

New 3,5-dimethylorsellinic acid-based meroterpenoids with BACE1 and AChE inhibitory activities from *Aspergillus terreus*

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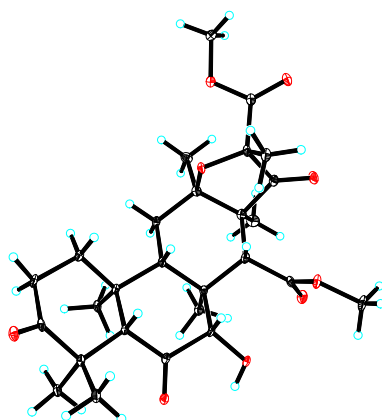
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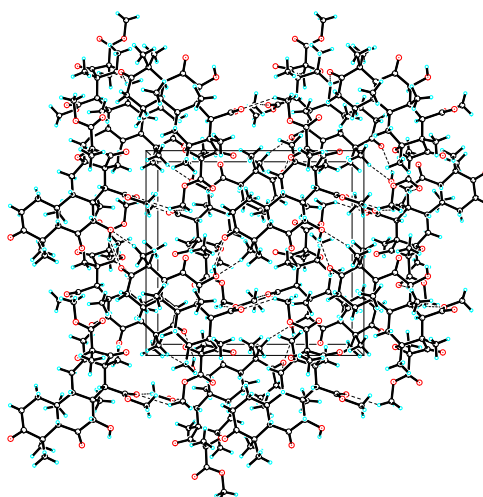
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Crystal data for compound **1**: $C_{27}H_{38}O_9$, $M = 506.57$, $a = 11.4298(6)$ Å, $b = 14.3863(8)$ Å, $c = 15.3115(8)$ Å, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, $V = 2517.7(2)$ Å³, $T = 100(2)$ K, space group $P212121$, $Z = 4$, $\mu(\text{CuK}\alpha) = 0.824$ mm⁻¹, 14247 reflections measured, 4526 independent reflections ($R_{\text{int}} = 0.0476$). The final R_1 values were 0.0376 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1013 ($I > 2\sigma(I)$). The final R_1 values were 0.0377 (all data). The final $wR(F^2)$ values were 0.1014 (all data). The goodness of fit on F^2 was 1.113. Flack parameter = 0.12(5).



View of a molecule of **1** with the atom-labelling scheme.

Displacement ellipsoids are drawn at the 30% probability level.



View of the pack drawing of **1**.

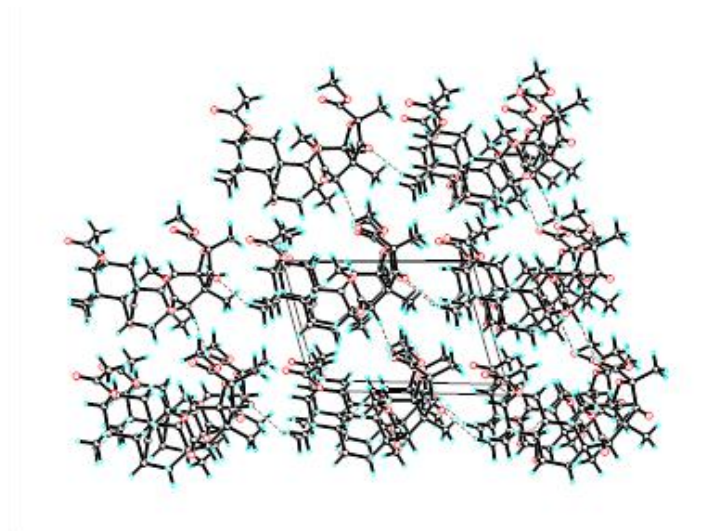
Hydrogen-bonds are shown as dashed lines.

Crystal data for compound **2**: $C_{29}H_{38}O_{10}$, $M = 546.59$, $a = 7.84890(10) \text{ \AA}$, $b = 7.85050(10) \text{ \AA}$, $c = 11.6784(2) \text{ \AA}$, $\alpha = 74.58^\circ$, $\beta = 73.43^\circ$, $\gamma = 87.86^\circ$, $V = 664.293(17) \text{ \AA}^3$, $T = 100(2) \text{ K}$, space group $P1$, $Z = 1$, $\mu(\text{CuK}\alpha) = 0.854 \text{ mm}^{-1}$, 10823 reflections measured, 3922 independent reflections ($R_{\text{int}} = 0.0281$). The final R_1 values were 0.0307 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0788 ($I > 2\sigma(I)$). The final R_1 values were 0.0308 (all data). The final $wR(F^2)$ values were 0.0788 (all data). The goodness of fit on F^2 was 1.058. Flack parameter = 0.17(5).



View of a molecule of **2** with the atom-labelling scheme.

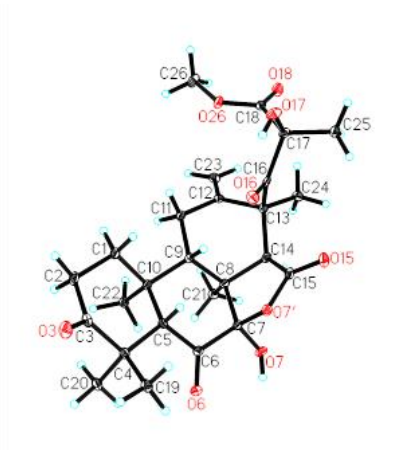
Displacement ellipsoids are drawn at the 30% probability level.



View of the pack drawing of **2**.

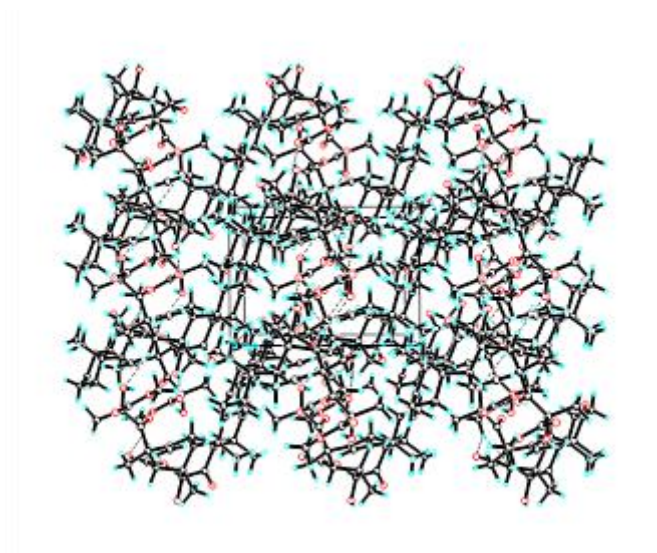
Hydrogen-bonds are shown as dashed lines.

Crystal data for compound **4**: $C_{26}H_{34}O_9$, $M = 490.53$, $a = 7.3751(3) \text{ \AA}$, $b = 15.7593(7) \text{ \AA}$, $c = 10.1577(4) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90.4660(10)^\circ$, $\gamma = 90^\circ$, $V = 1180.55(8) \text{ \AA}^3$, $T = 100(2) \text{ K}$, space group $P21$, $Z = 2$, $\mu(\text{CuK}\alpha) = 0.863 \text{ mm}^{-1}$, 13065 reflections measured, 4201 independent reflections ($R_{\text{int}} = 0.0271$). The final R_1 values were 0.0339 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0825 ($I > 2\sigma(I)$). The final R_1 values were 0.0340 (all data). The final $wR(F^2)$ values were 0.0825 (all data). The goodness of fit on F^2 was 3.155. Flack parameter = 0.10(4).



View of a molecule of **4** with the atom-labelling scheme.

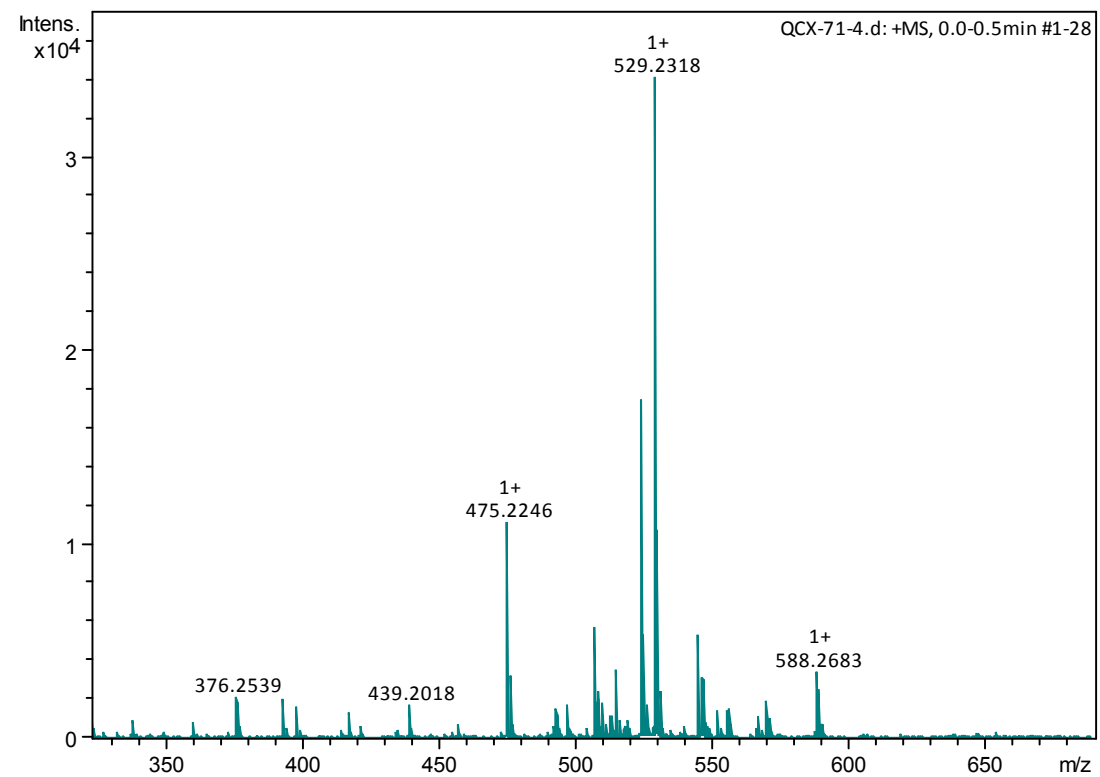
Displacement ellipsoids are drawn at the 30% probability level.



View of the packing motif of **4**.

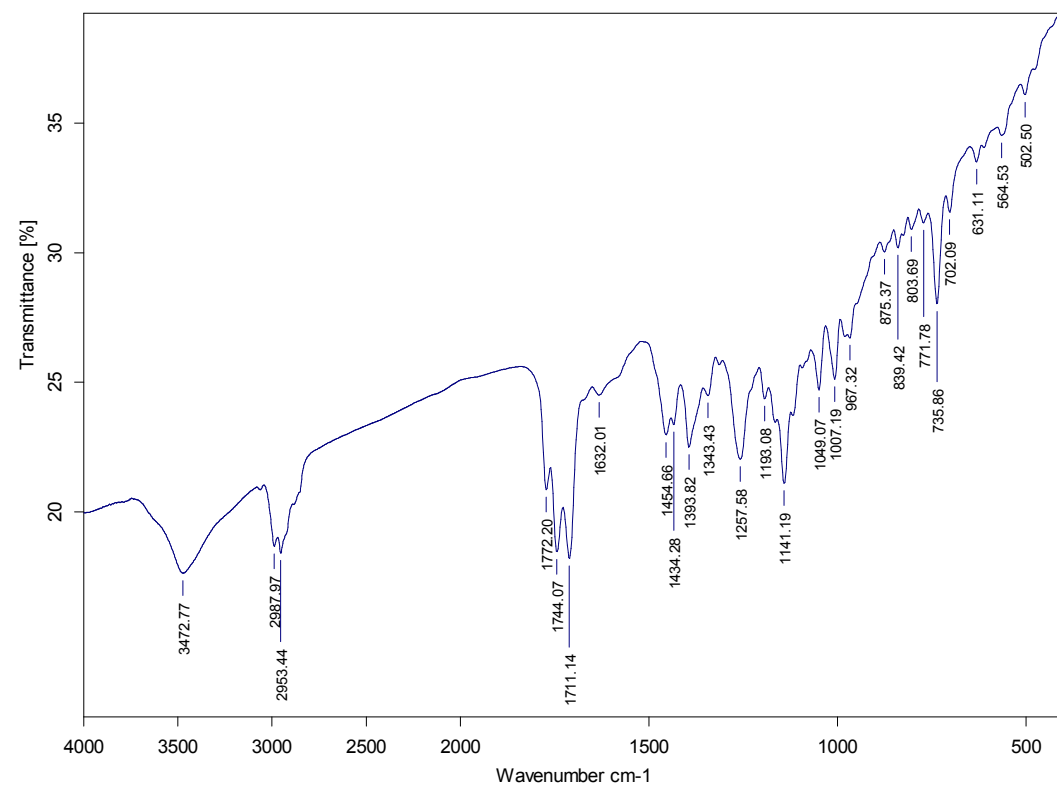
Hydrogen-bonds are shown as dashed lines.

HRESIMS of compound **1**



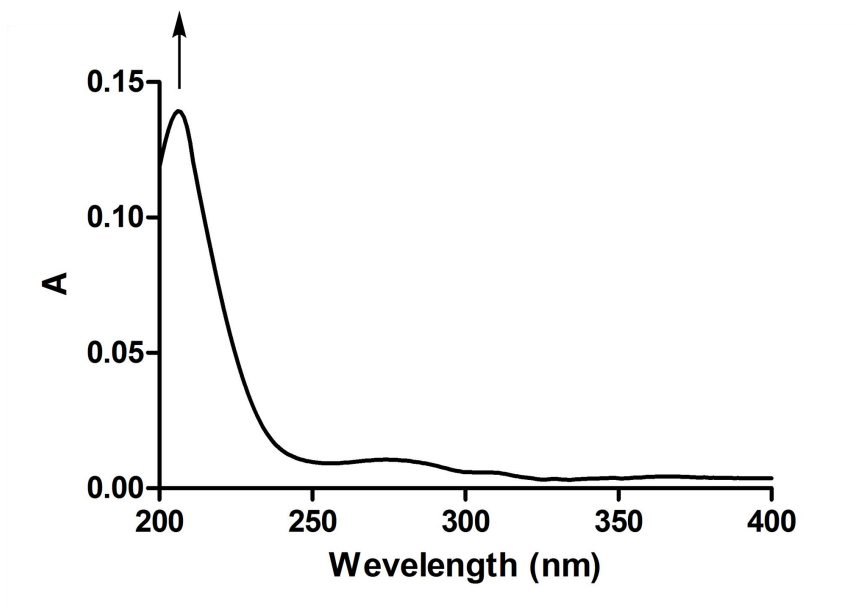
IR of compound 1

E:\20160330\齐昌兴20160330\QCX-71-4.0

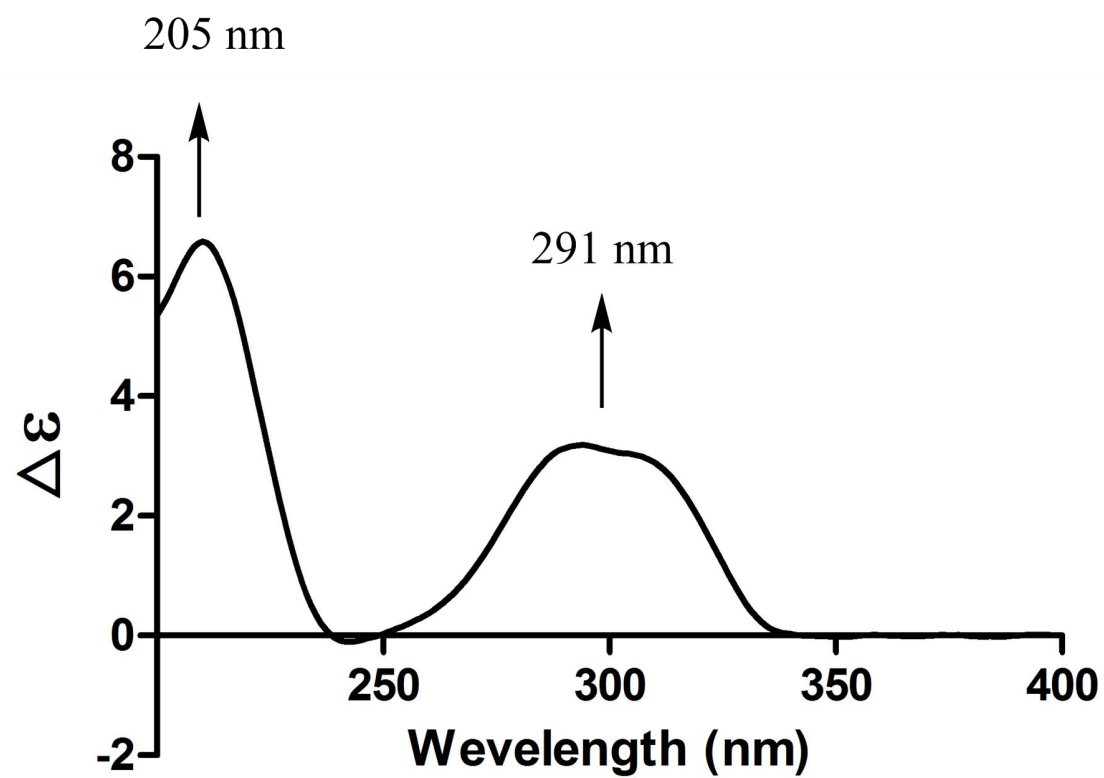


UV of compound 1

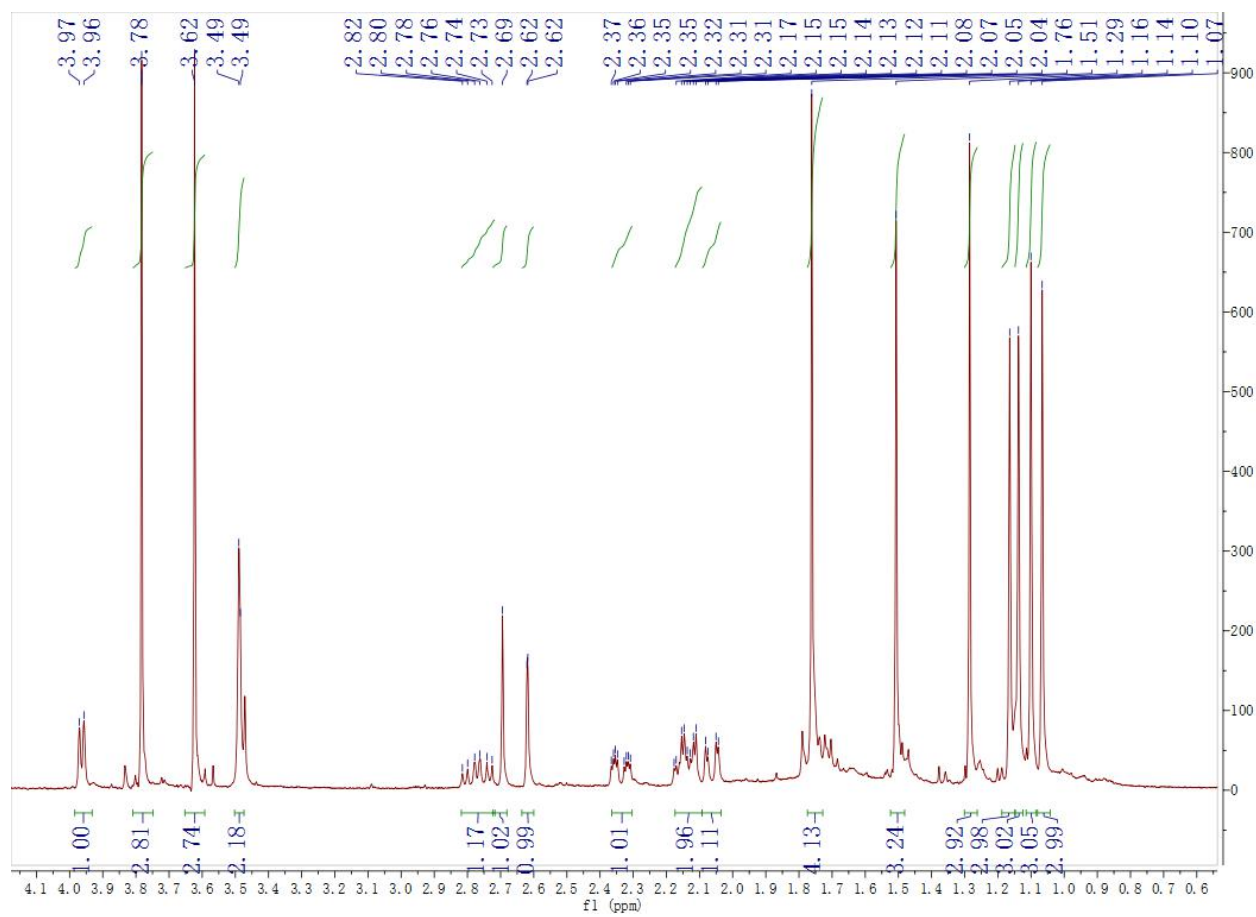
204 nm



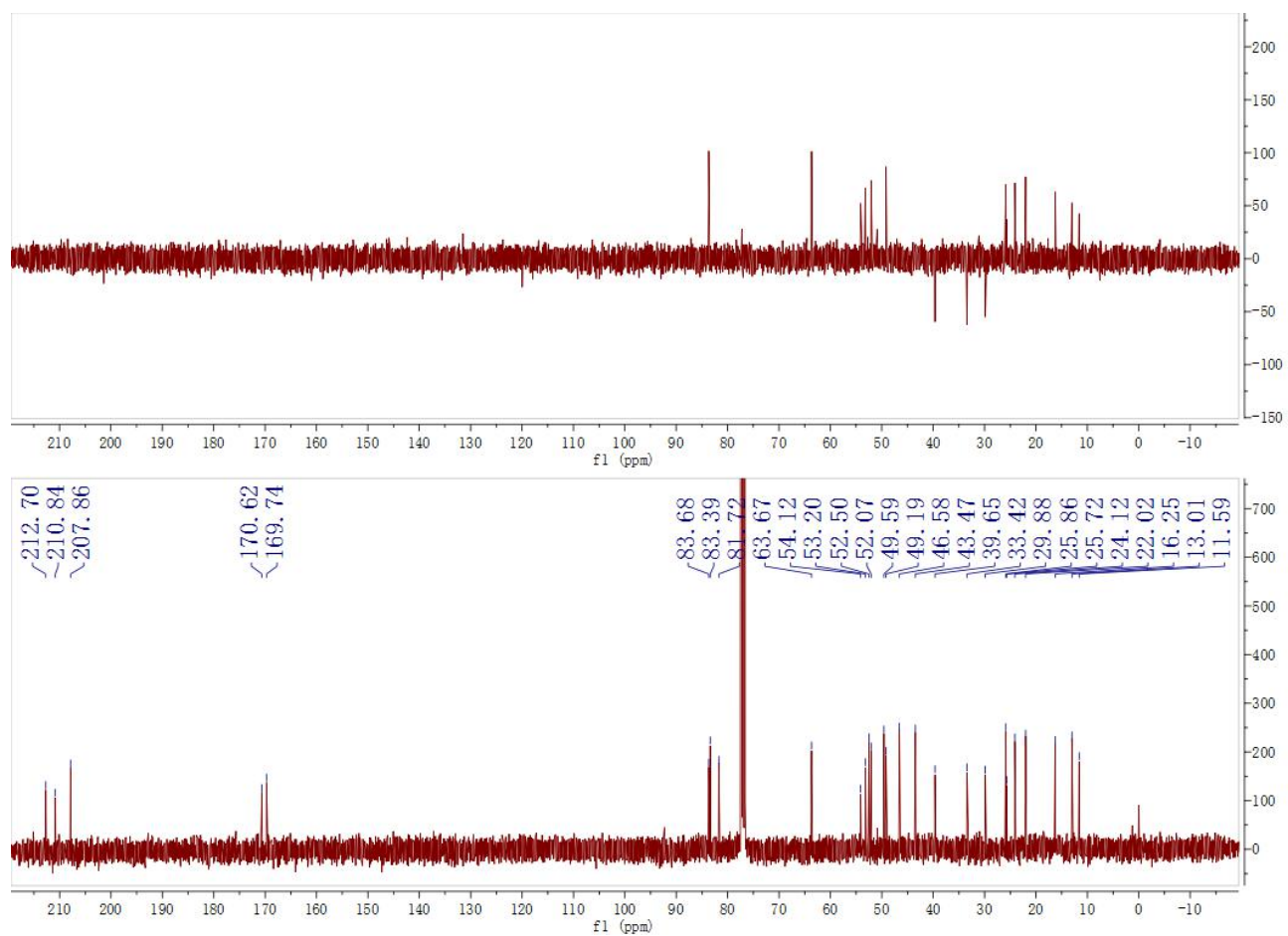
CD of compound 1



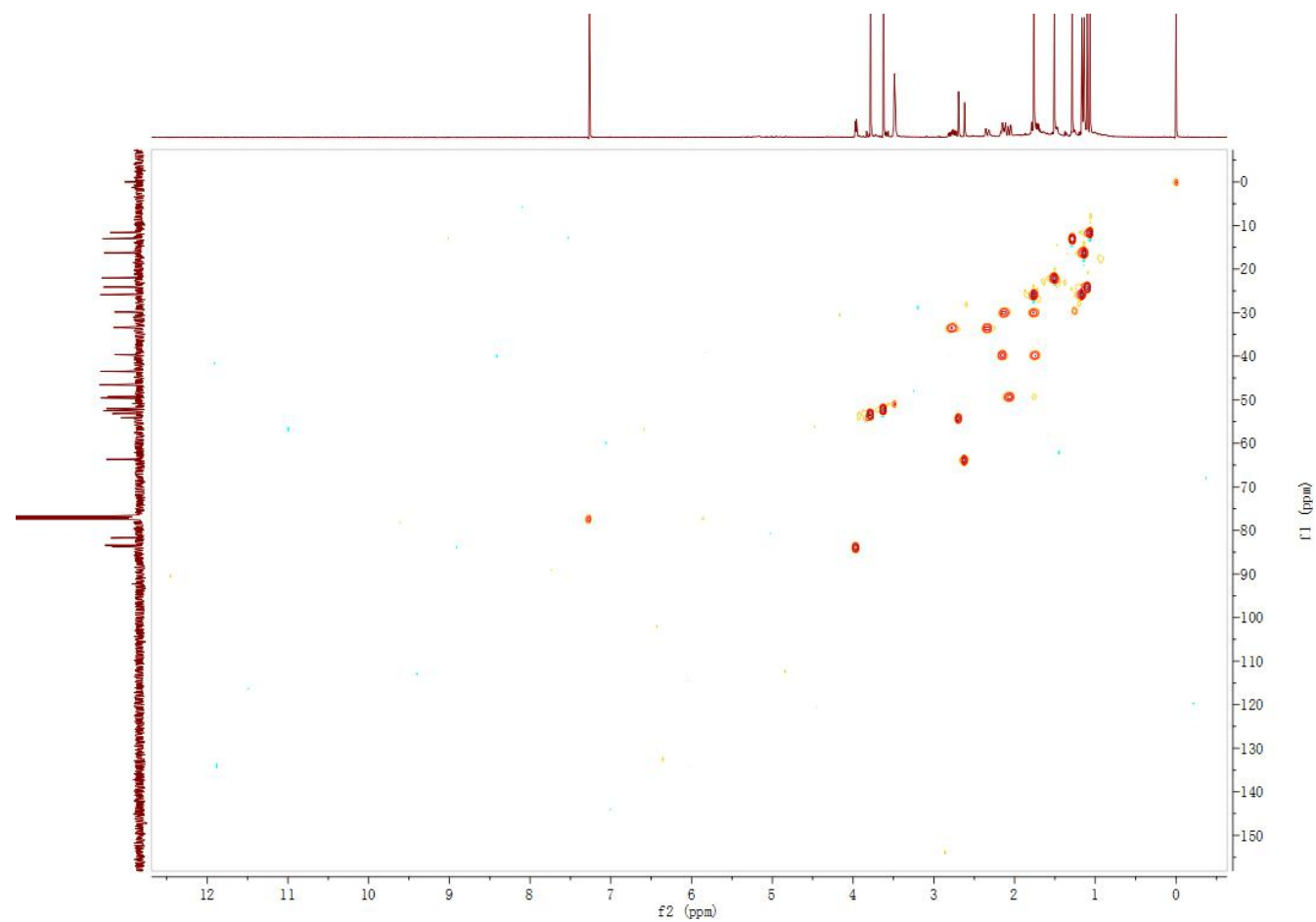
^1H NMR of compound **1** (in CDCl_3)



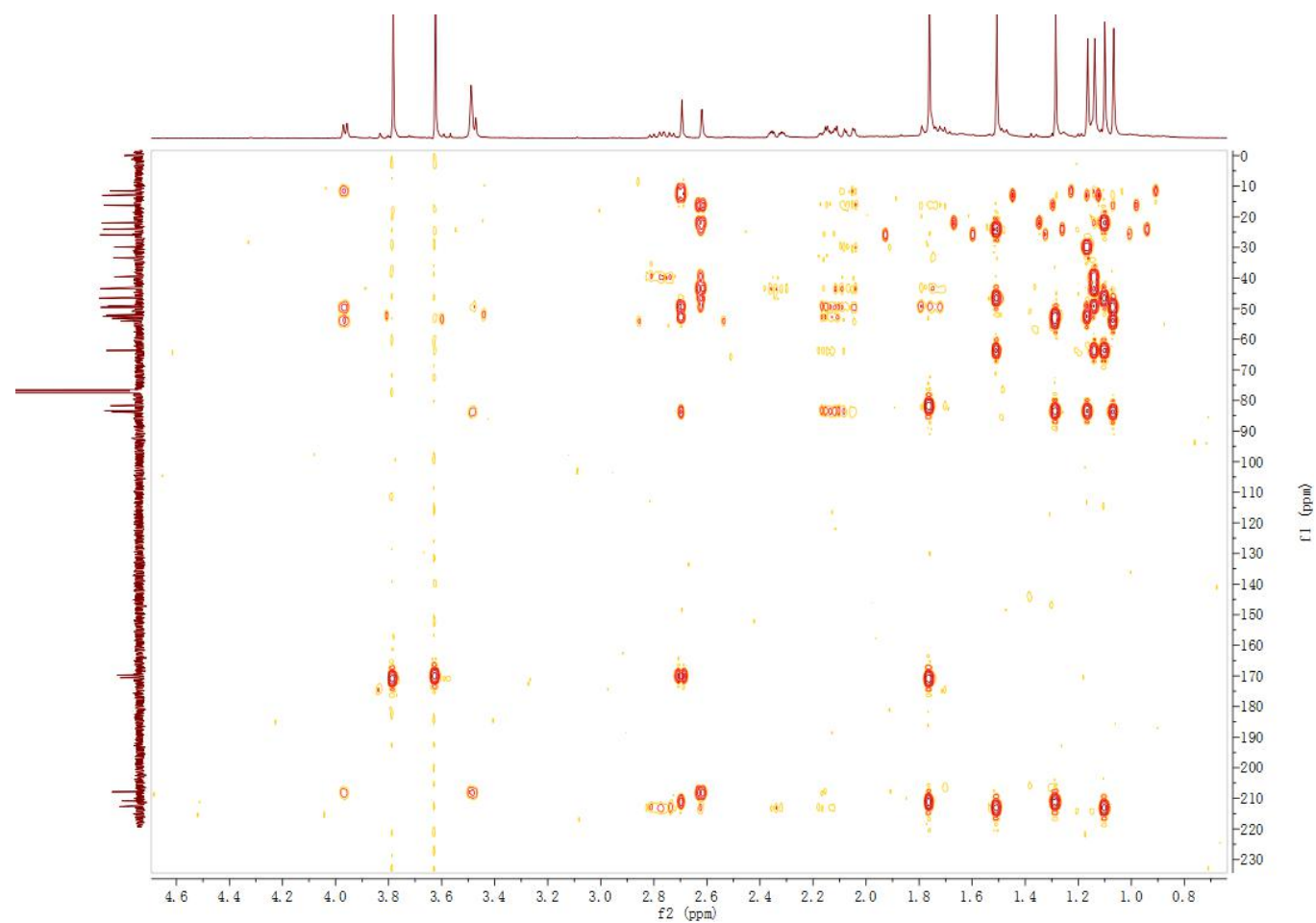
^{13}C NMR of compound **1** (in CDCl_3)



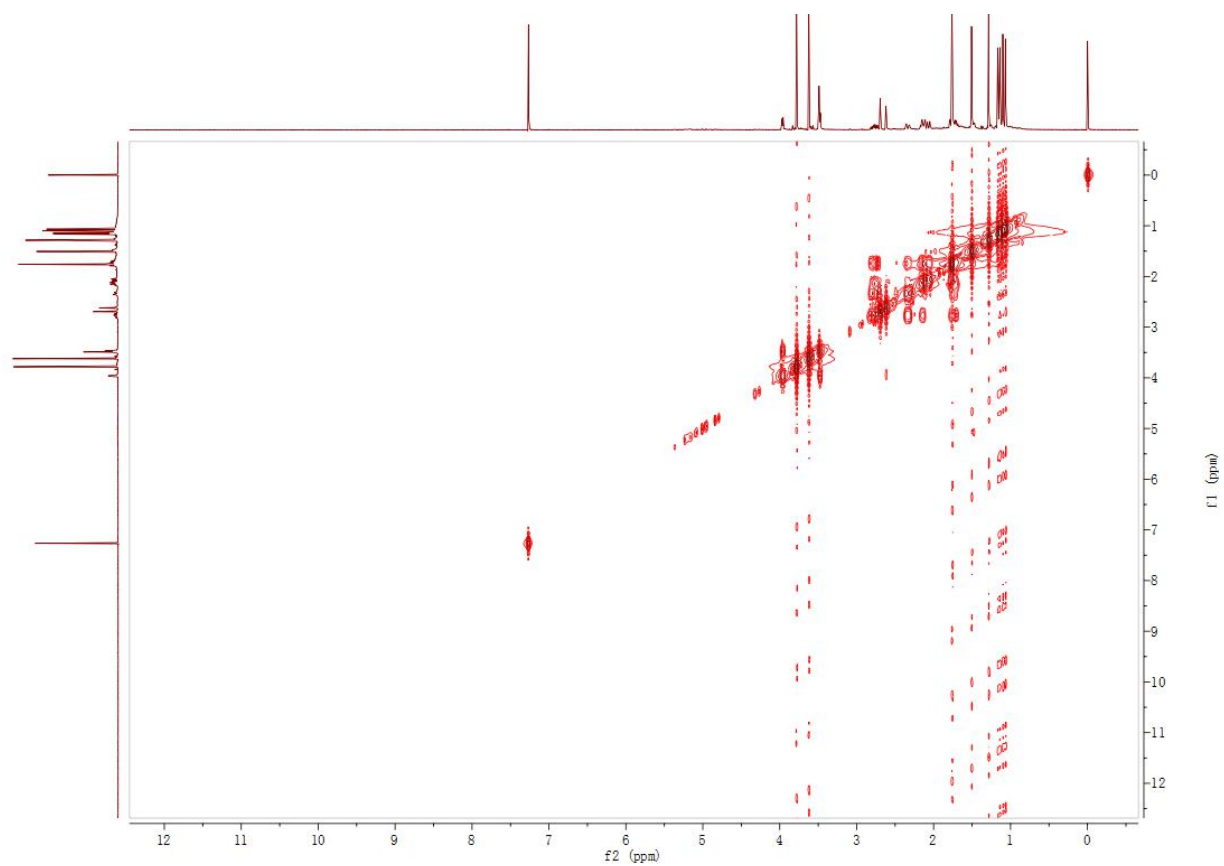
HSQC of compound **1** (in CDCl₃)



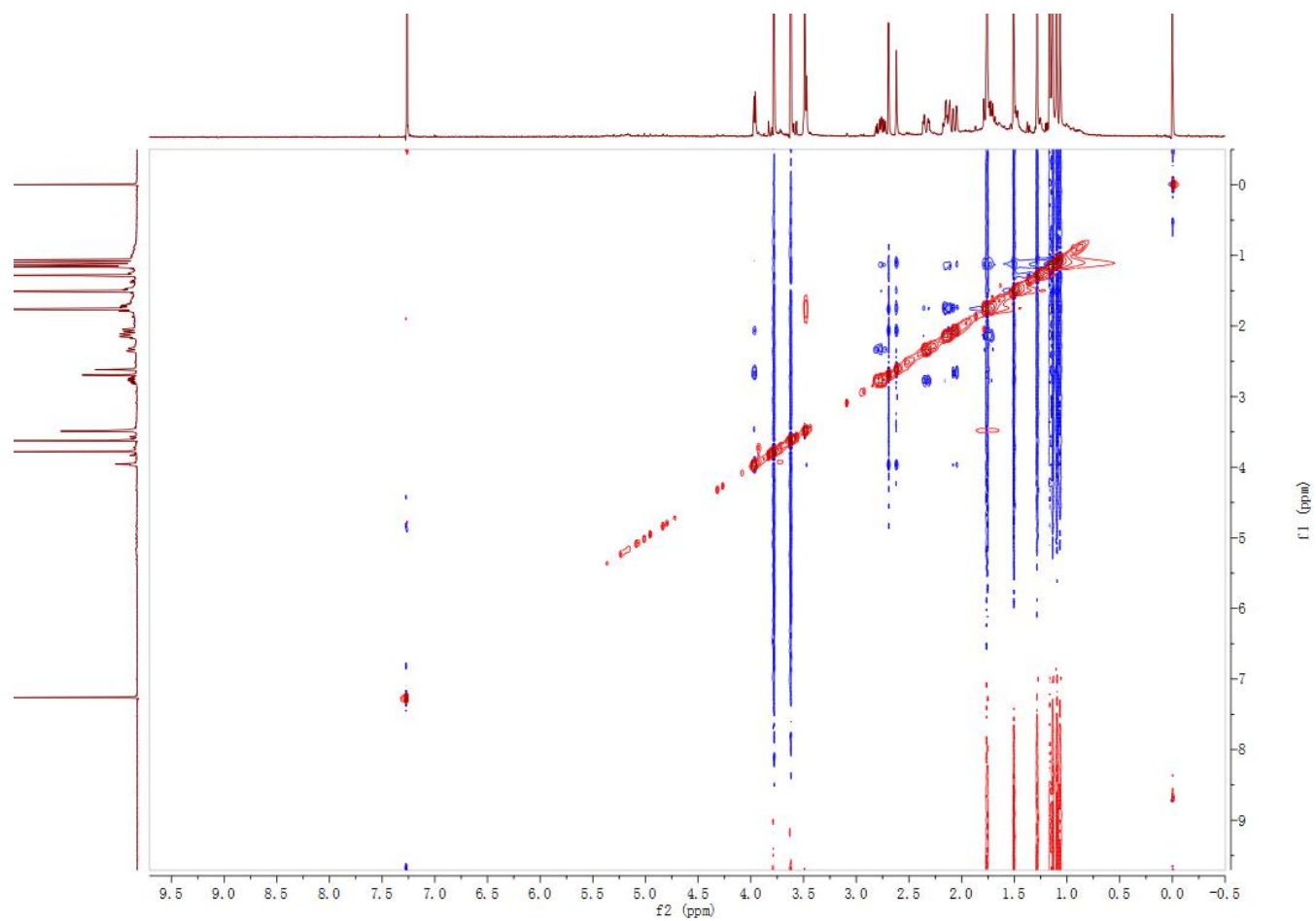
HMBC of compound **1** (in CDCl₃)



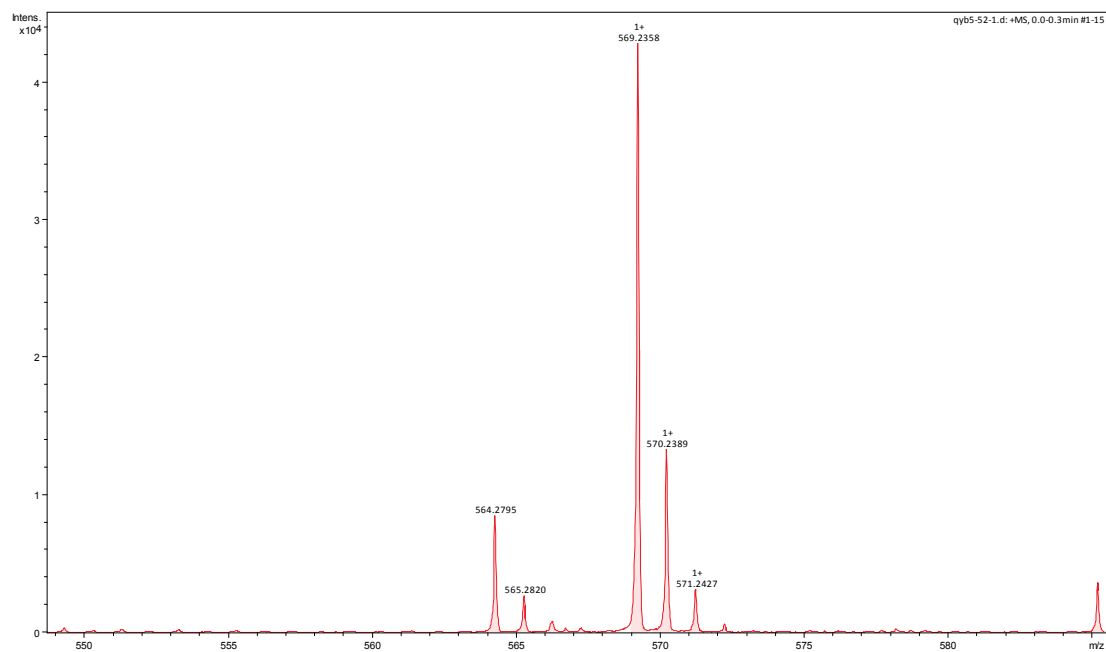
^1H - ^1H COSY of compound **1** (in CDCl_3)



NOESY of compound **1** (in CDCl₃)



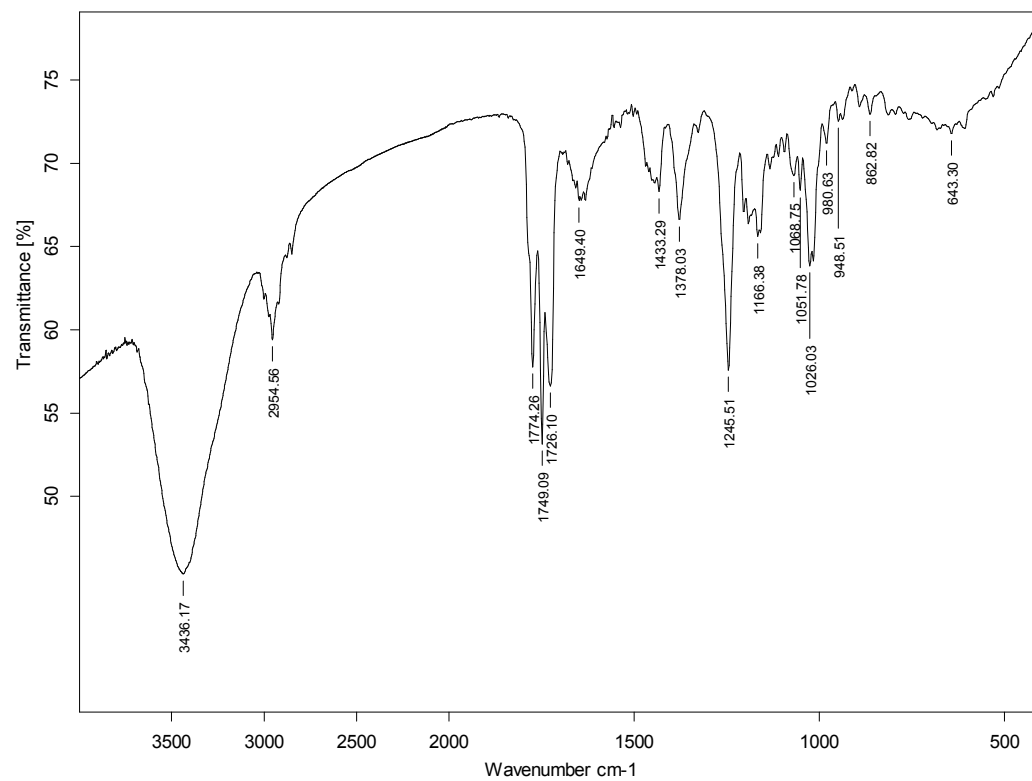
HRESIMS of compound **2**



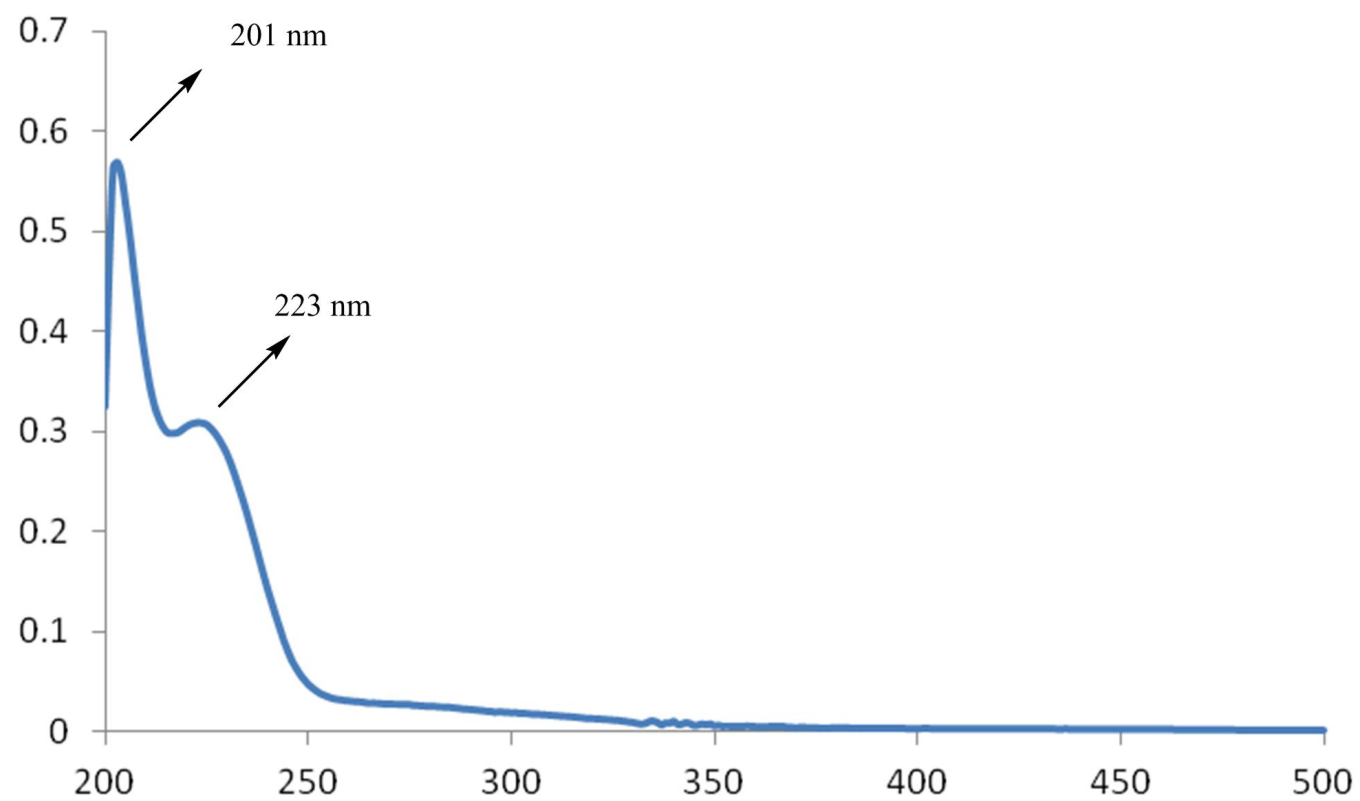
IR of compound 2

E:\20170912\20170912同济\11f-8.0

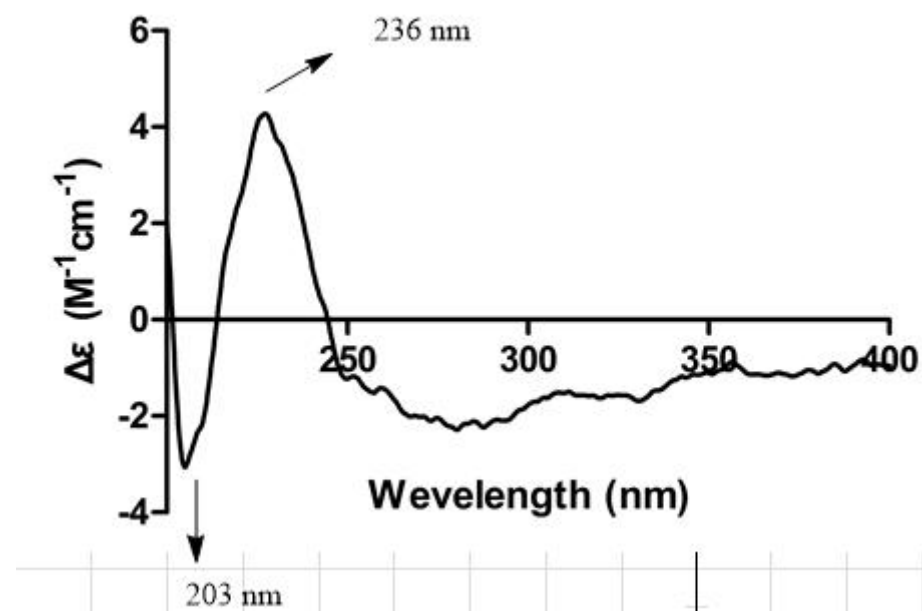
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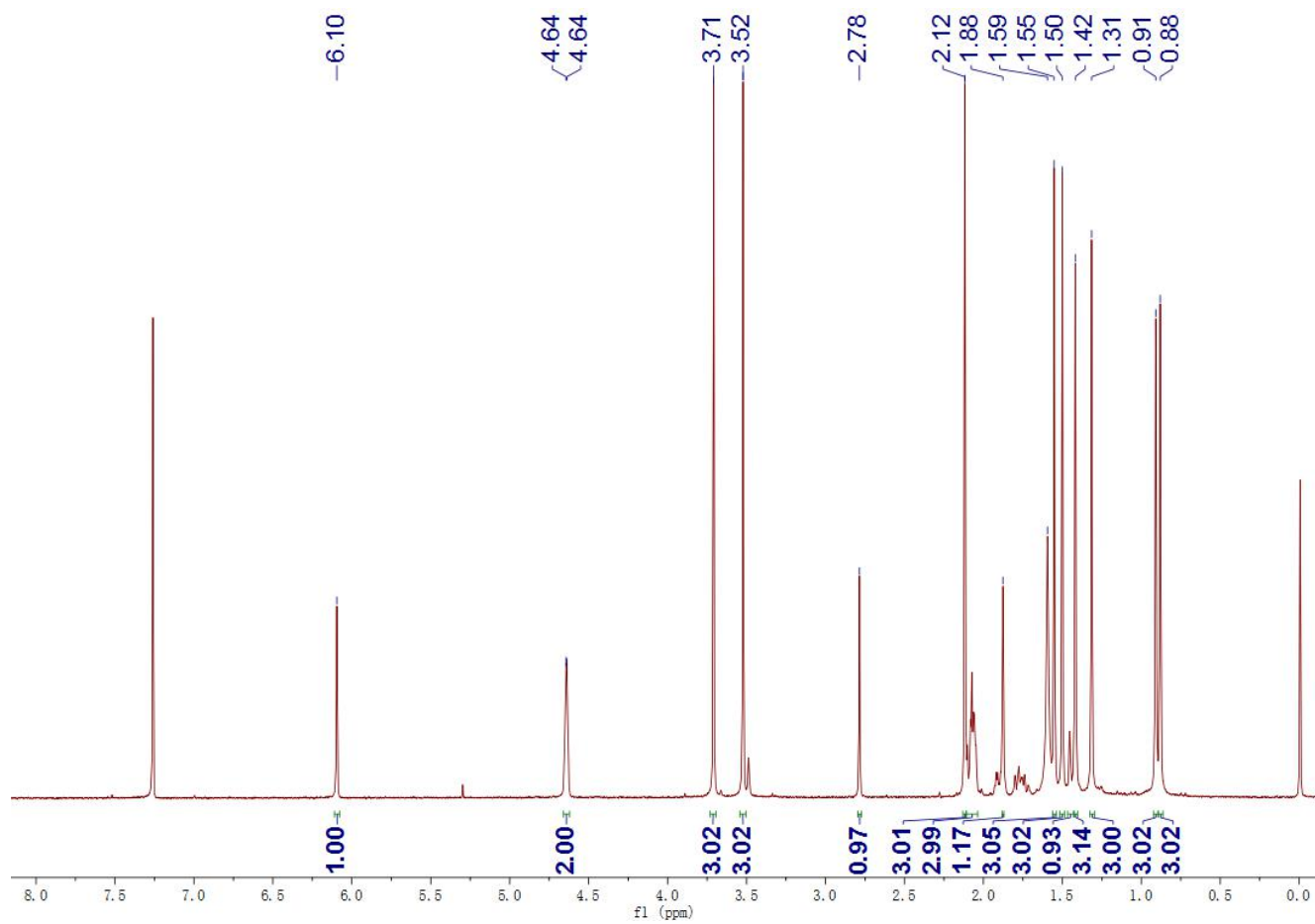
UV of compound **2**



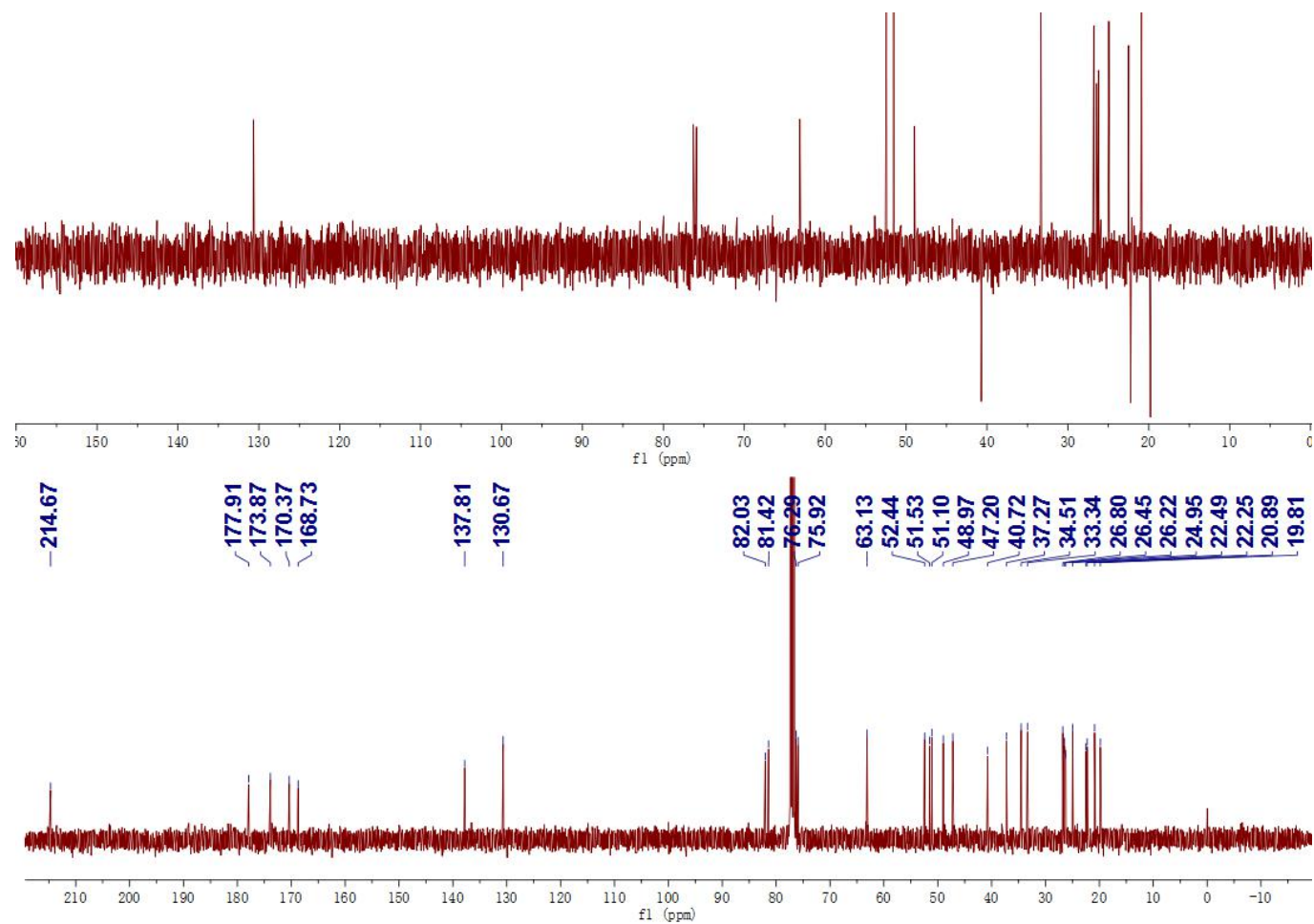
CD of compound 2



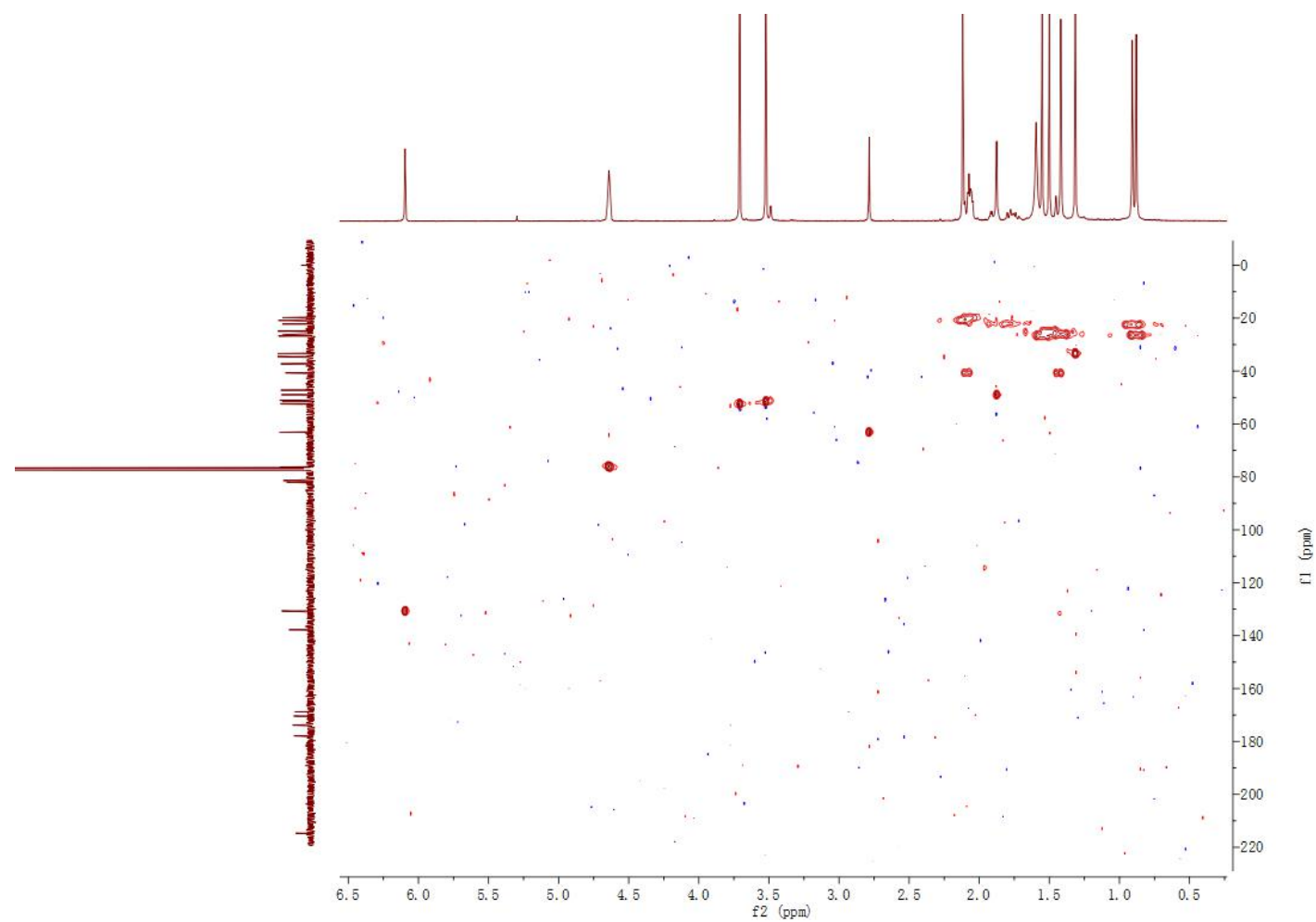
^1H NMR of compound **2** (in CDCl_3)



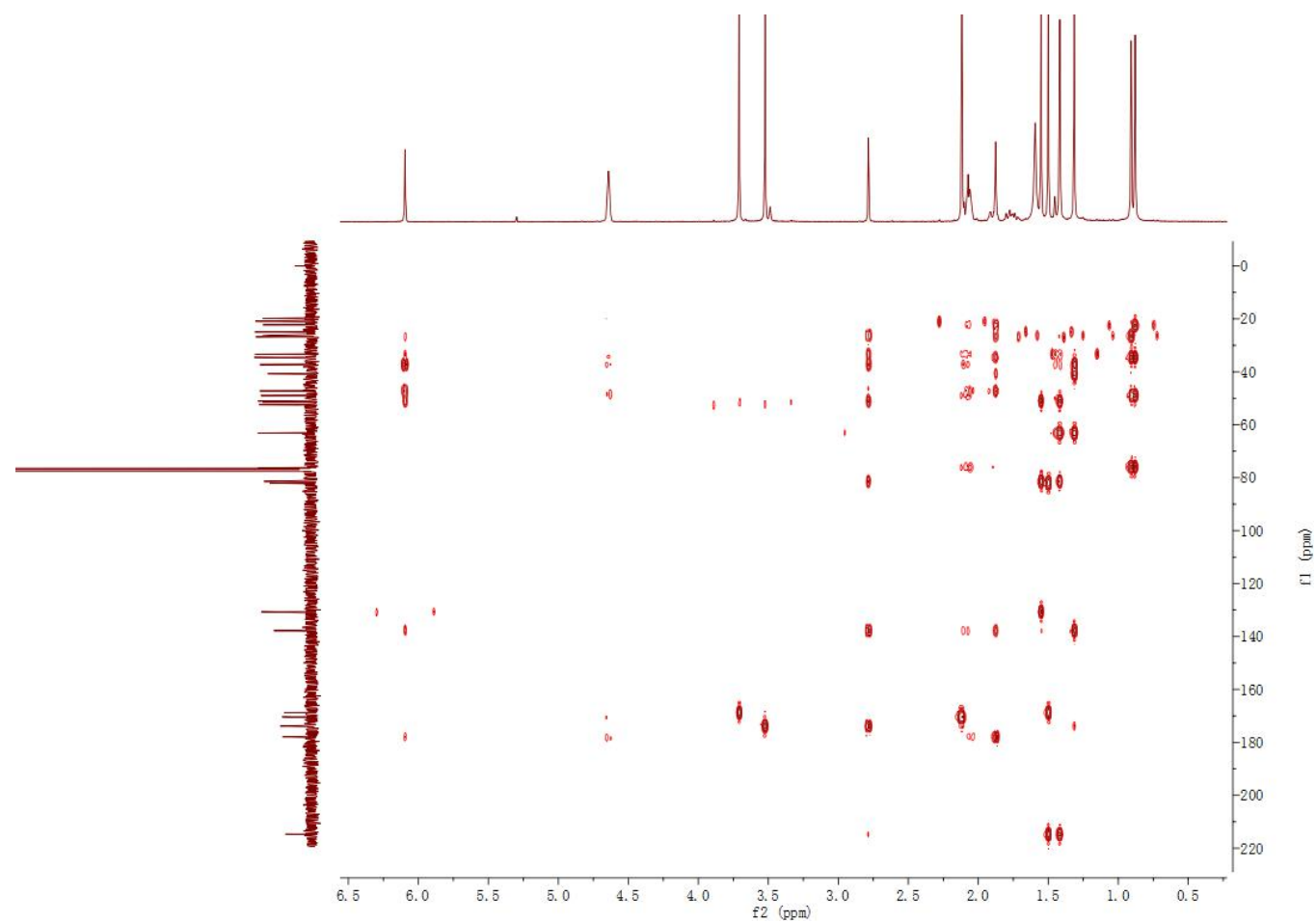
^{13}C NMR of compound **2** (in CDCl_3)



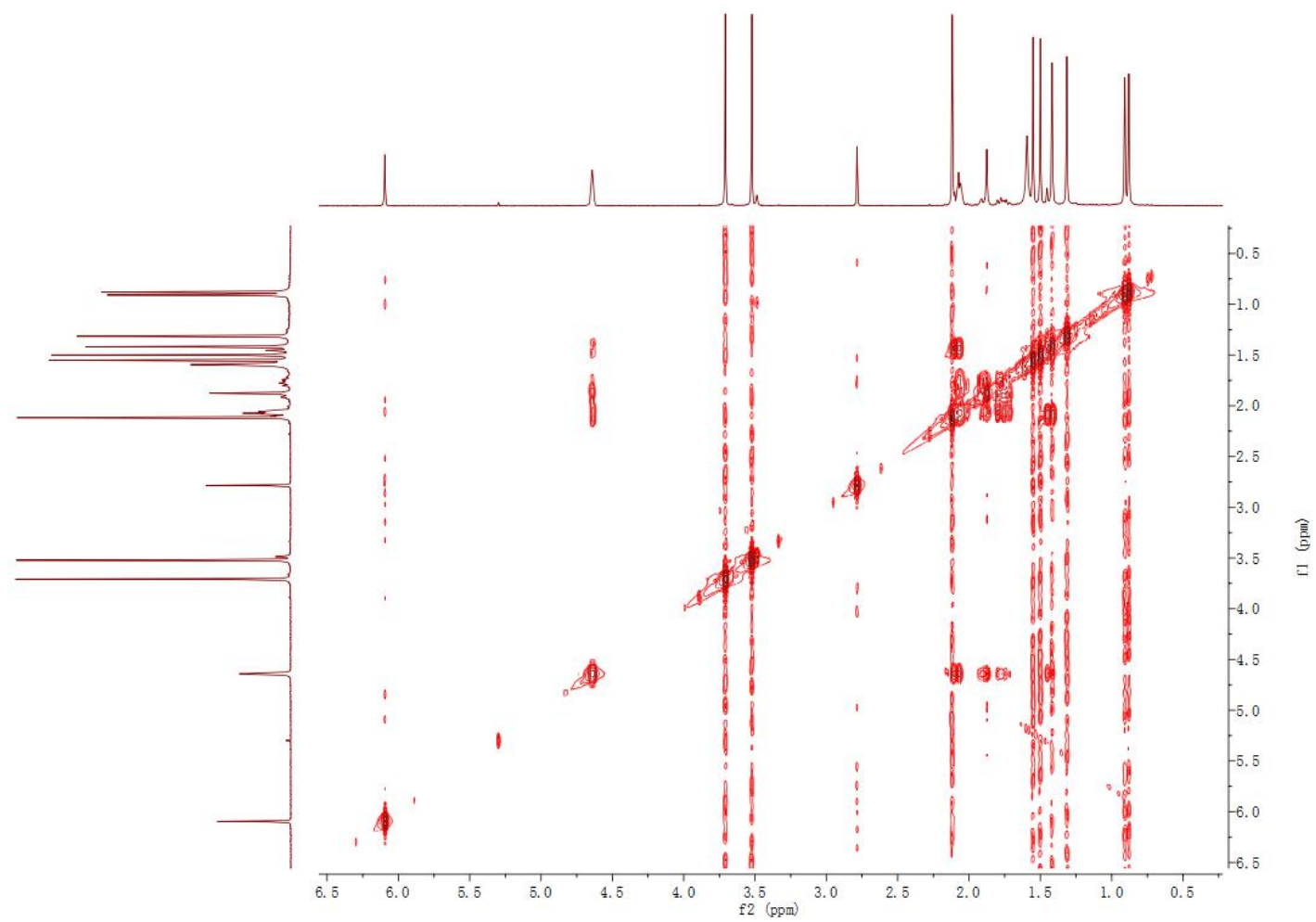
HSQC of compound **2** (in CDCl₃)



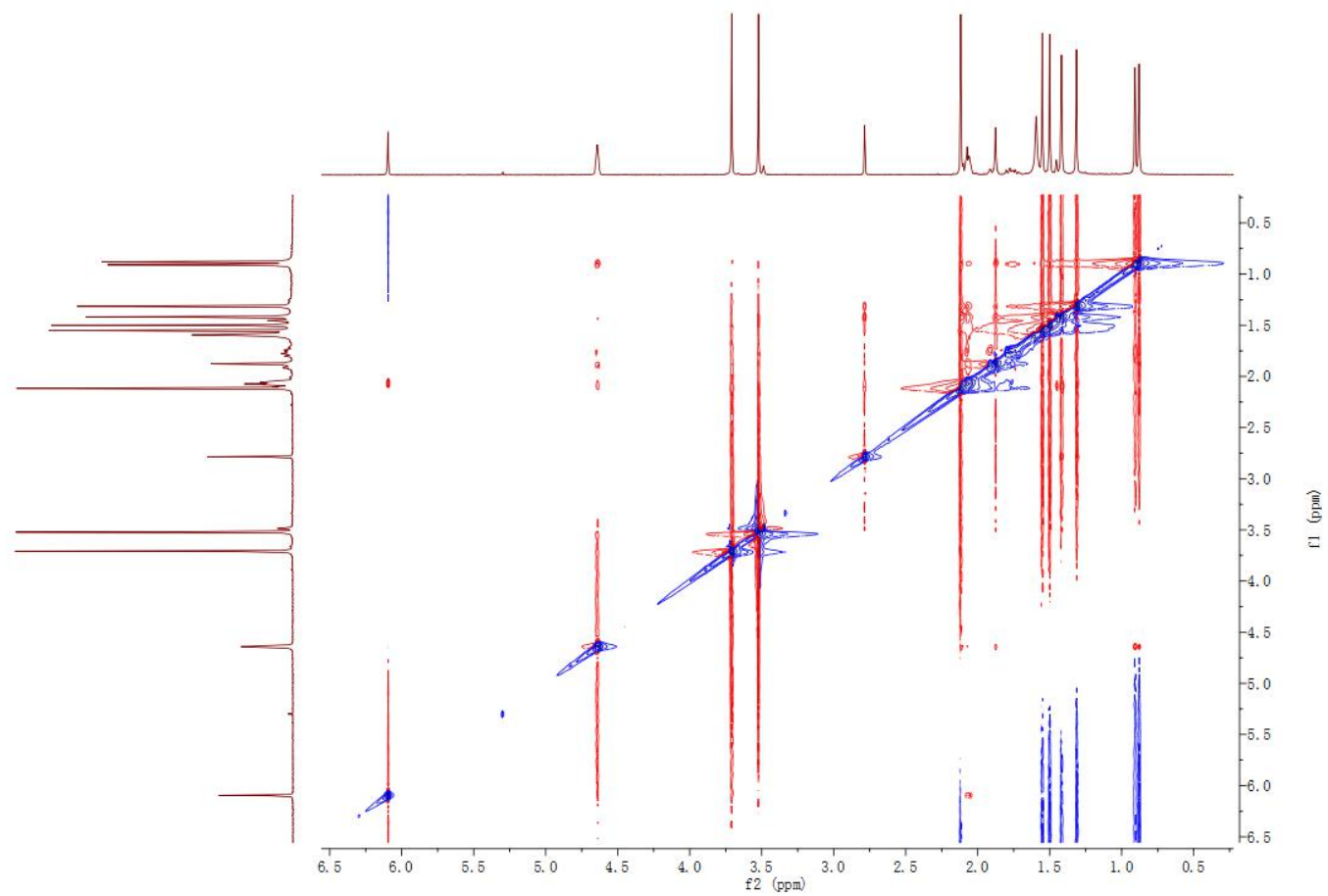
HMBC of compound **2** (in CDCl₃)



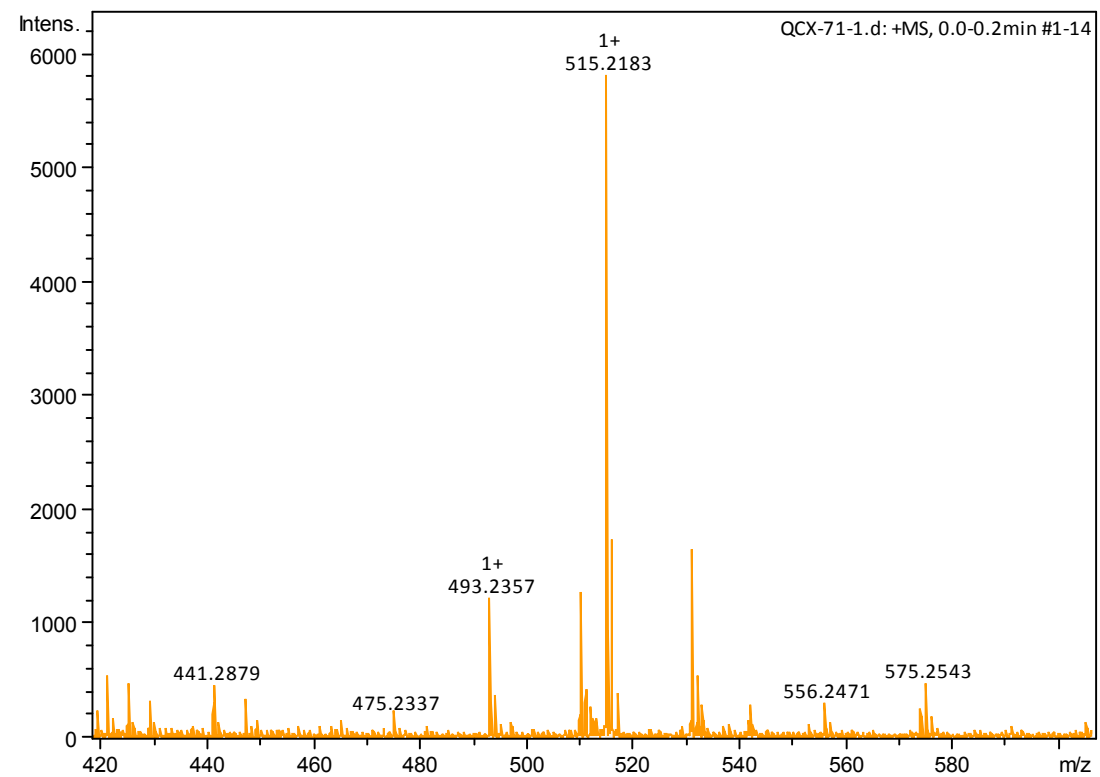
^1H – ^1H COSY of compound **2** (in CDCl_3)



NOESY of compound **2** (in CDCl₃)

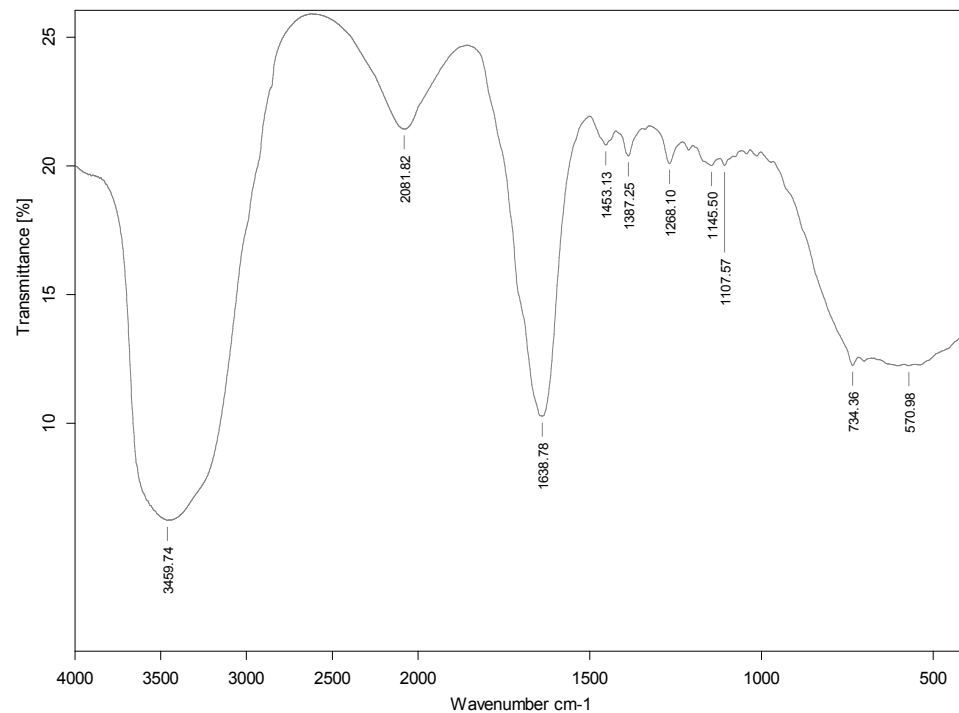


HRESIMS of compound **3**

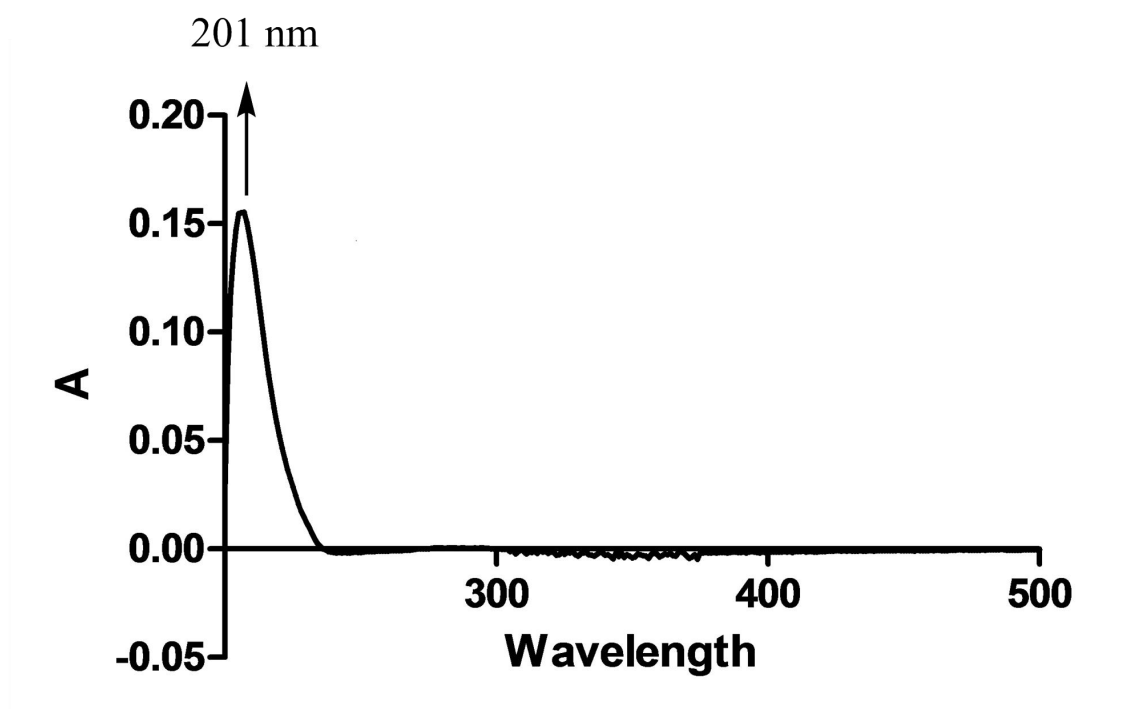


IR of compound 3

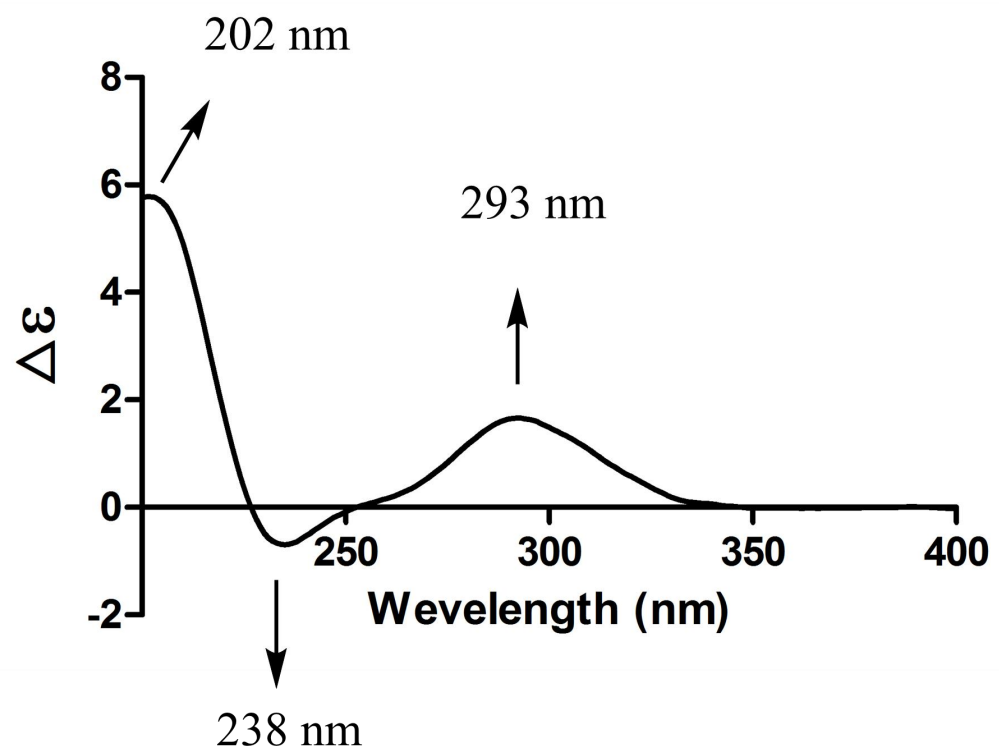
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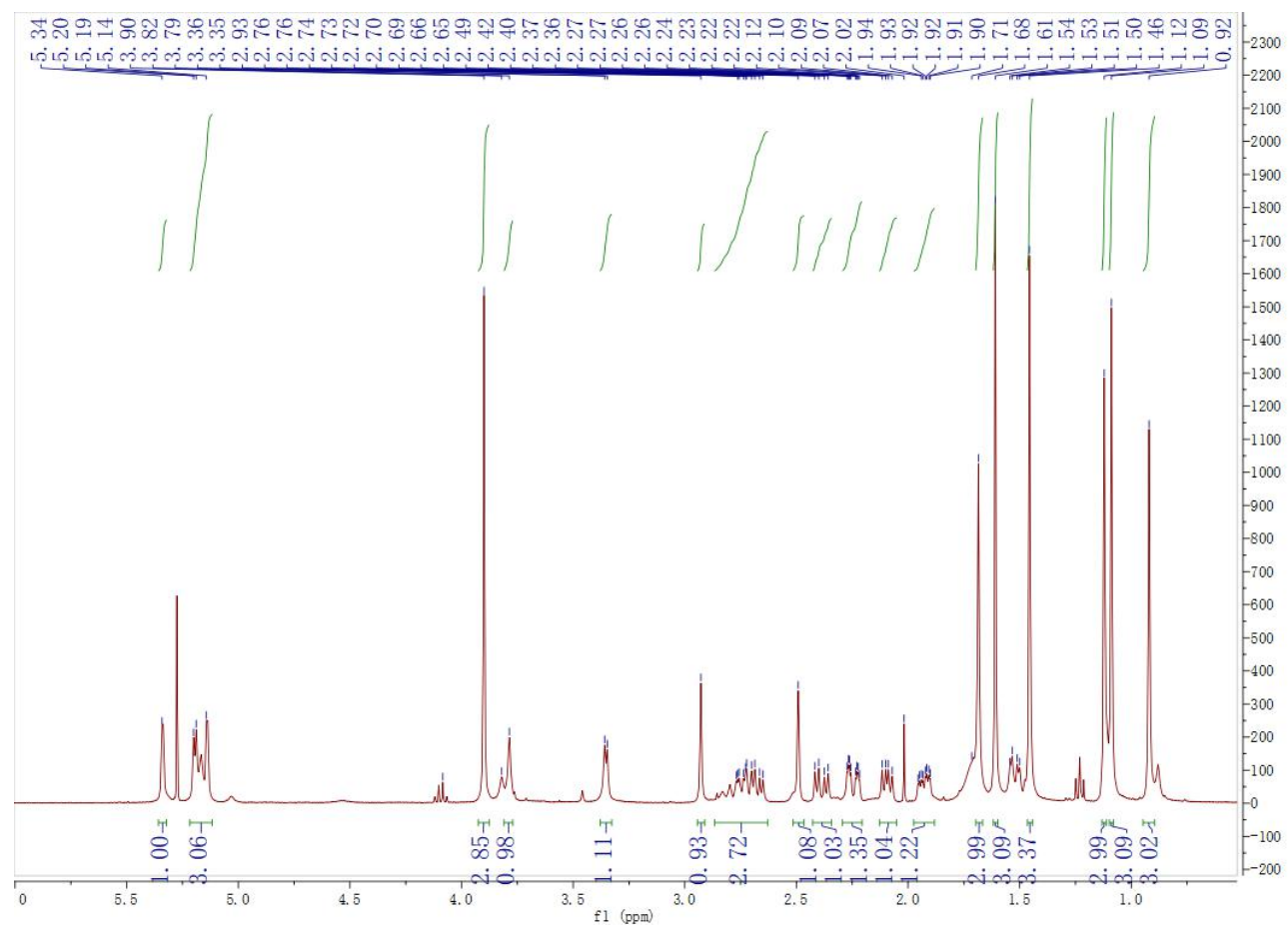
UV of compound 3



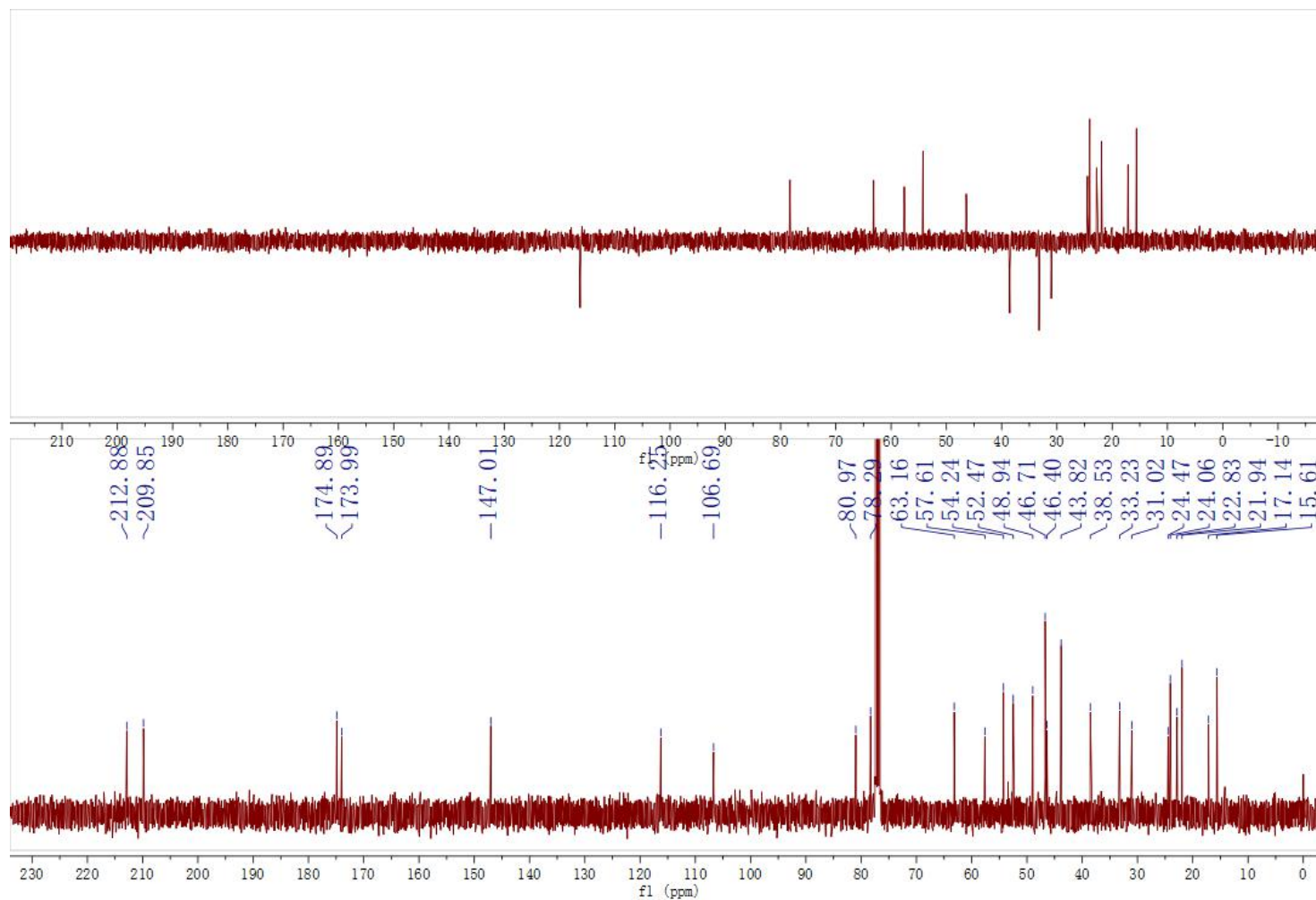
CD of compound 3



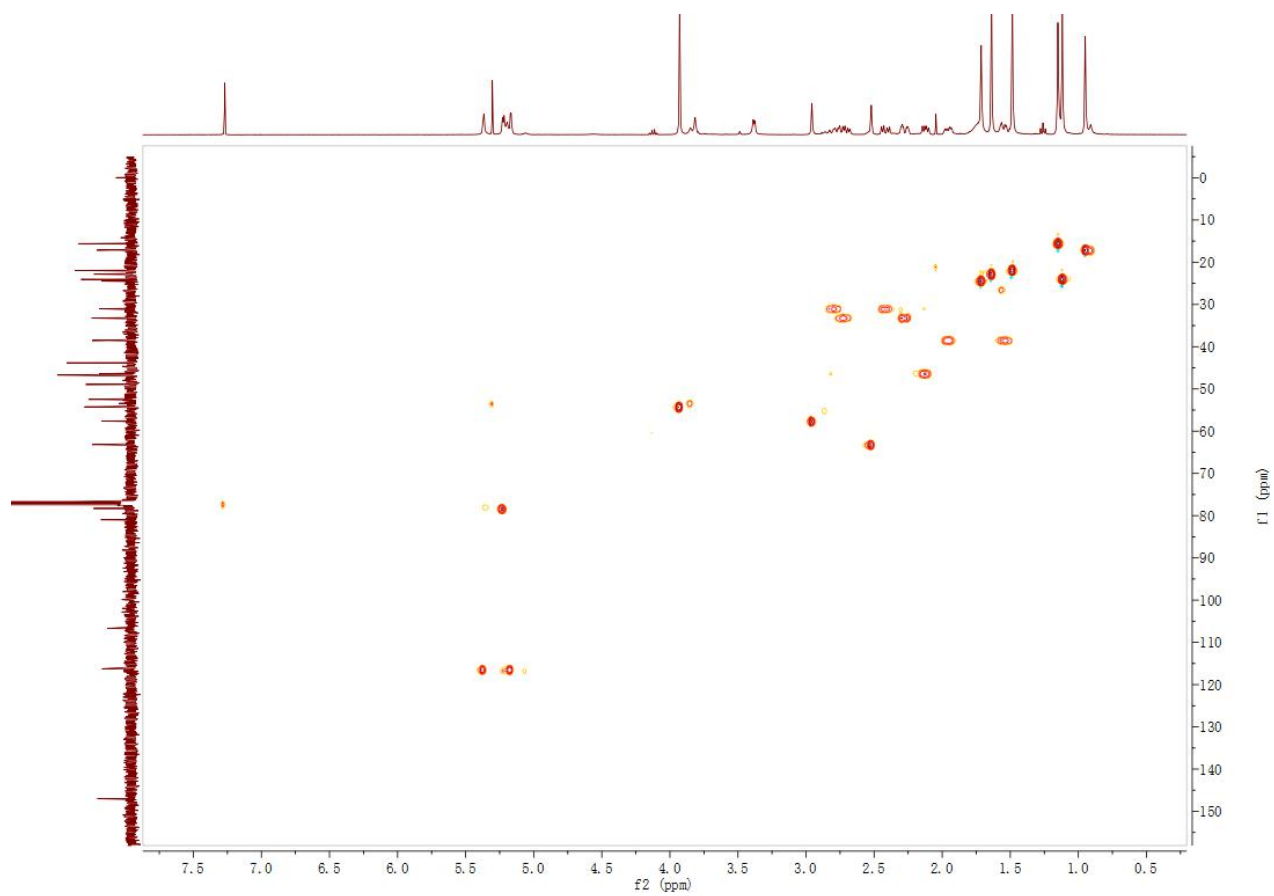
^1H NMR of compound **3** (in CDCl_3)



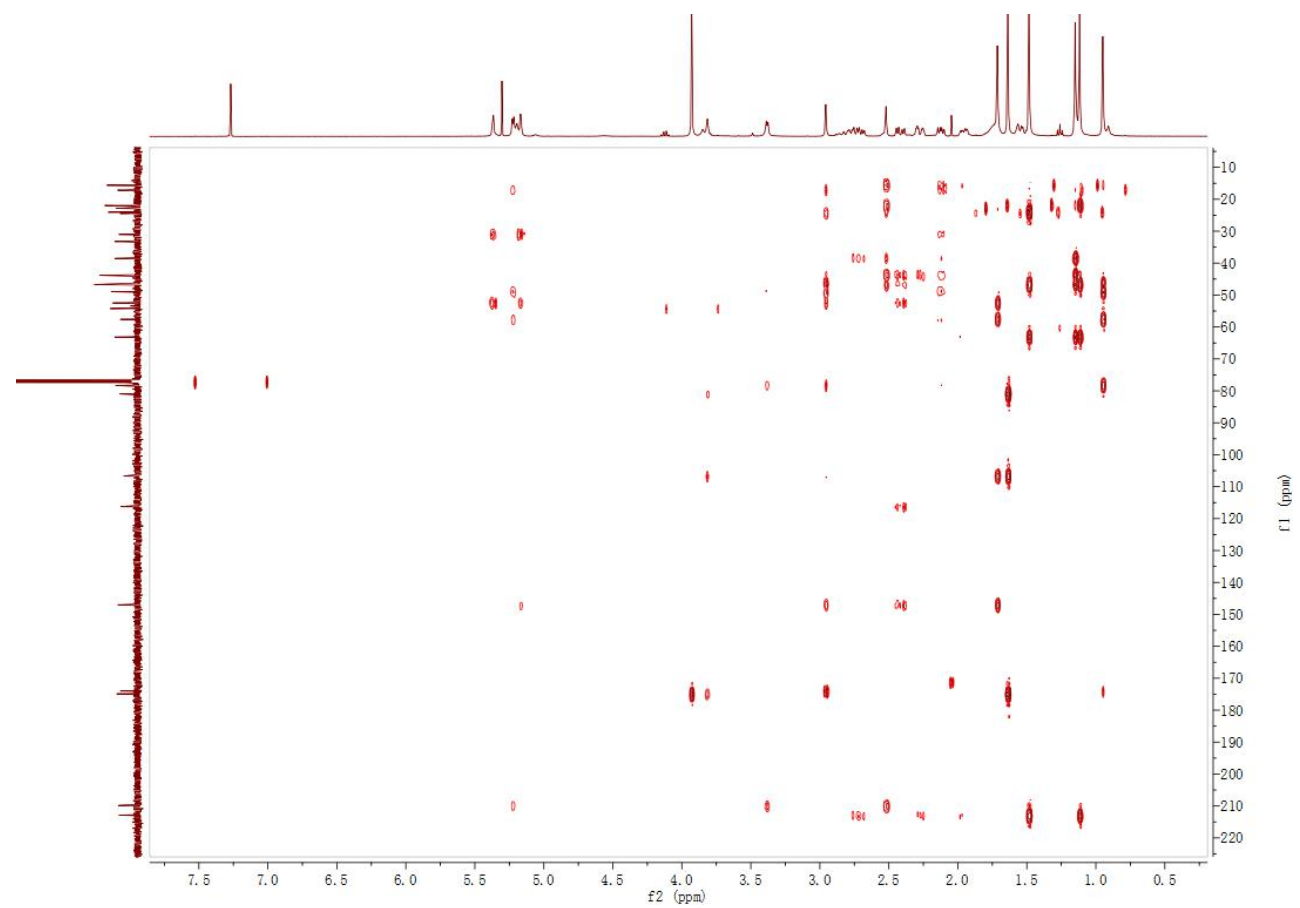
^{13}C NMR of compound **3** (in CDCl_3)



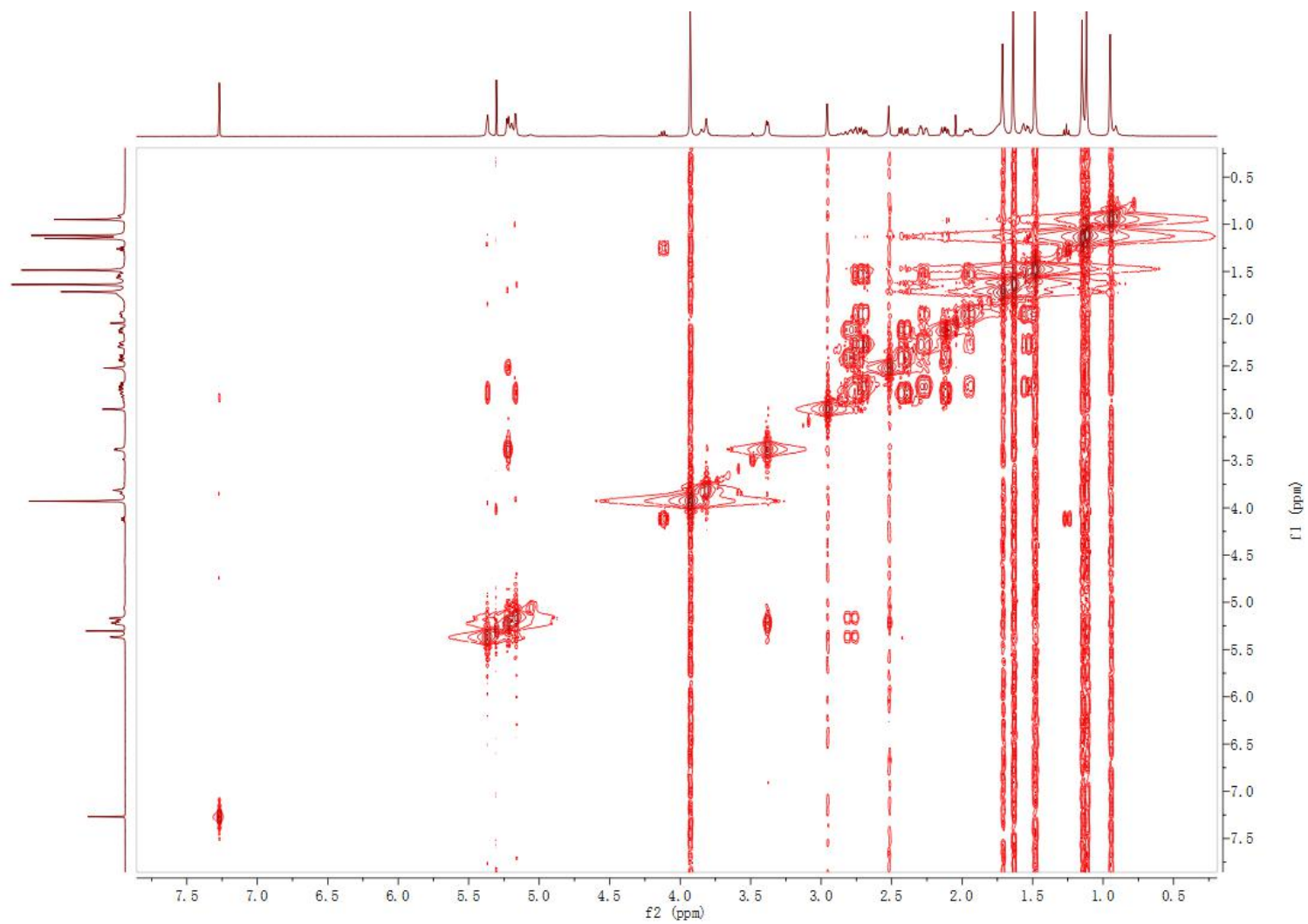
HSQC of compound **3** (in CDCl₃)



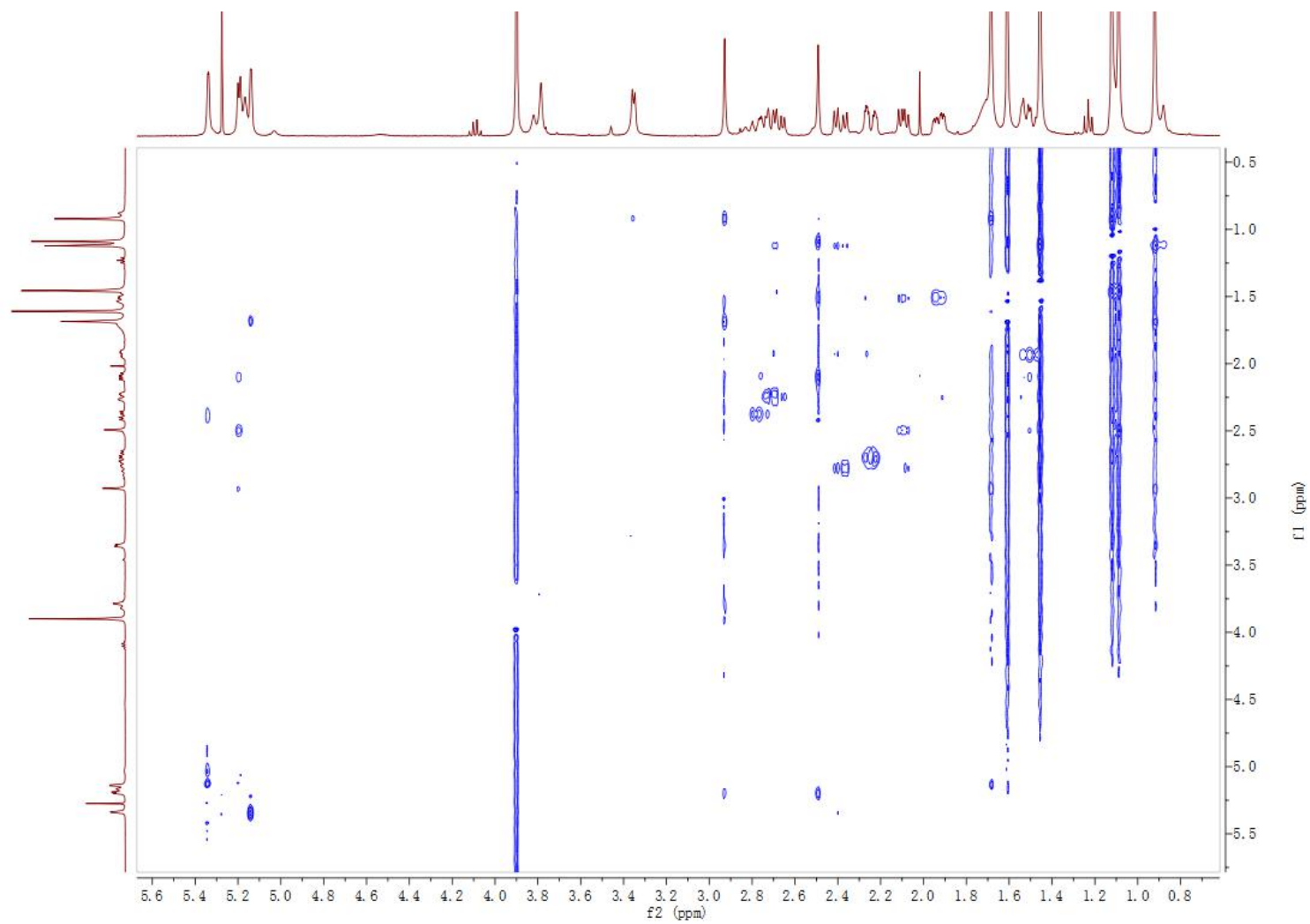
HMBC of compound **3** (in CDCl₃)



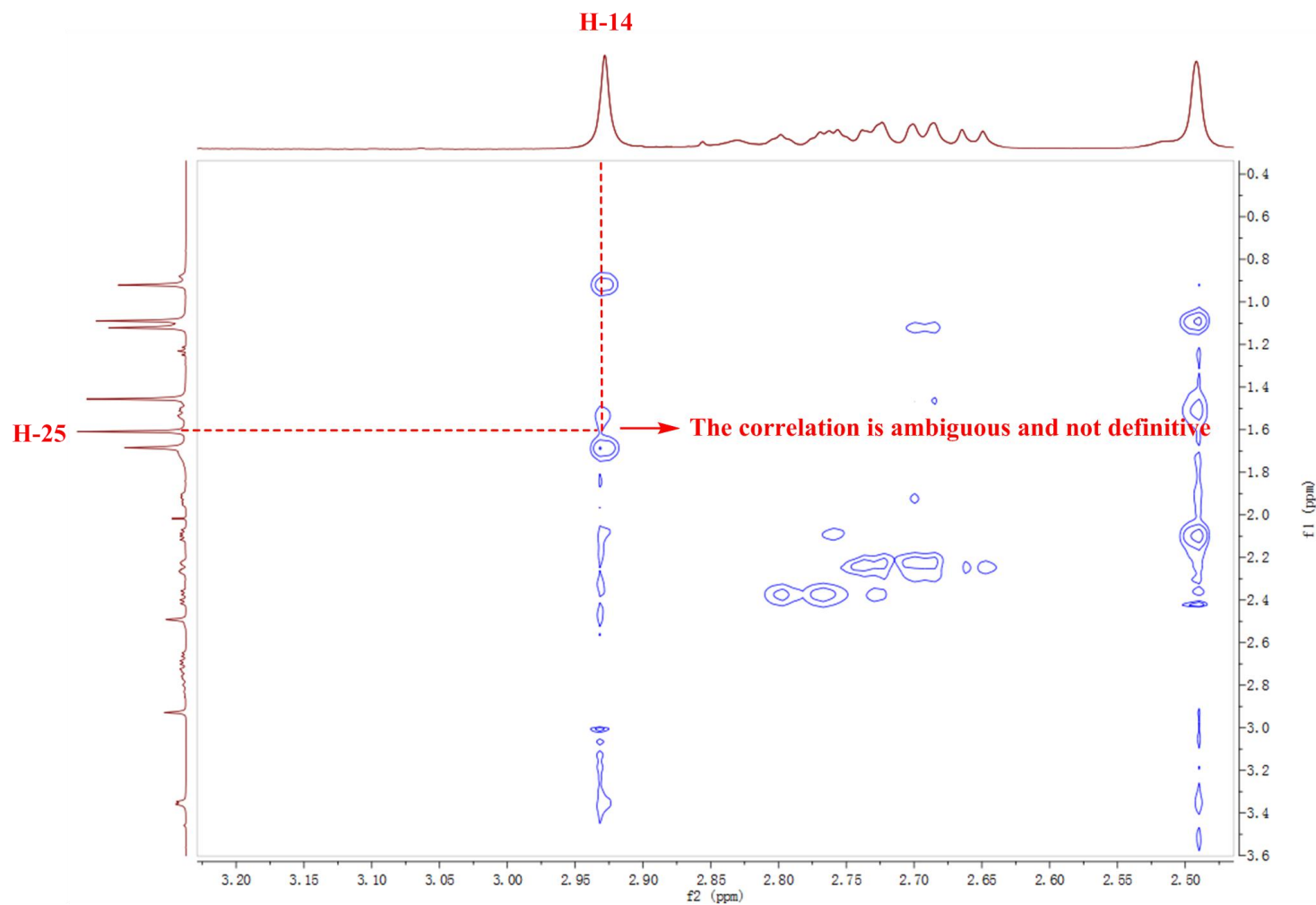
^1H - ^1H COSY of compound **3** (in CDCl_3)



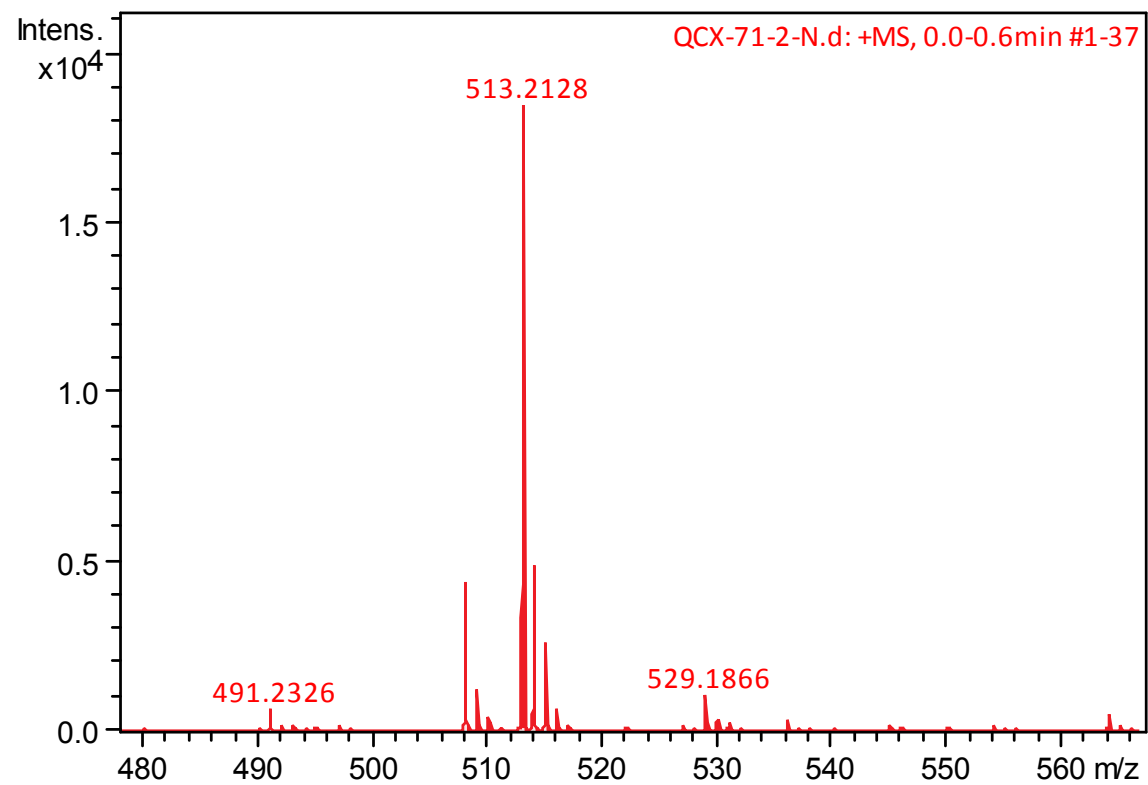
NOESY of compound **3** (in CDCl₃)



Enlarged NOESY of compound **3** (in CDCl₃)



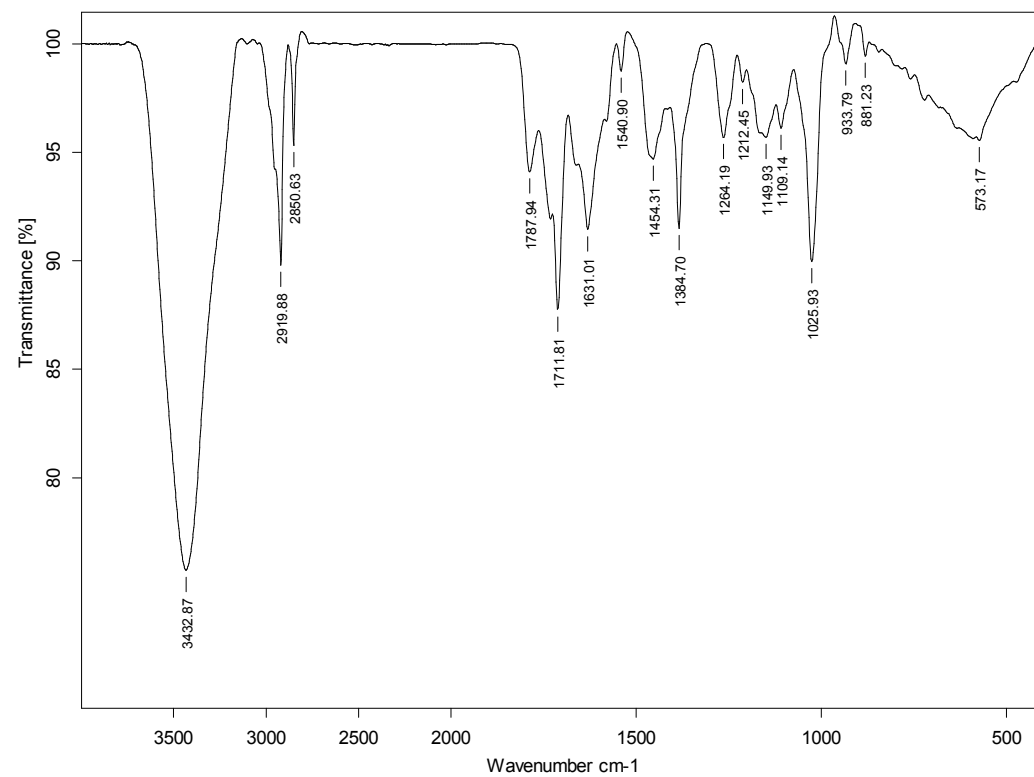
HRESIMS of compound **4**



IR of compound 4

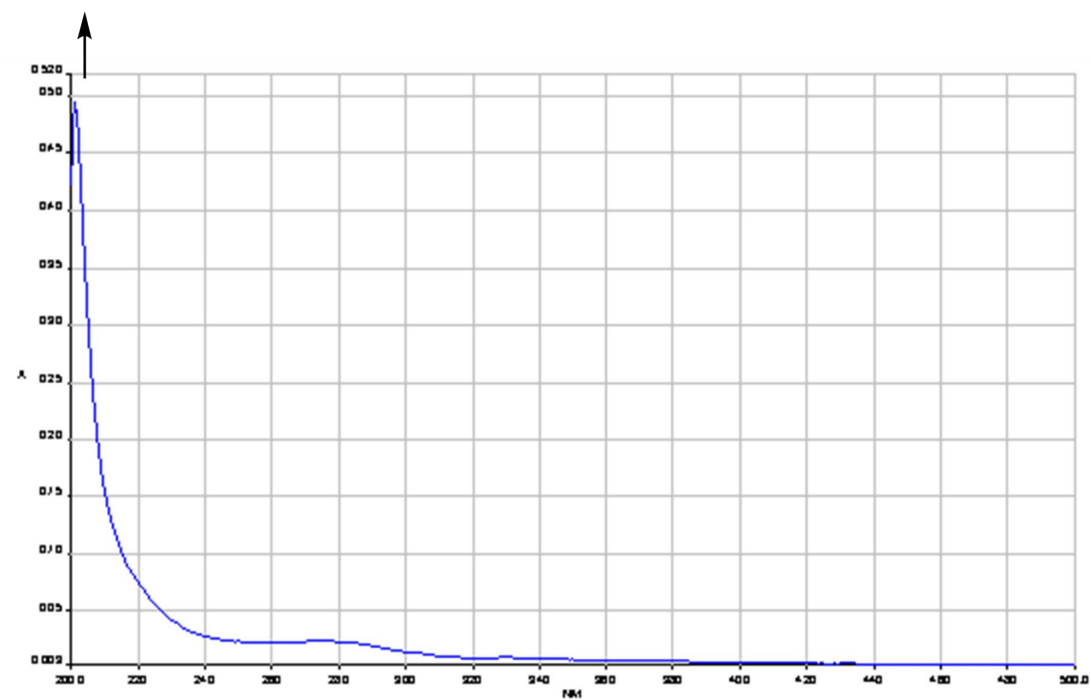
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11:14:03 2017-3-15

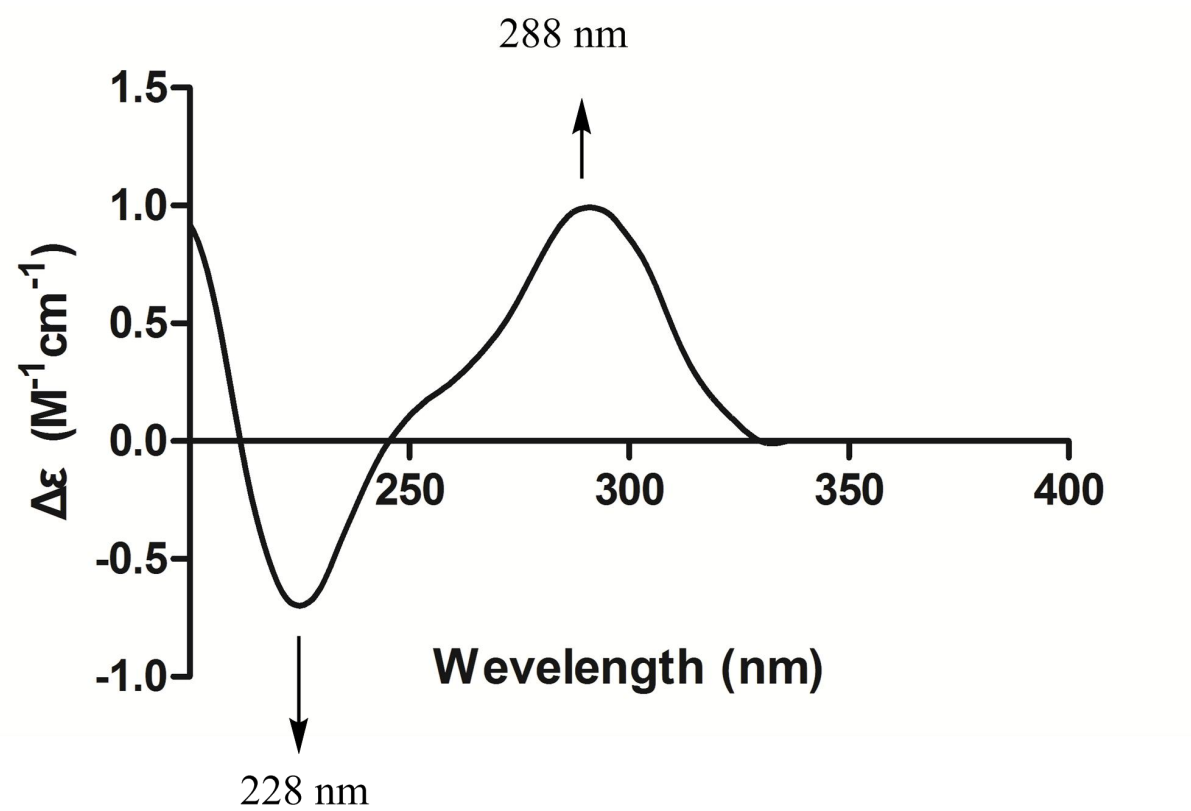


UV of compound **4**

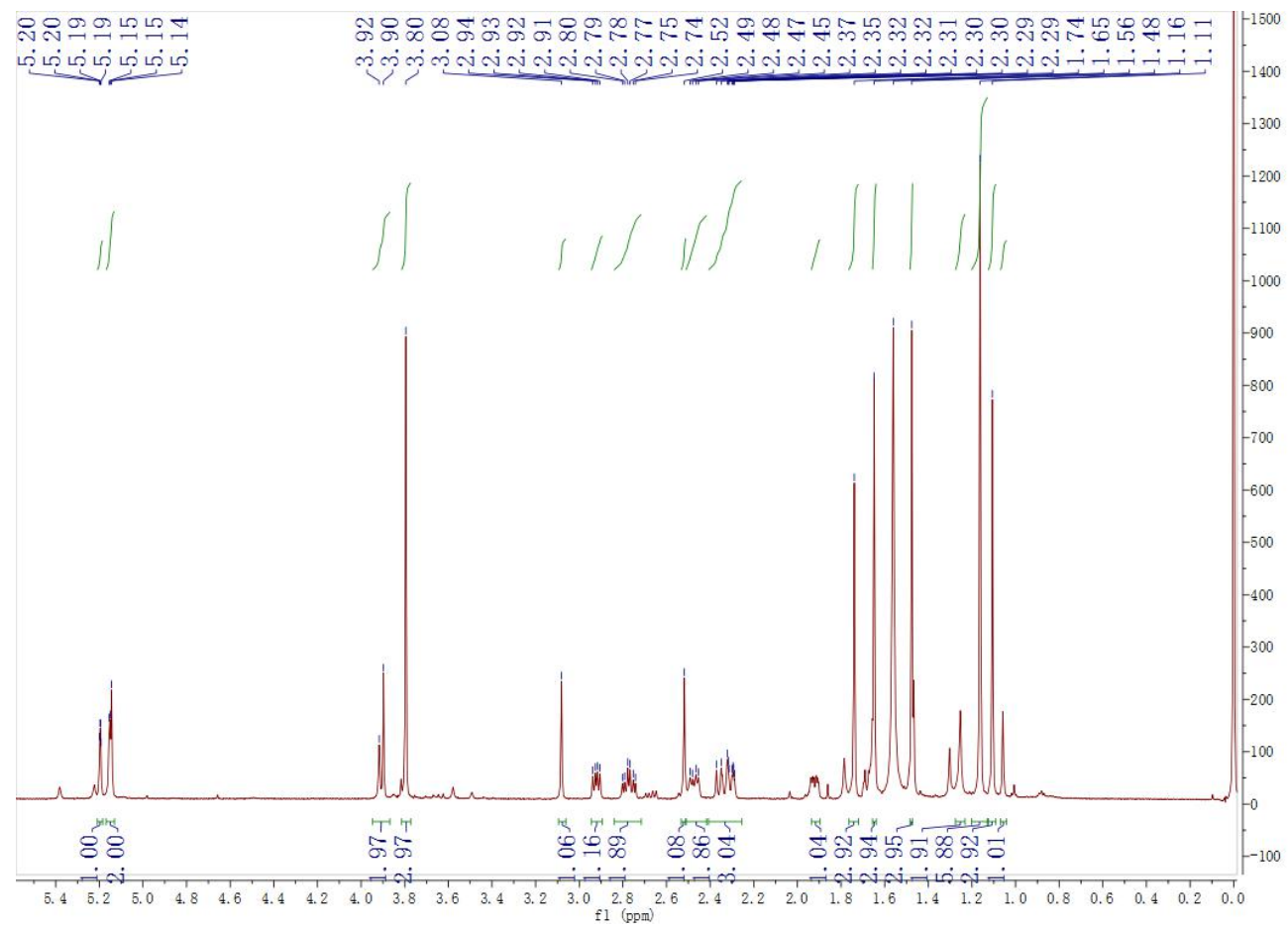
201 nm



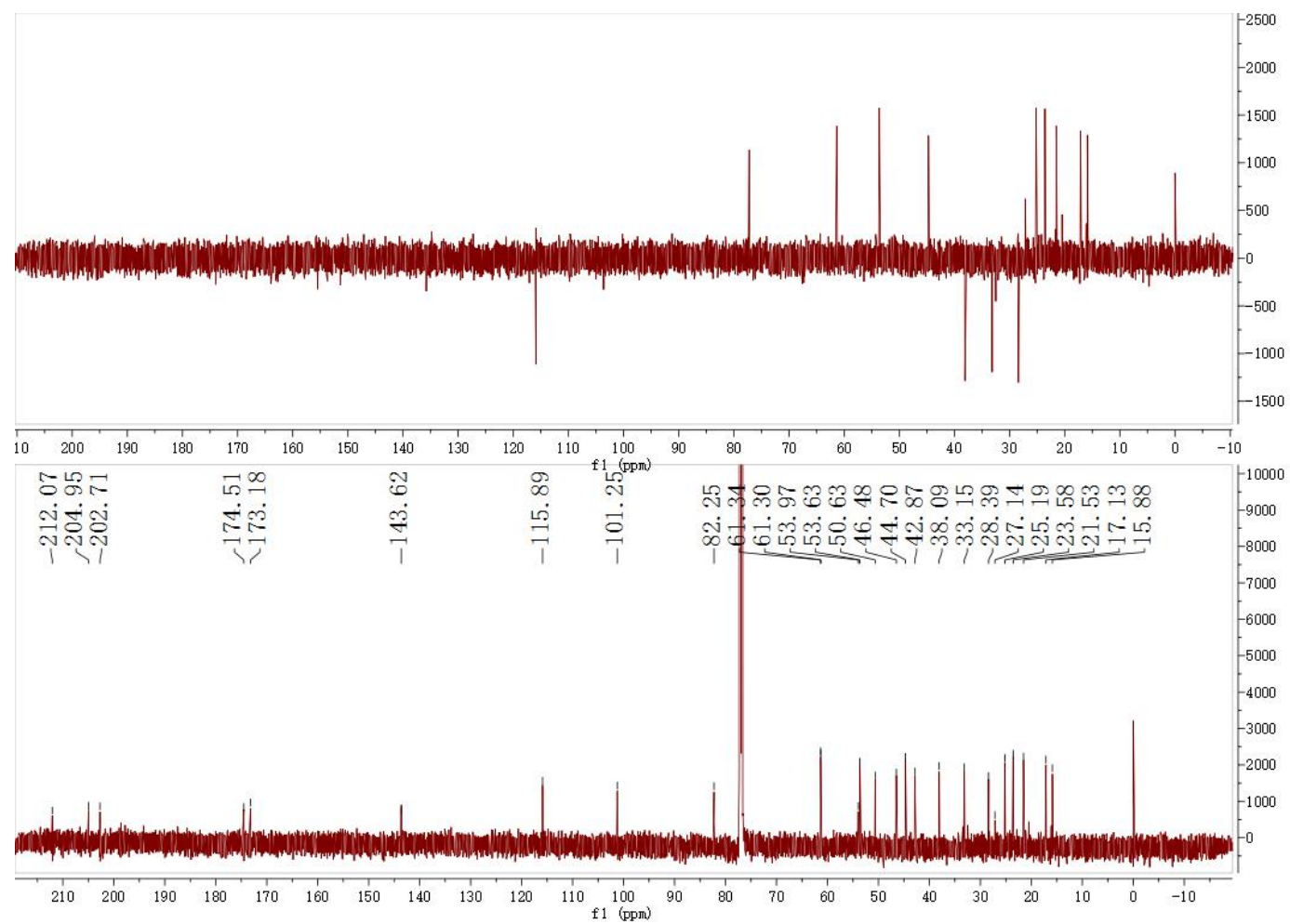
CD of compound 4



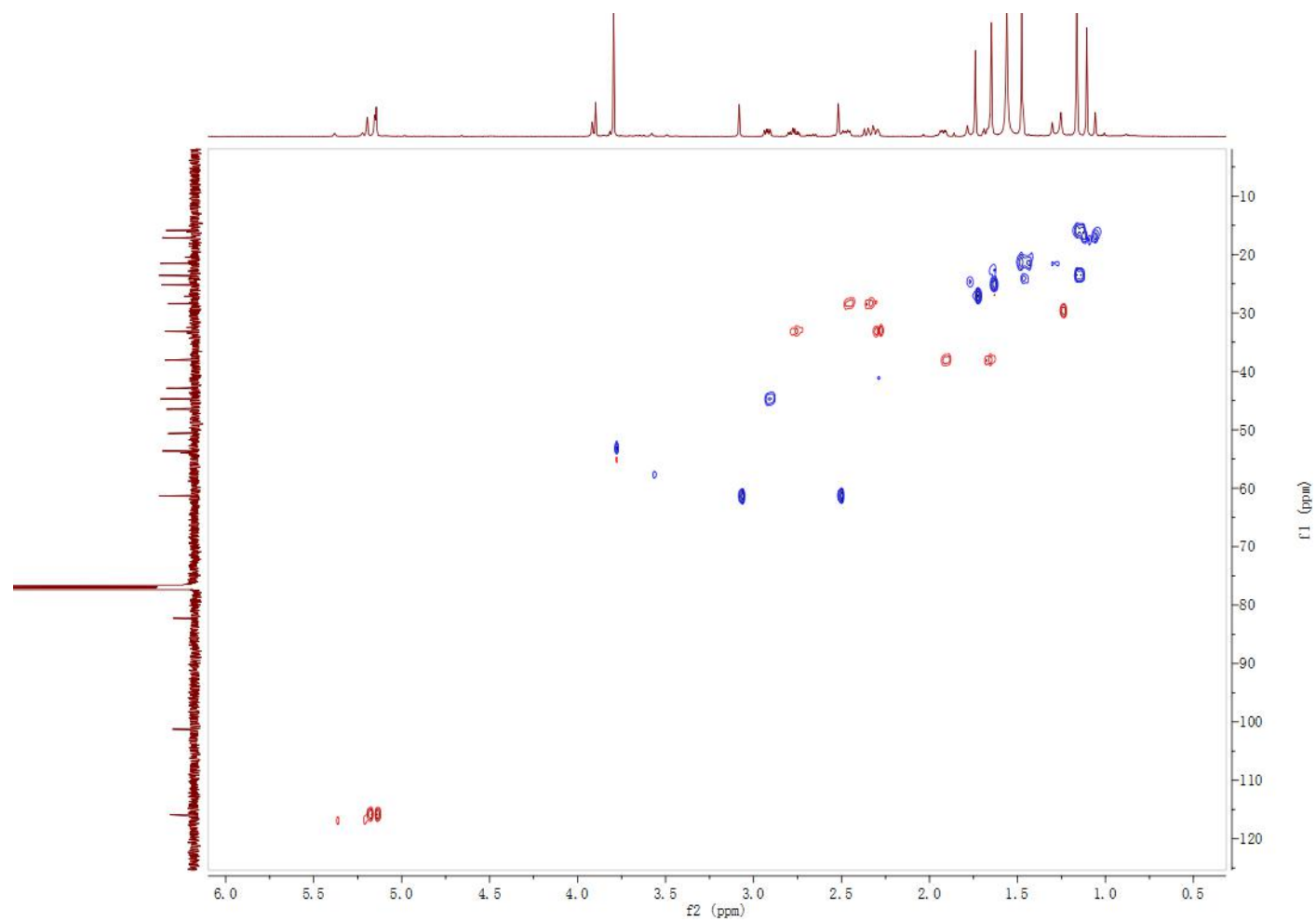
^1H NMR of compound **4** (in CDCl_3)



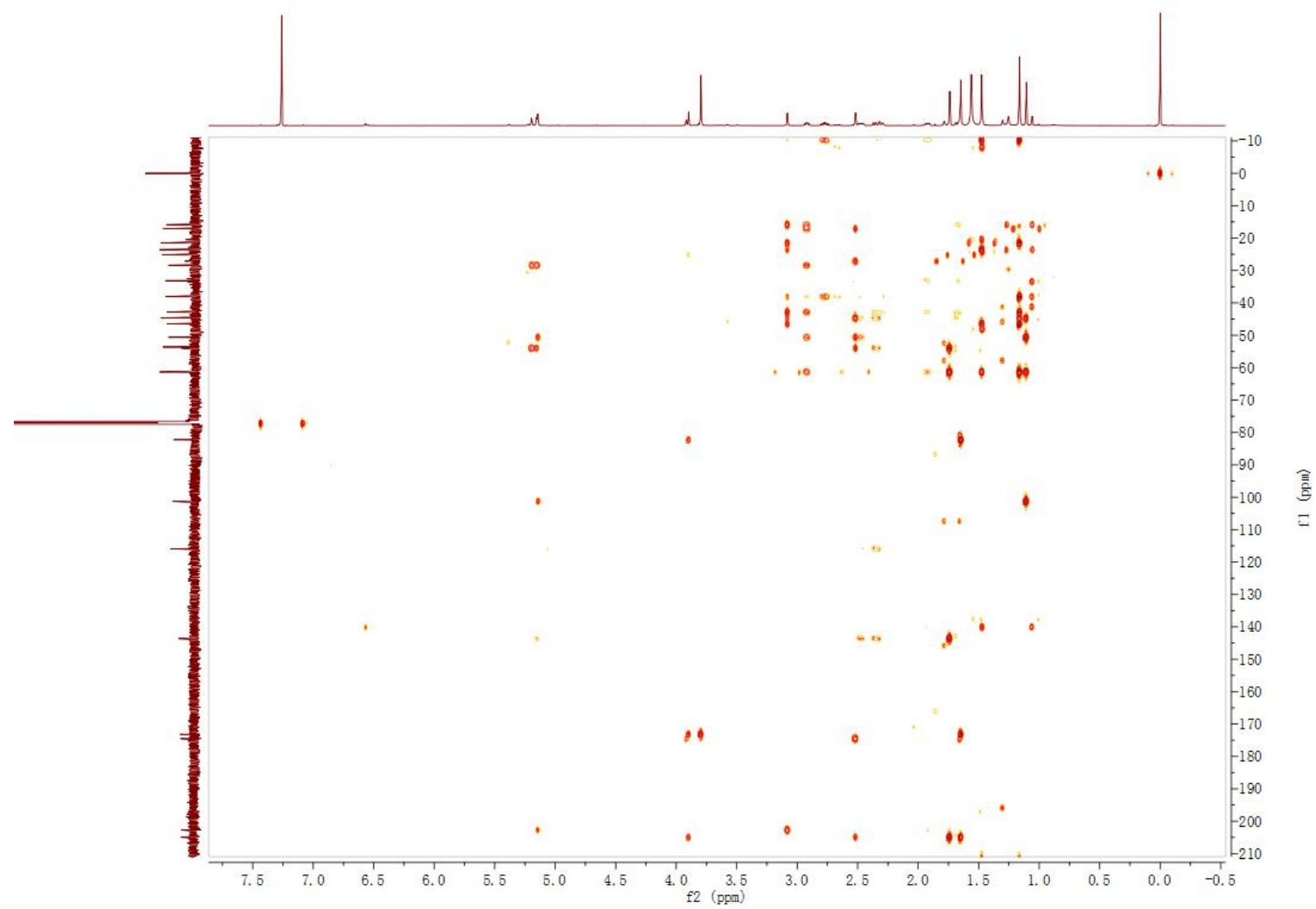
^{13}C NMR of compound **4** (in CDCl_3)



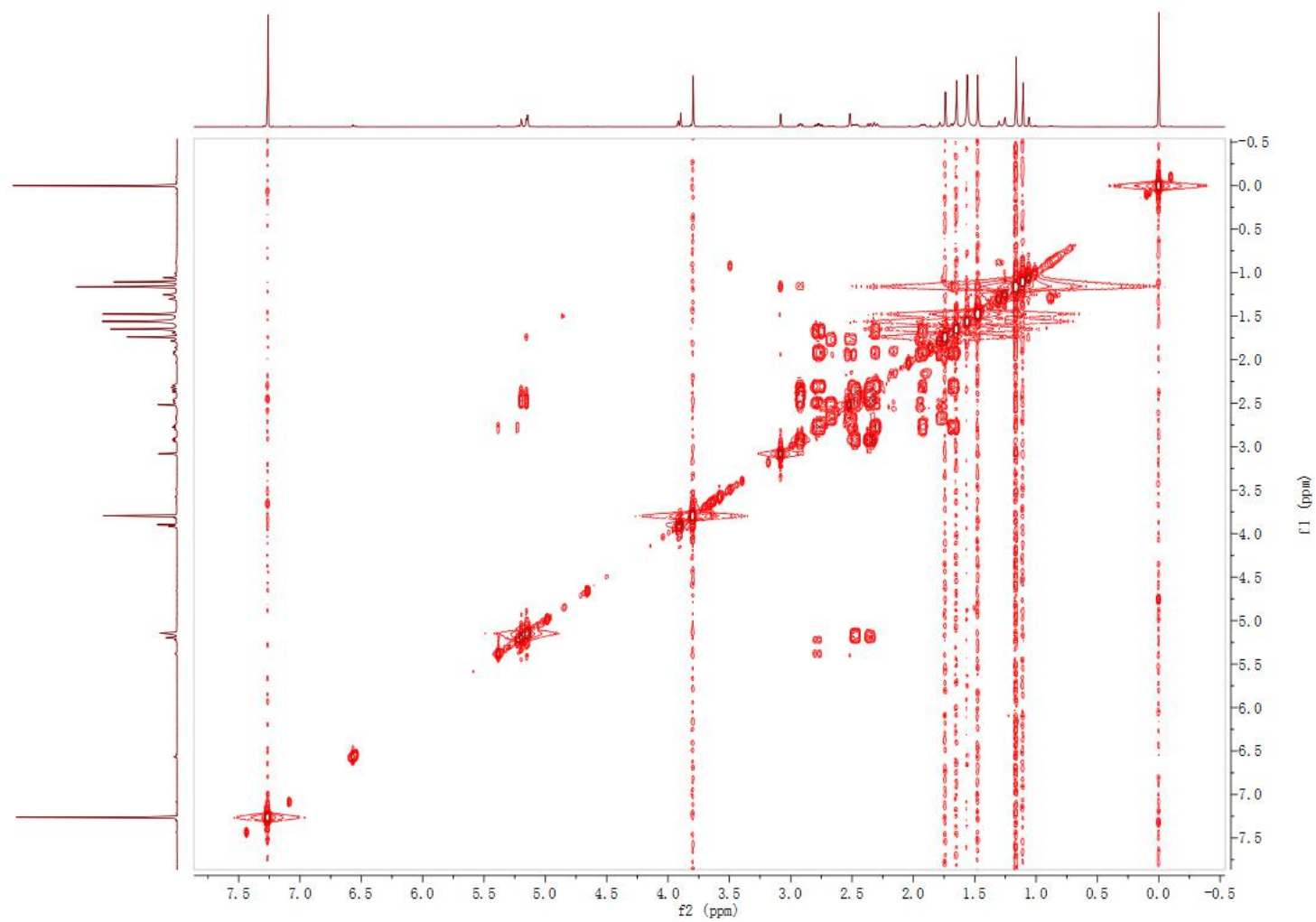
HSQC of compound **4** (in CDCl₃)



HMBC of compound **4** (in CDCl₃)



^1H - ^1H COSY of compound **4** (in CDCl_3)



NOESY of compound **4** (in CDCl₃)

