Supporting Information

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

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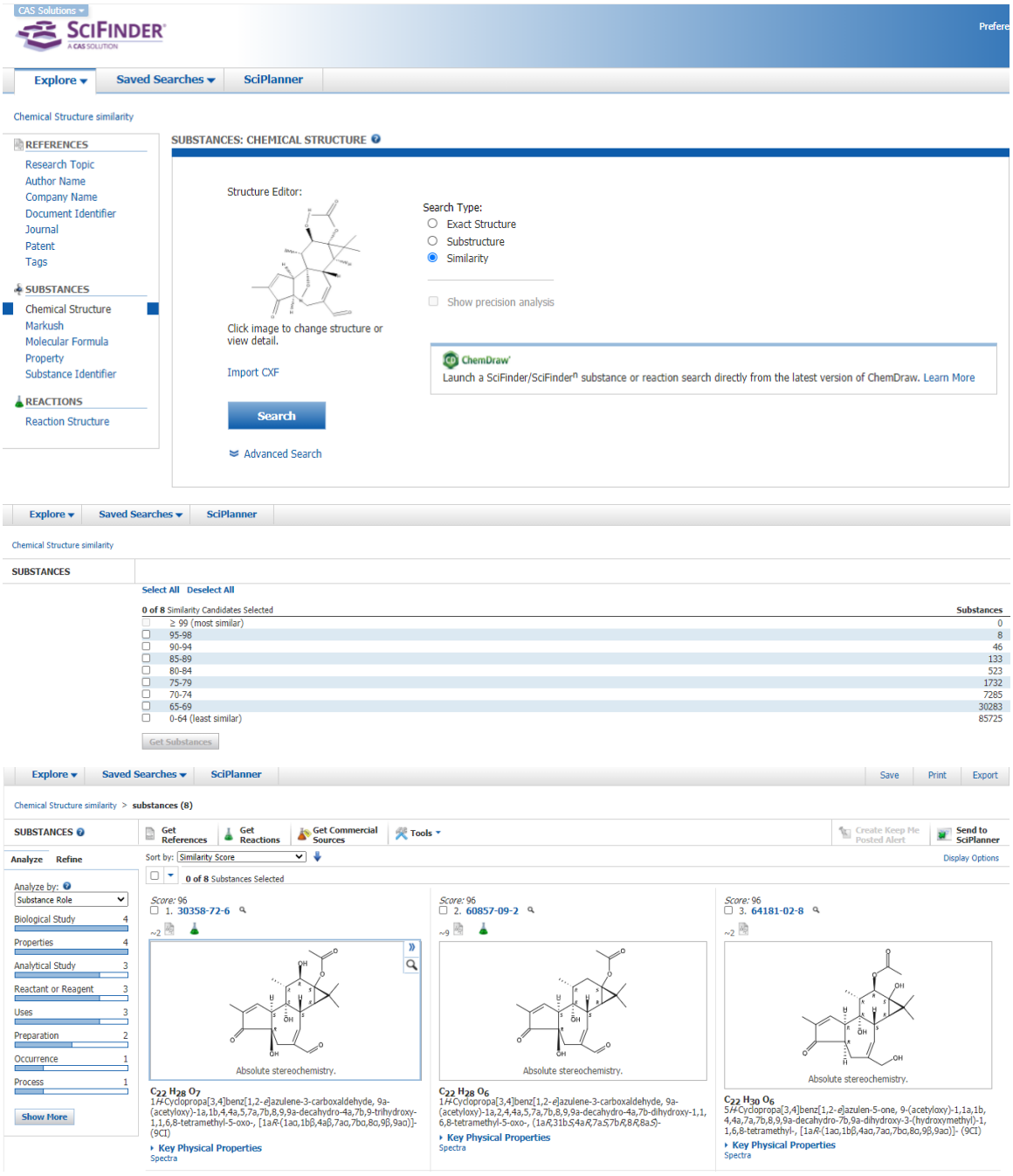
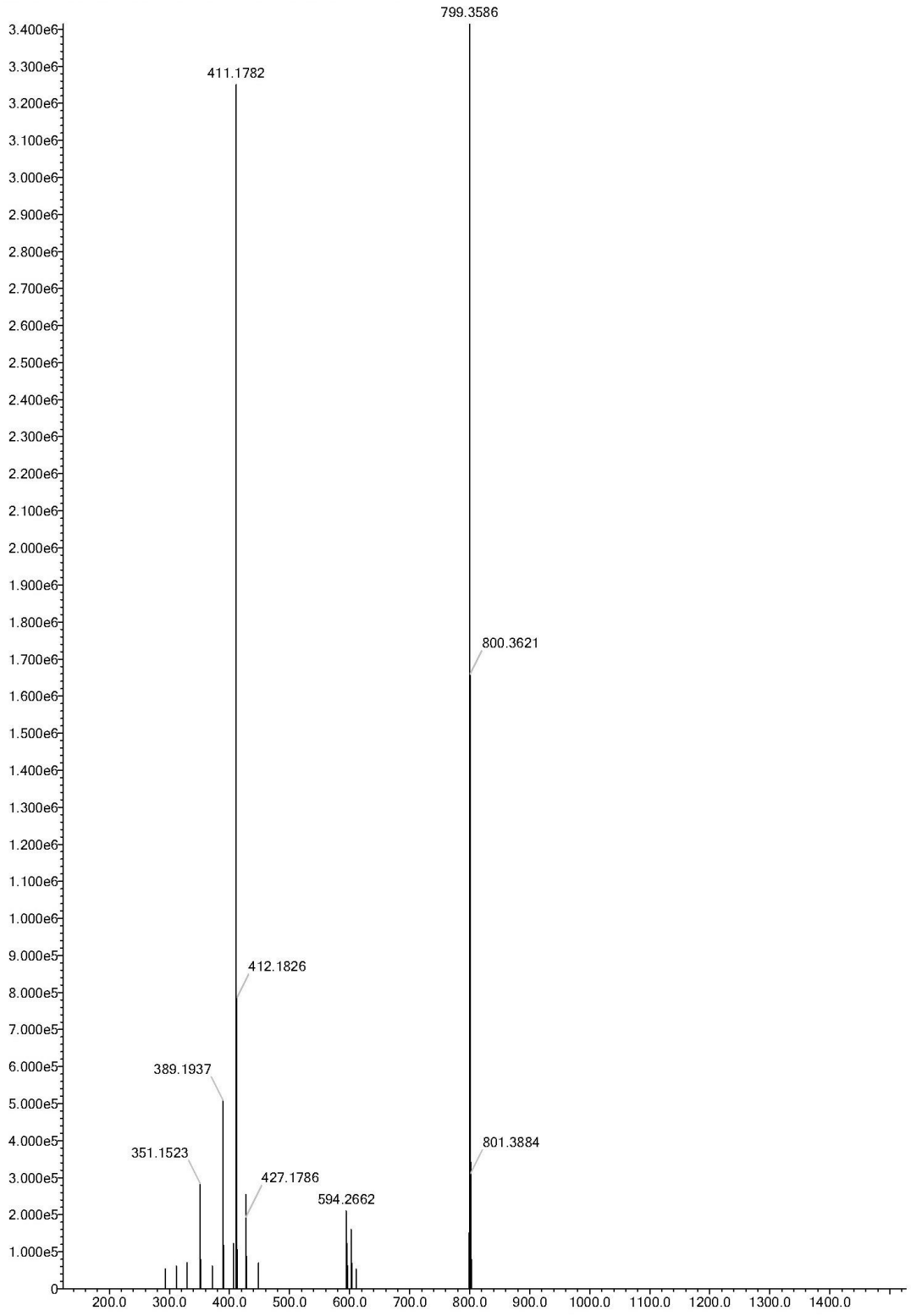


Figure S1: Scifinder search of compound **1**



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

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

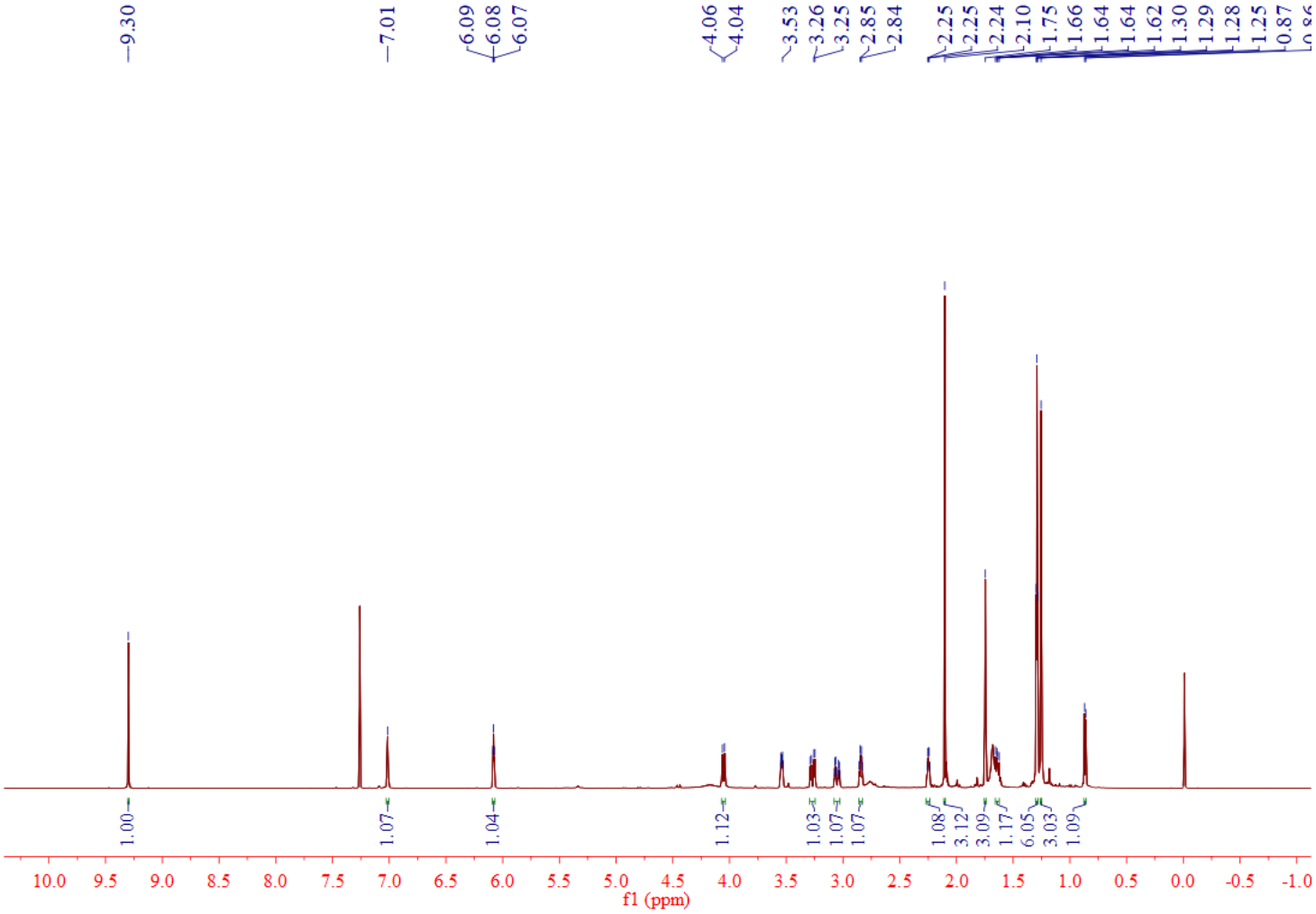


Figure S3: ^{1}H-NMR (500 MHz, $CDCl_3$) spectrum of compound **1**

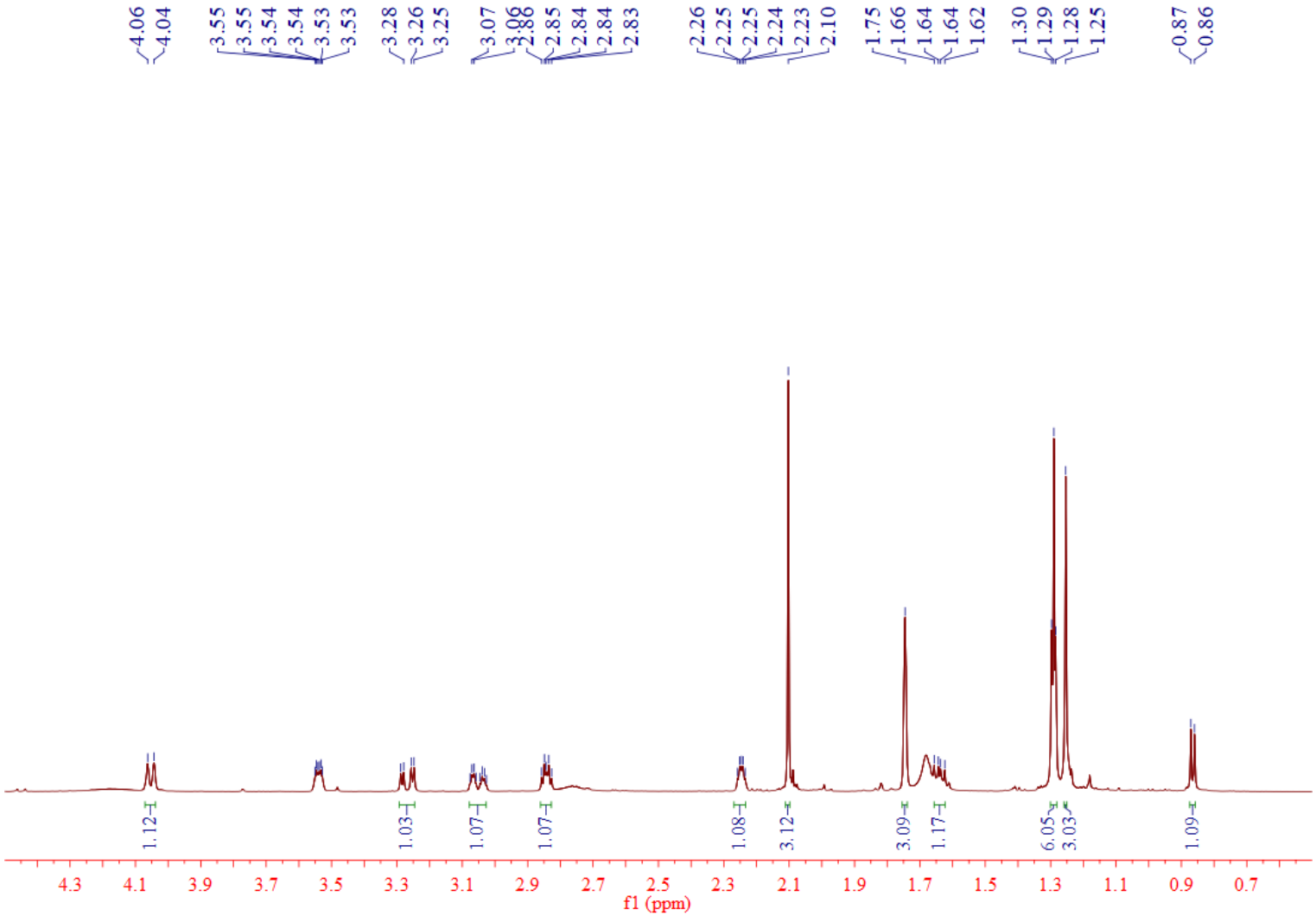


Figure S4: Enlarged ^{1}H-NMR (500 MHz, $CDCl_3$) spectrum of compound **1** (δ_H 0.5–4.5 ppm)

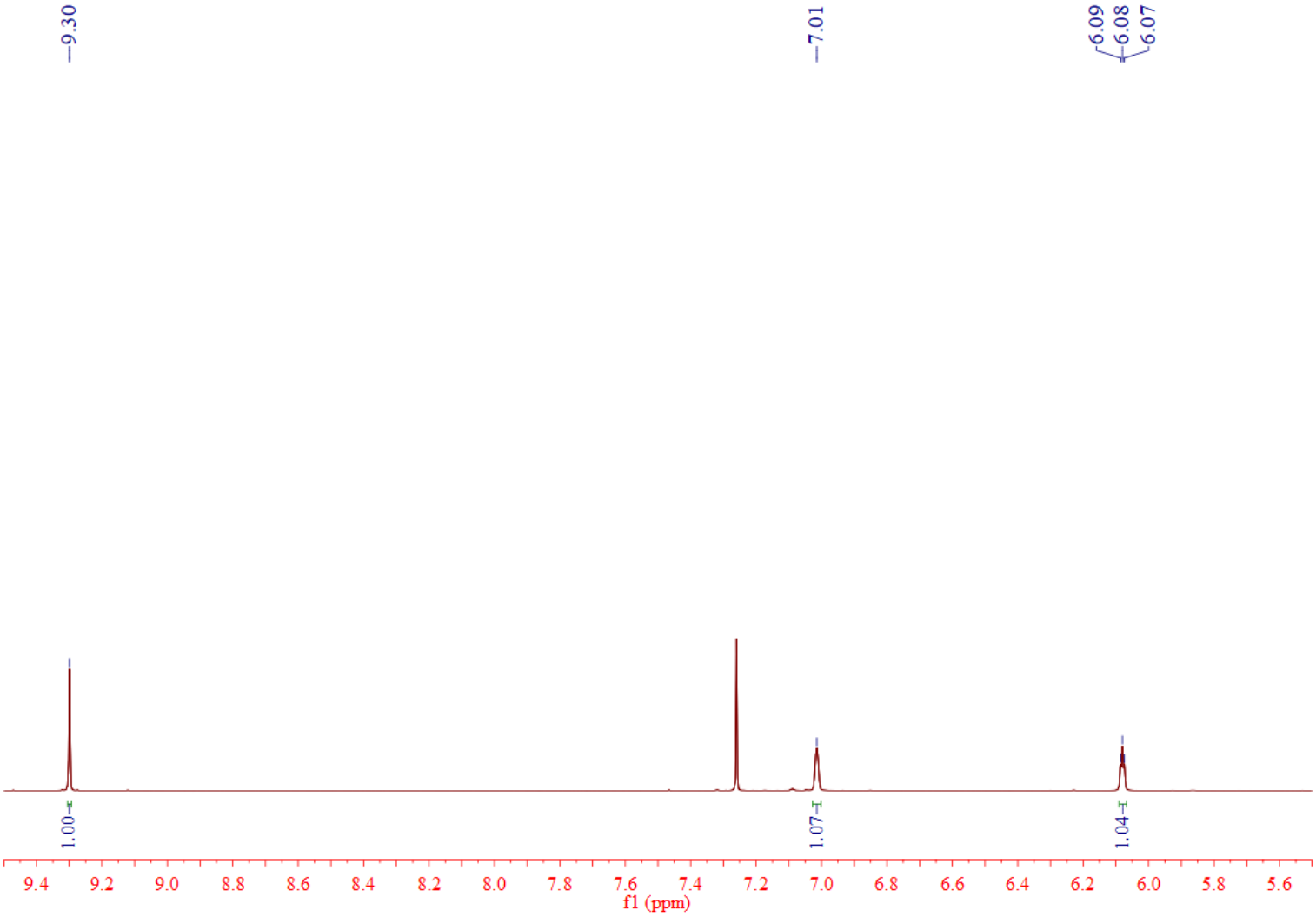


Figure S5: Enlarged ^{1}H-NMR (500 MHz, $CDCl_3$) spectrum of compound **1** (δ_H 5.5–9.5 ppm)

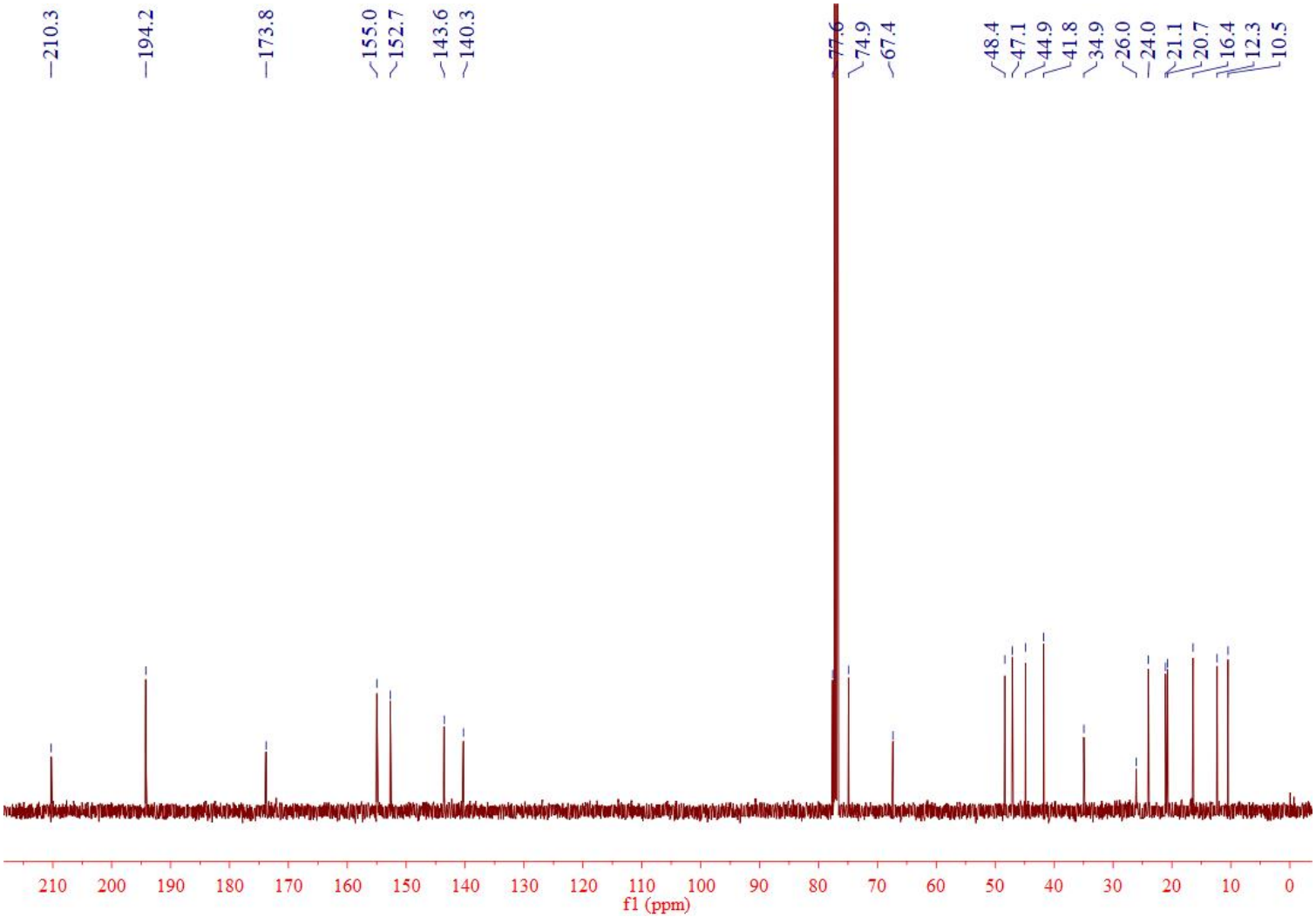


Figure S6: ^{13}C-NMR (125 MHz, $CDCl_3$) spectrum of compound **1**

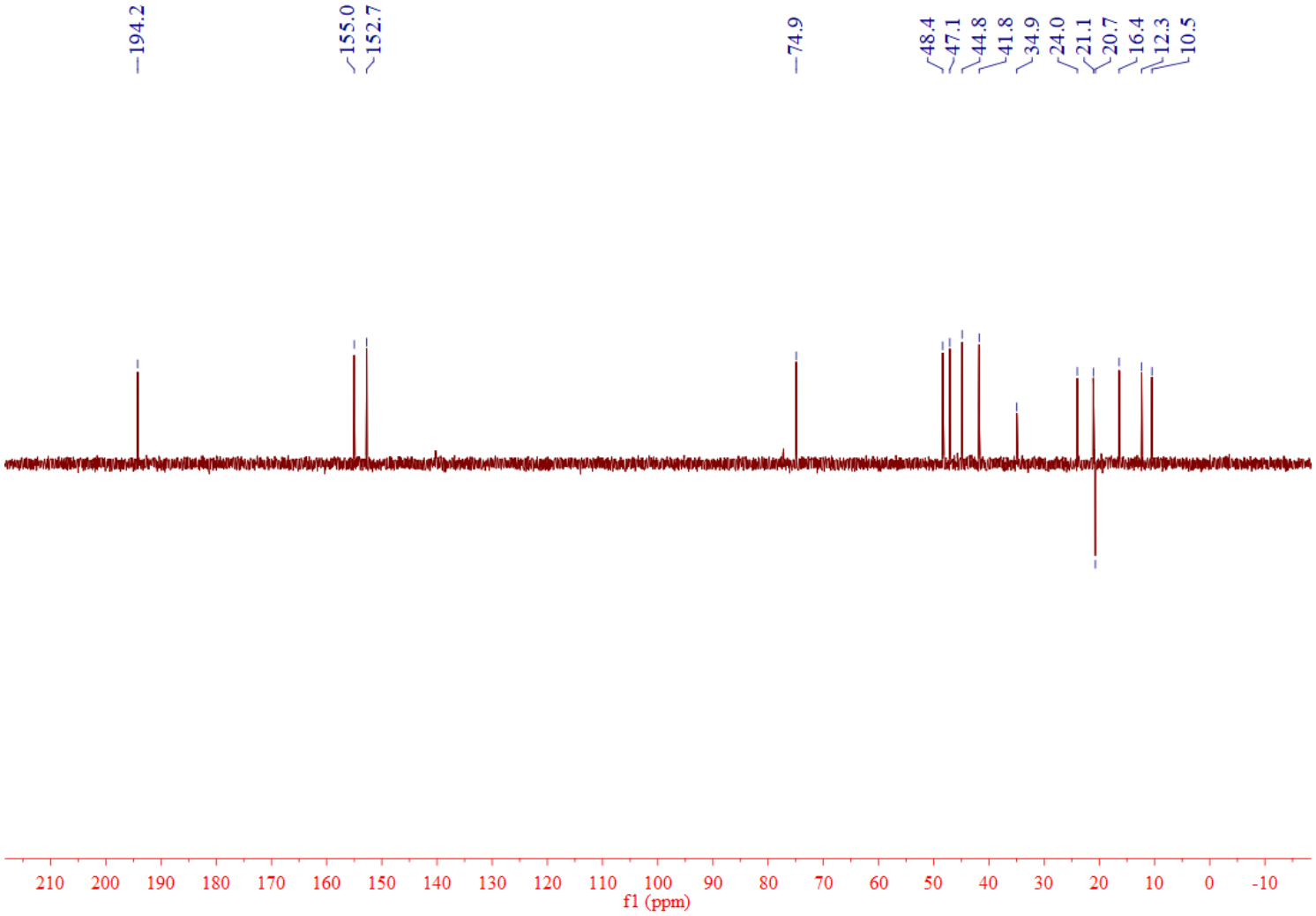


Figure S7: DEPT135 (125 MHz, $CDCl_3$) spectrum of compound **1**

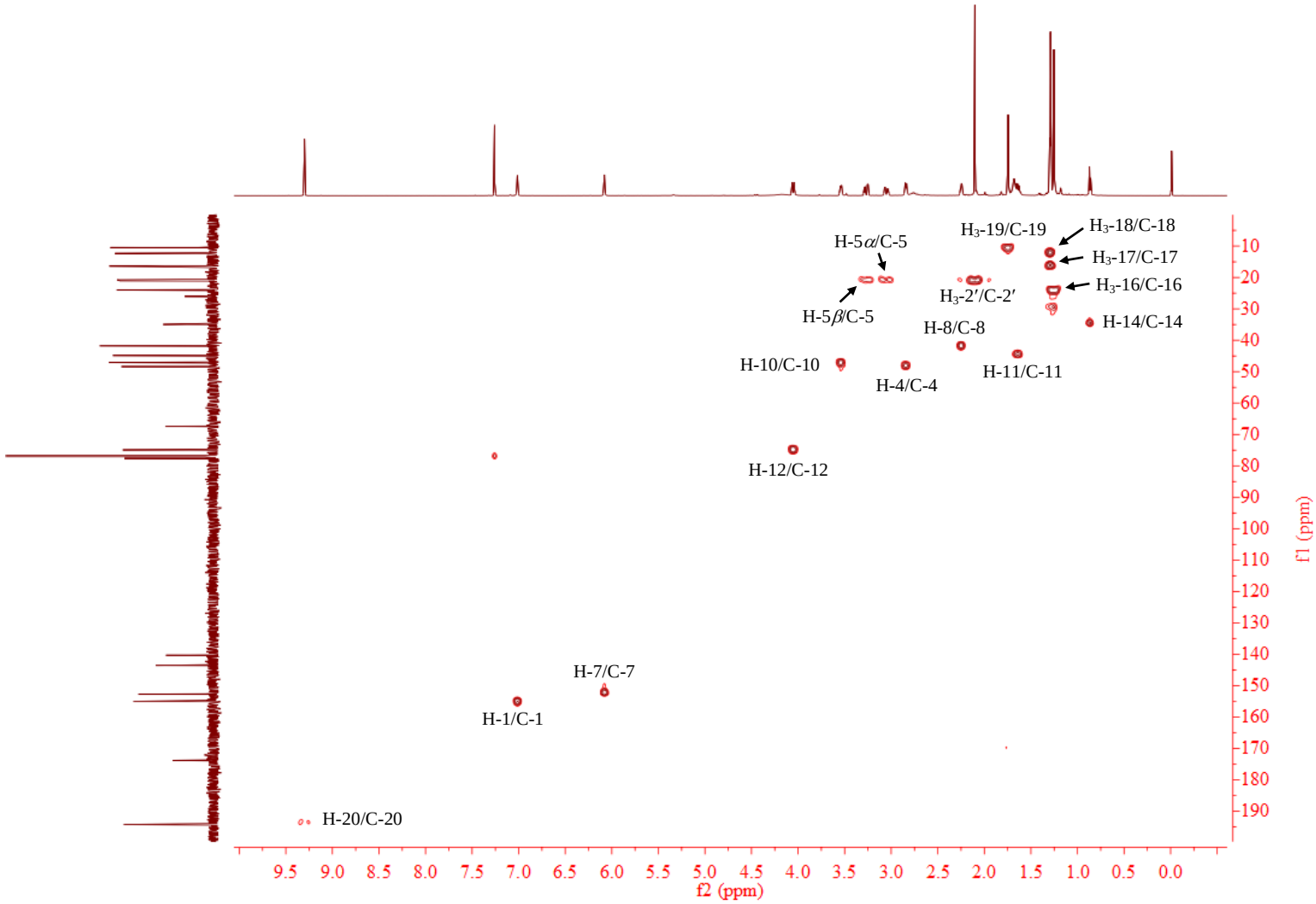


Figure S8: HSQC spectrum of compound **1**

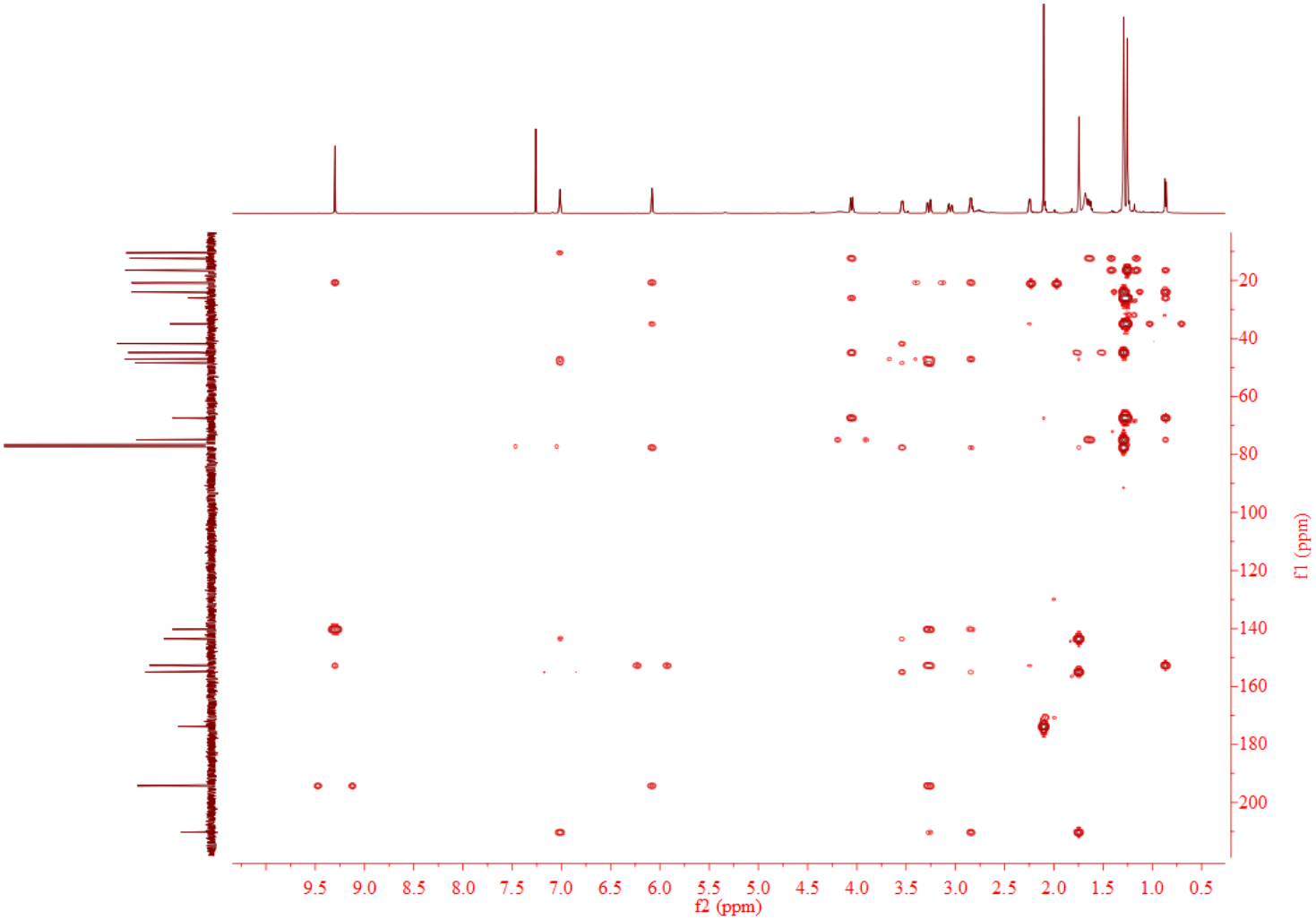


Figure S9: HMBC spectrum of compound **1**

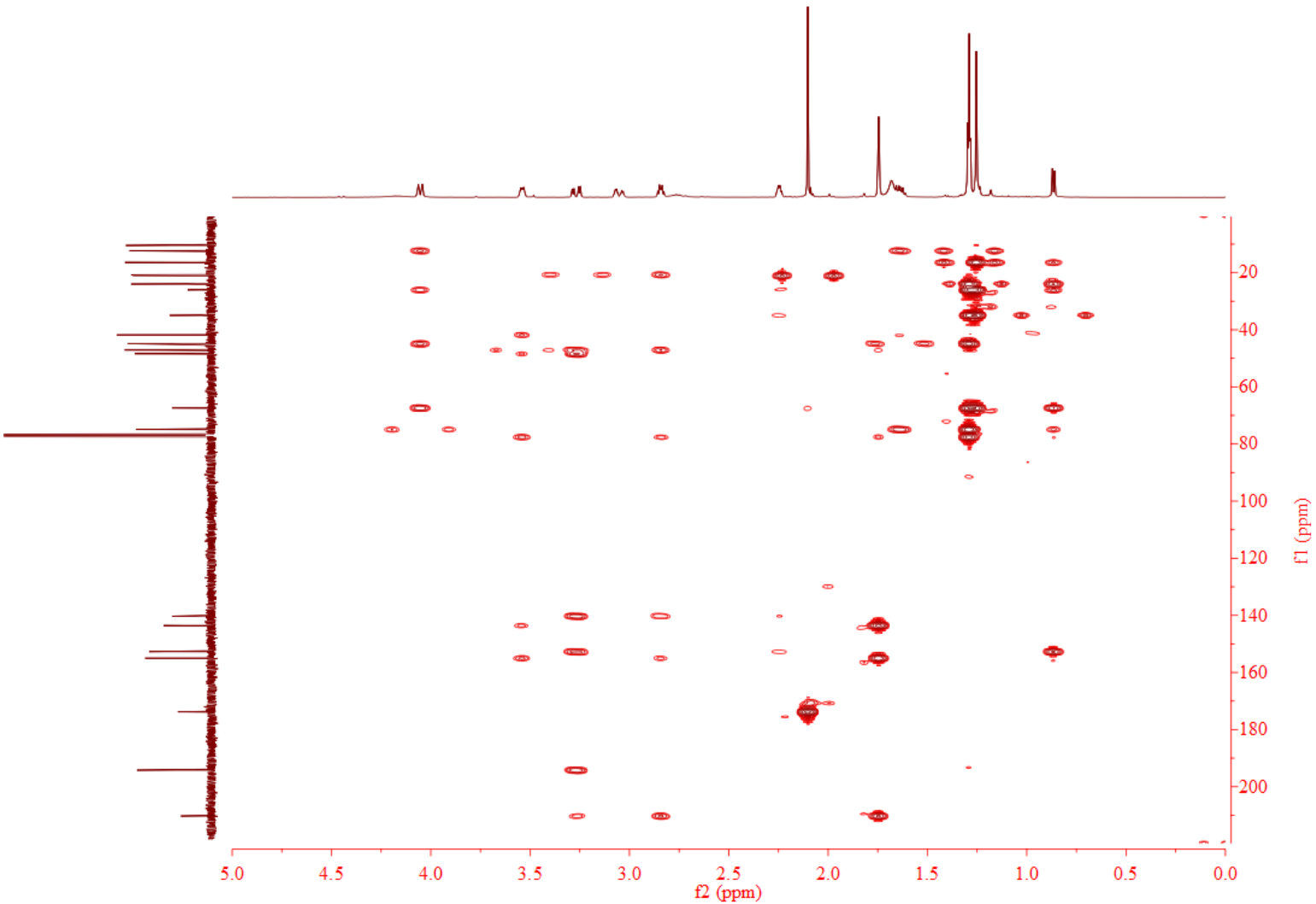


Figure S10: HMBC spectrum of compound **1** (δ_H 0–5 ppm)

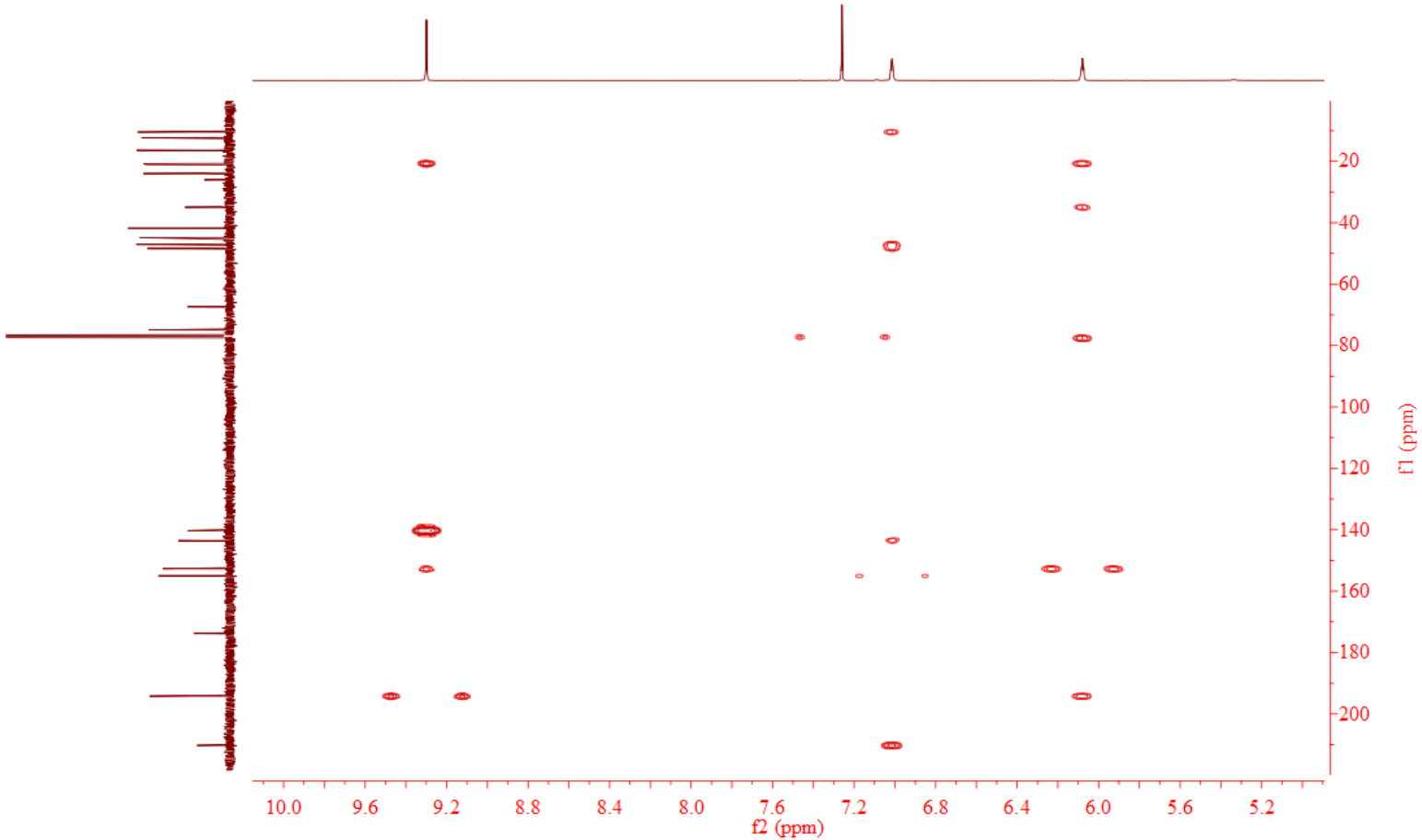


Figure S11: HMBC spectrum of compound **1** (δ_H 5–10 ppm)

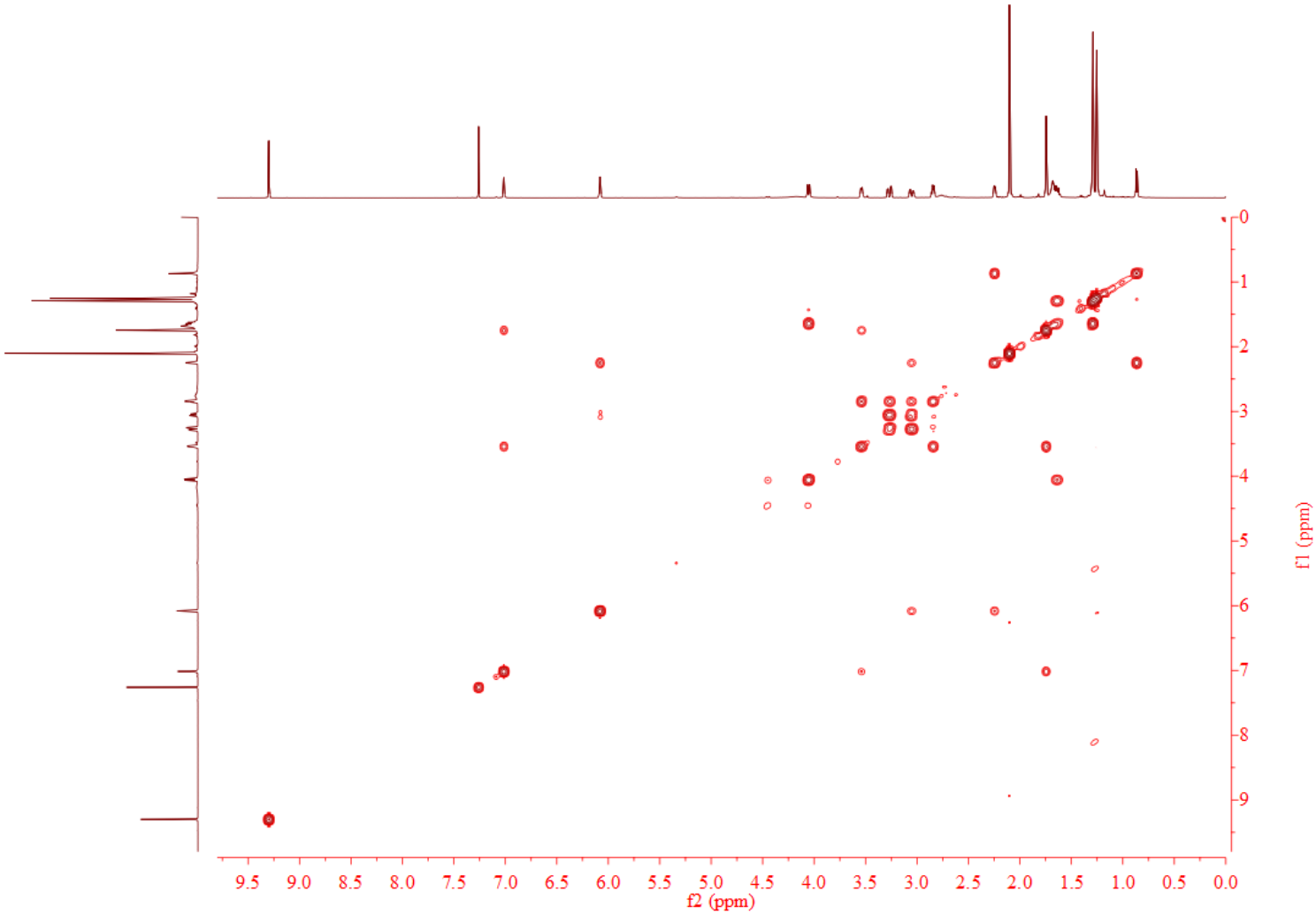


Figure S12: $^{1}H–^{1}H$ COSY spectrum of compound **1**

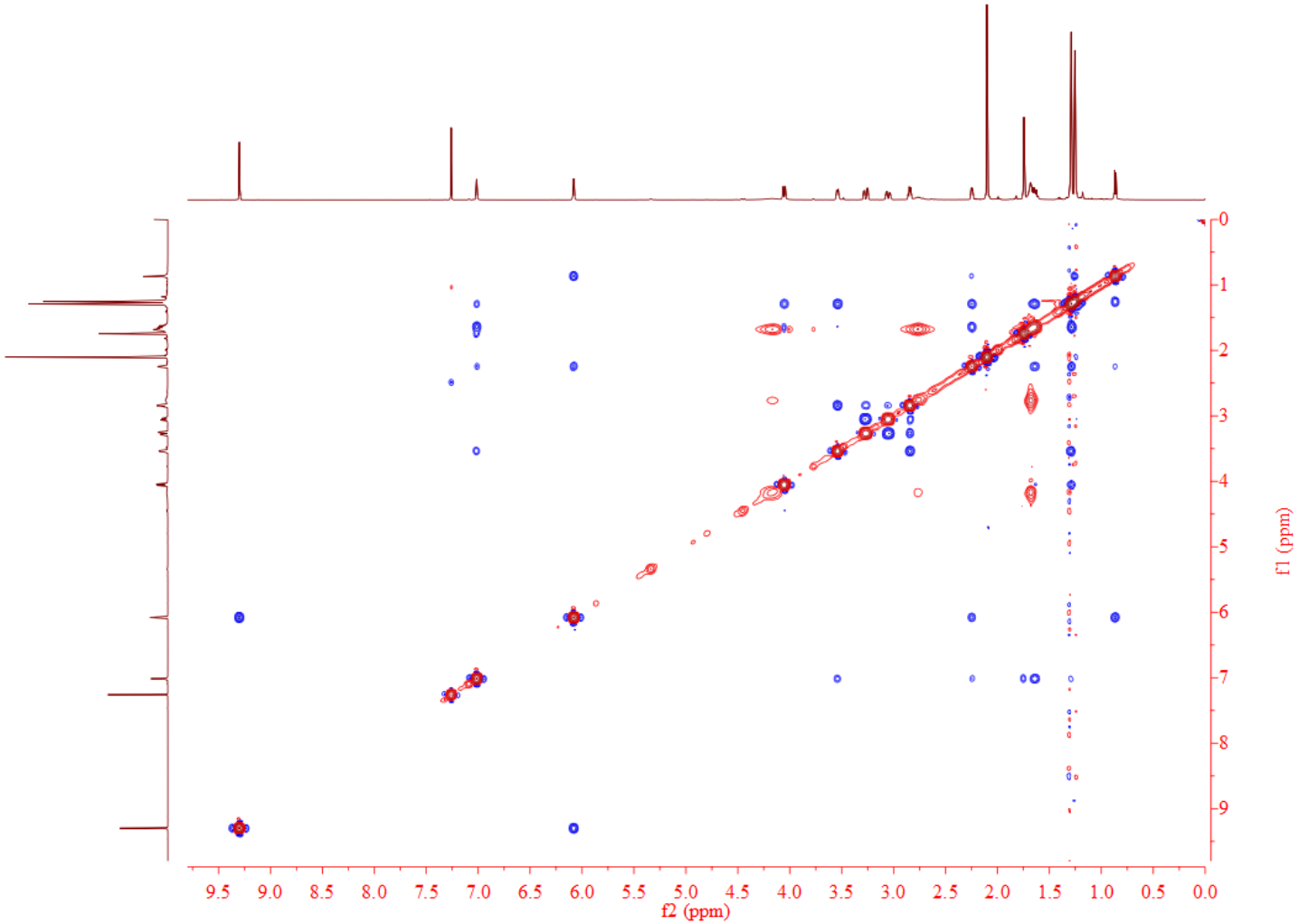


Figure S13: NOESY spectrum of compound **1**

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

```
Bond precision:   C-C = 0.0027 A          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)=
                                                 0.0824( 4323)
S = 1.050                  Npar= 261
```

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