm)

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**Figure S6:**  $^{13}\text{C}$ -NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound **1**

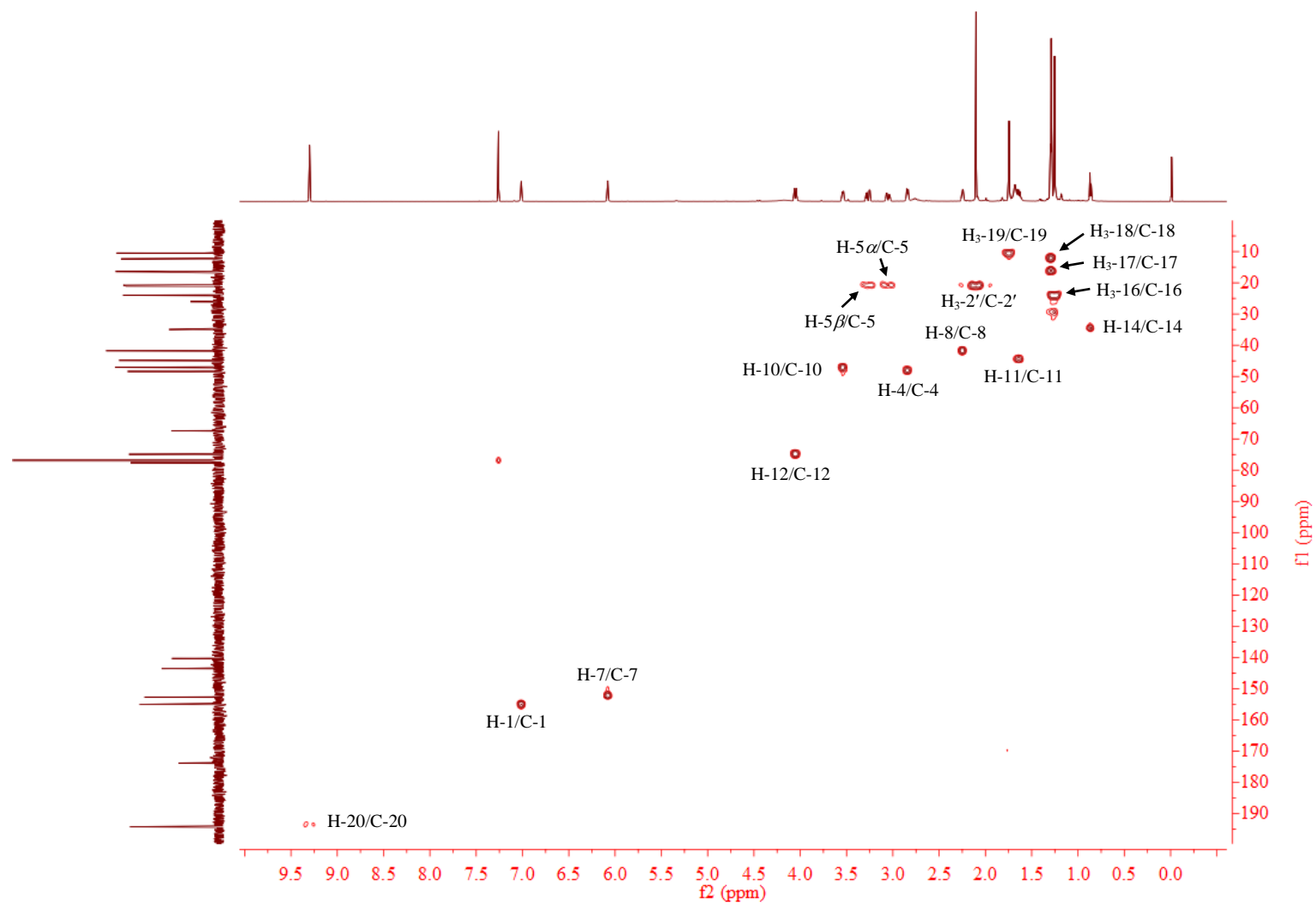
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**Figure S7:** DEPT135 (125 MHz, CDCl<sub>3</sub>) spectrum of compound **1**

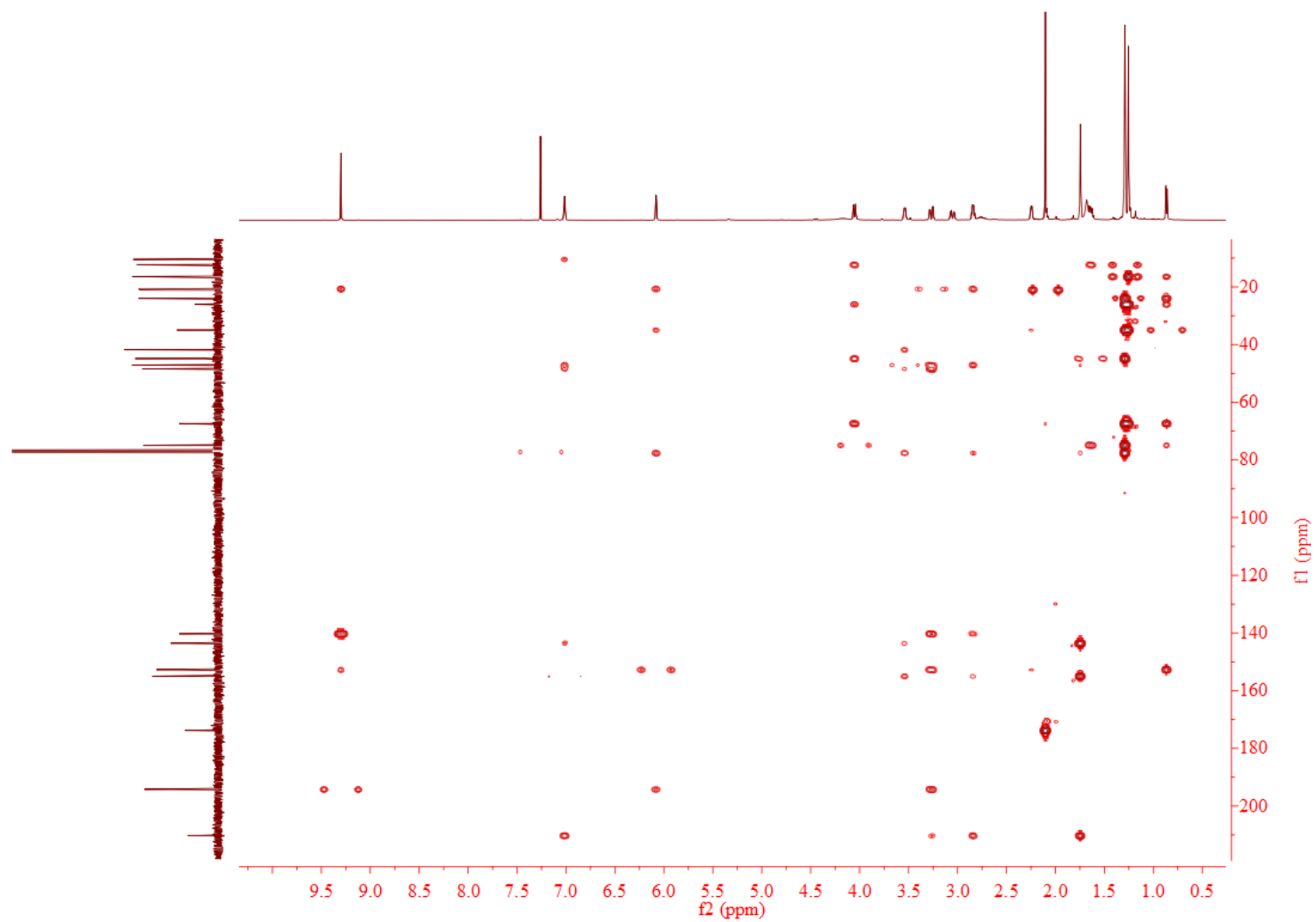
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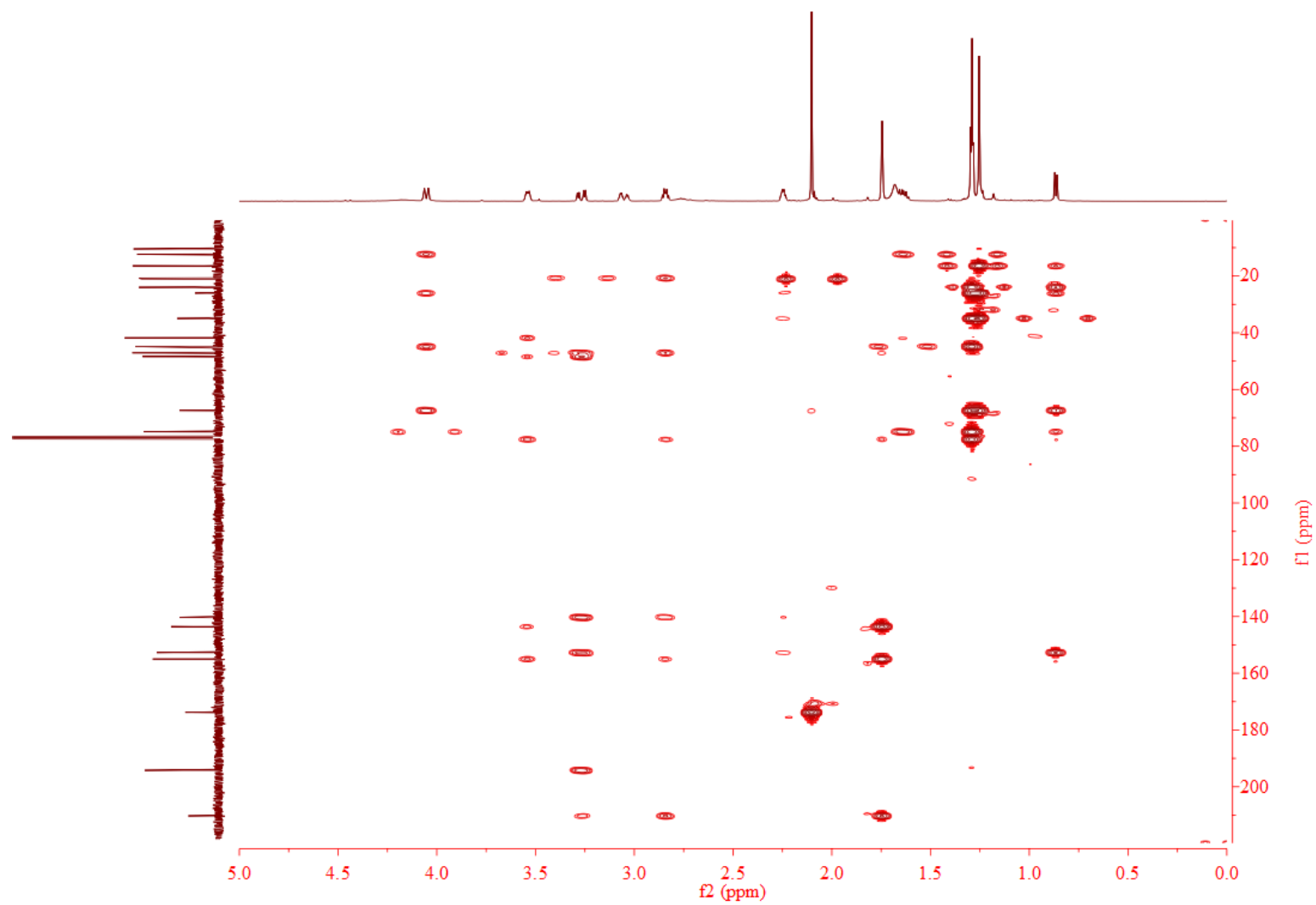
**Figure S8:** HSQC spectrum of compound **1**

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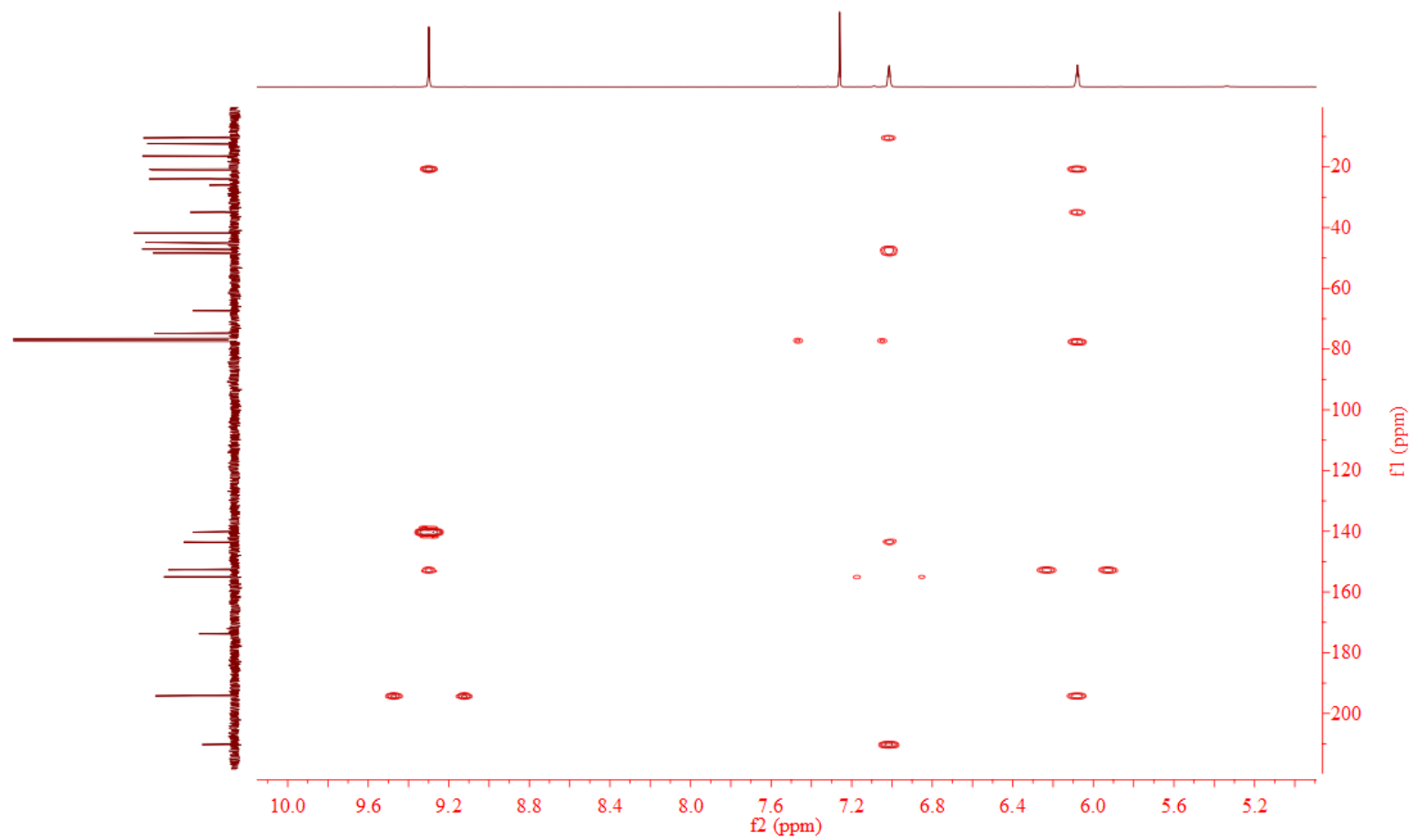
**Figure S9:** HMBC spectrum of compound **1**

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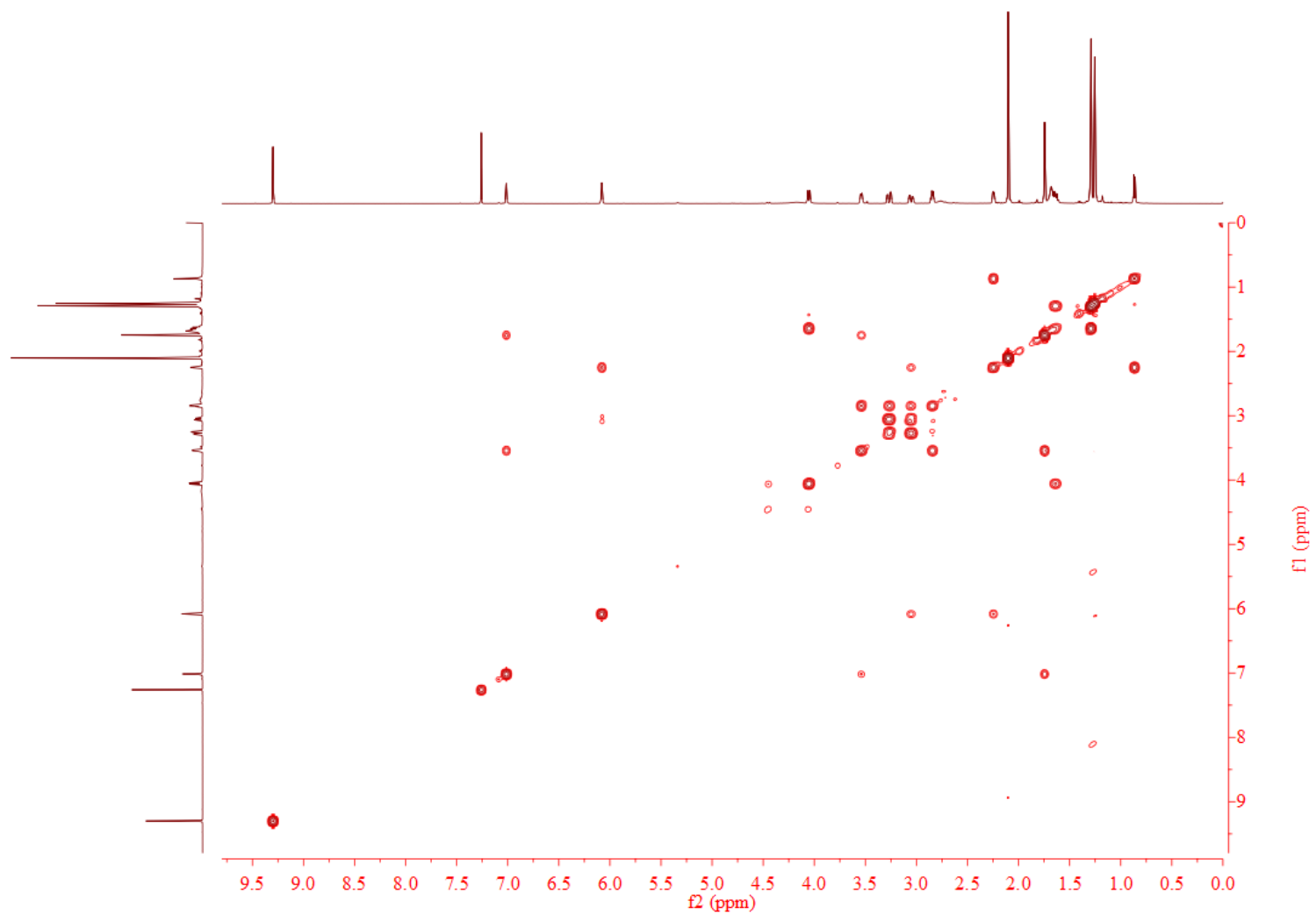
**Figure S10:** HMBC spectrum of compound **1** ( $\delta_{\text{H}}$  0–5 ppm)

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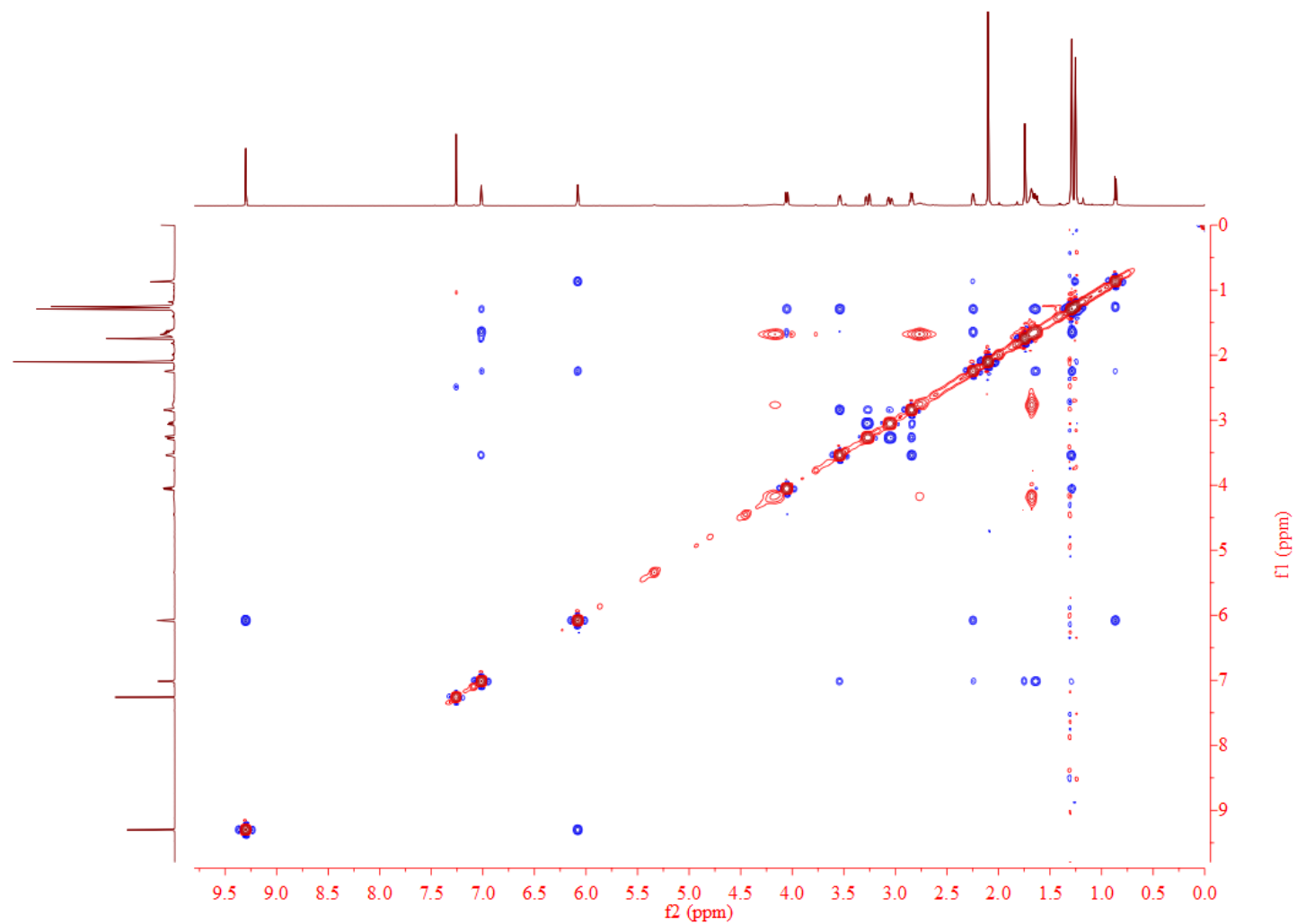
**Figure S11:** HMBC spectrum of compound **1** ( $\delta_{\text{H}}$  5–10 ppm)

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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-3     1.263             1.263
Z              4                 4
Mu (mm-1)     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**