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

Changxing Qi,[a,†] Yuben Qiao,[a,†] Weixi Gao,[a] Mengting Liu,[a] Qun Zhou,[a] Chunmei Chen,[a] Yongji Lai,[b] Yongbo Xue,[a] Jinwen Zhang,[c] Dongyan Li,[c] Jianping Wang,[a] Hucheng Zhu,[a] Zhengxi Hu,[a,*] Yuan Zhou,[a,*] and Yonghui Zhang[a,*]

[a]Hubei Key Laboratory of Natural Medicinal Chemistry and Resource Evaluation, School of Pharmacy, Tongji Medical College, Huazhong University of Science and Technology, Wuhan 430030, Hubei Province, People's Republic of China. E-mail: zhangyh@mails.tjmu.edu.cn (Y. Zhang); zhouyuan@mail.hust.edu.cn (Y. Zhou); hzx616@126.com (Z. Hu). Fax: 86-27-83692762; Tel: 86-27-83692892.

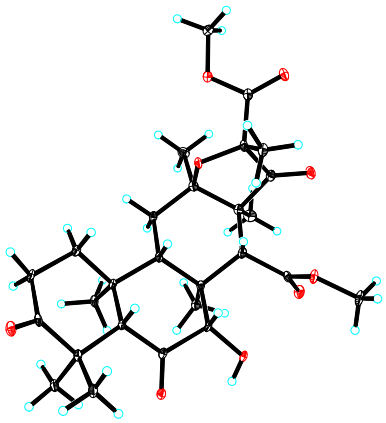
[b]Department of Pharmacy, the Central Hospital of Wuhan, Wuhan 430014, Hubei Province, People's Republic of China.

[c]Department of Pharmacy, Tongji Hospital, Tongji Medical College, Huazhong University of Science and Technology, Wuhan 430030, Hubei Province, People's Republic of China

[†]These authors contributed equally to this work.

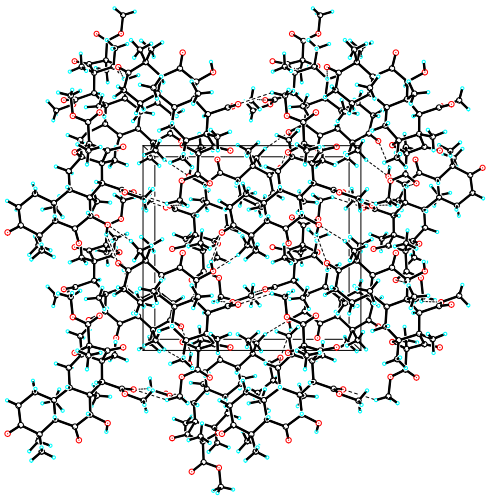
CONTENTS

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, α = 90°, β = 90°, γ = 90°, V = 2517.7(2) Å^3, T = 100(2) K, space group $P212121$, Z = 4, μ(CuKα) = 0.824 mm^{-1}, 14247 reflections measured, 4526 independent reflections (R_{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.



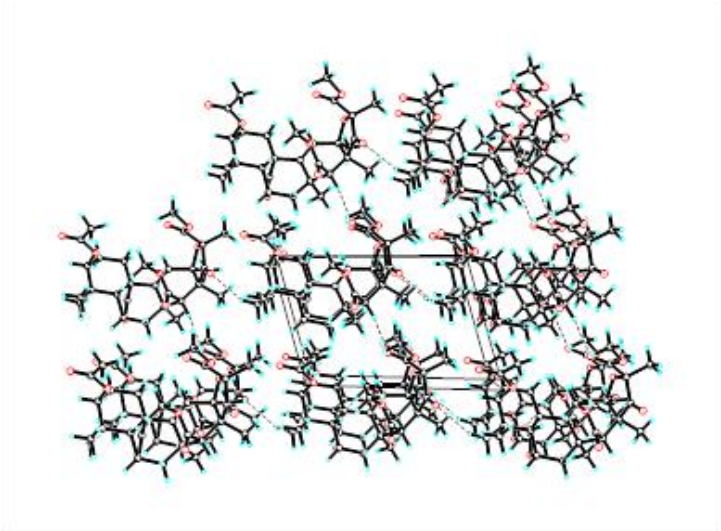
View of the pack drawing of **1**.

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) Å, b = 7.85050(10) Å, c = 11.6784(2) Å, α = 74.58°, β = 73.43°, γ = 87.86°, V = 664.293(17) Å^3, T = 100(2) K, space group $P1$, Z = 1, μ(CuKα) = 0.854 mm^{-1}, 10823 reflections measured, 3922 independent reflections (R_{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.

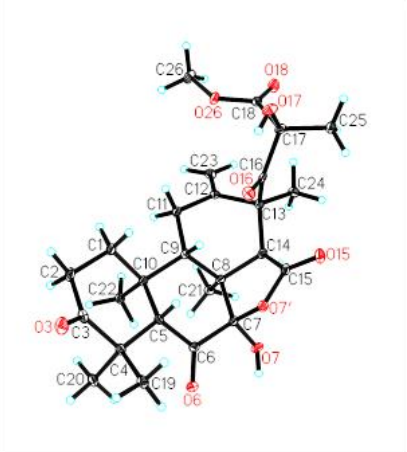
Displacement ellipsoids are drawn at the 30% probability level.



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

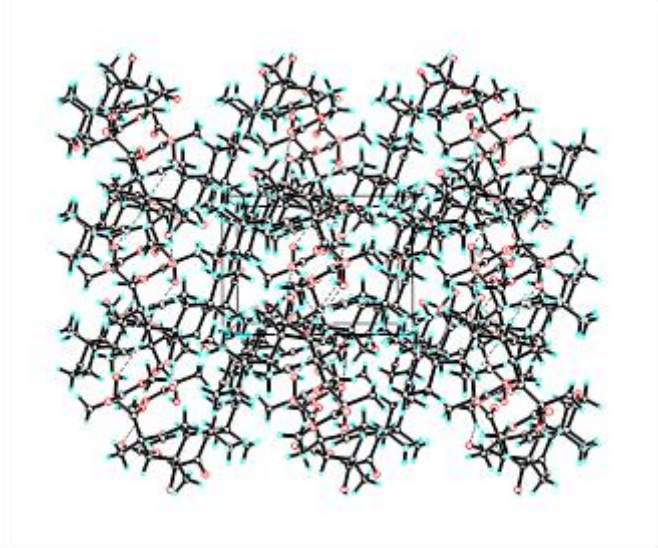
Hydrogen-bonds are shown as dashed lines.

Crystal data for compound **4**: $C_{26}H_{34}O_9$, M = 490.53, a = 7.3751(3) Å, b = 15.7593(7) Å, c = 10.1577(4) Å, α = 90°, β = 90.4660(10)°, γ = 90°, V = 1180.55(8) Å^3, T = 100(2) K, space group $P21$, Z = 2, μ(CuKα) = 0.863 mm^{-1}, 13065 reflections measured, 4201 independent reflections (R_{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.

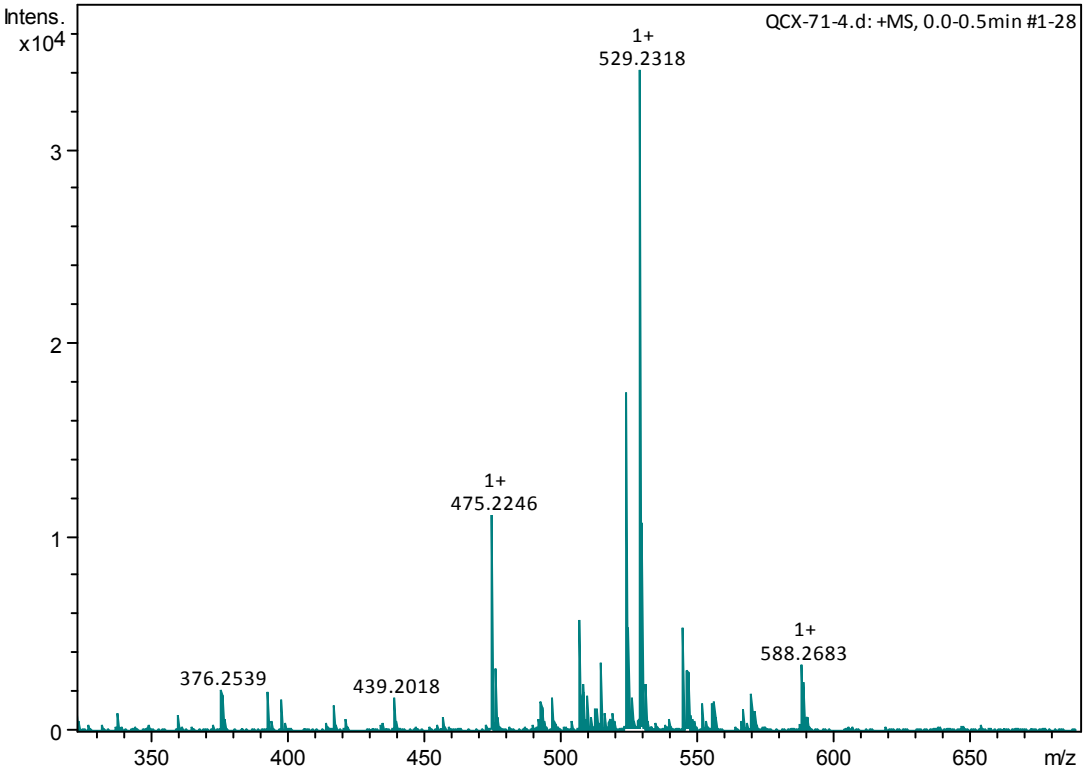
Displacement ellipsoids are drawn at the 30% probability level.



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

Hydrogen-bonds are shown as dashed lines.

HRESIMS of compound **1**



IR of compound **1**

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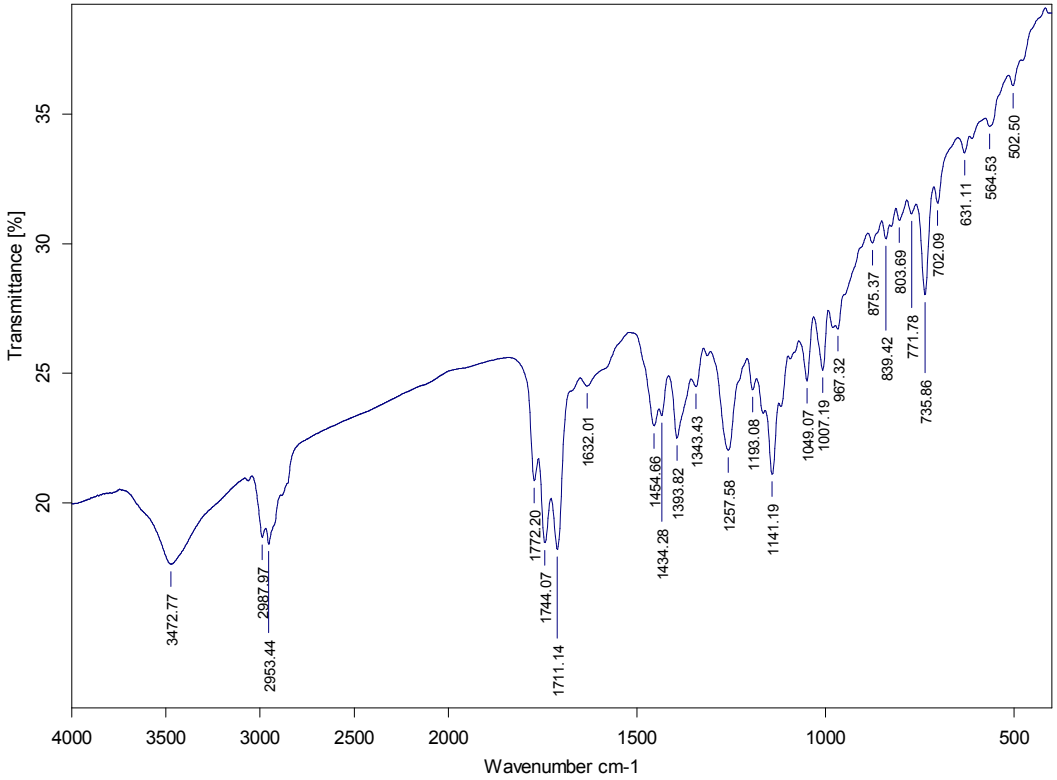
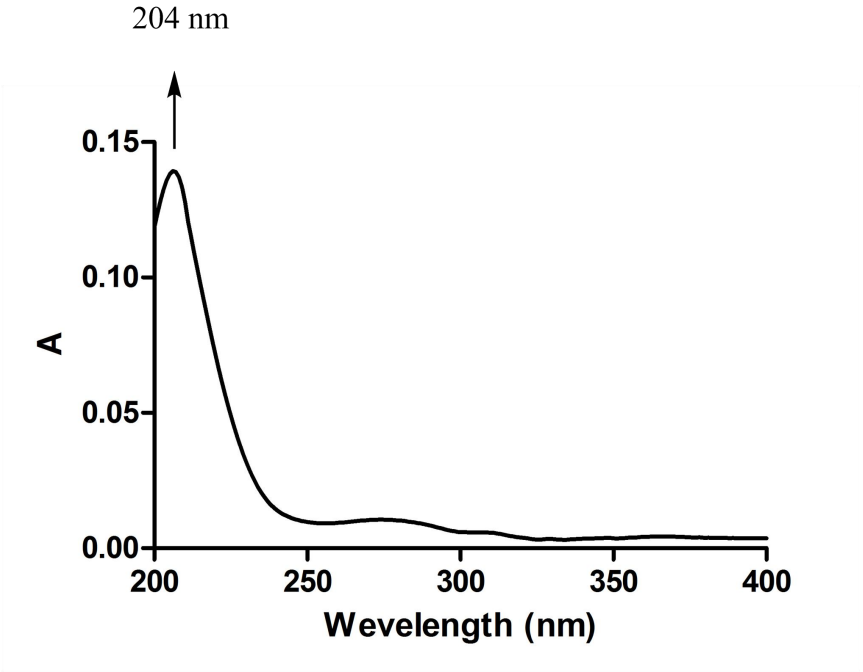
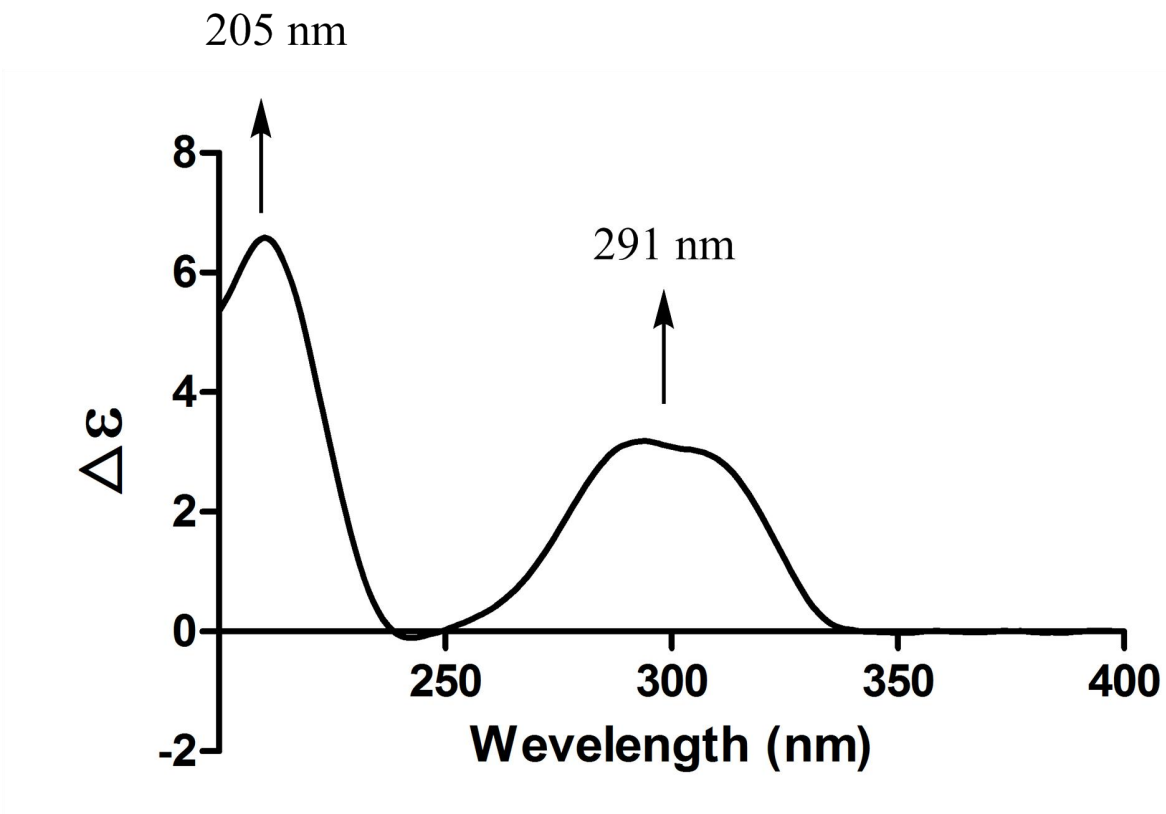


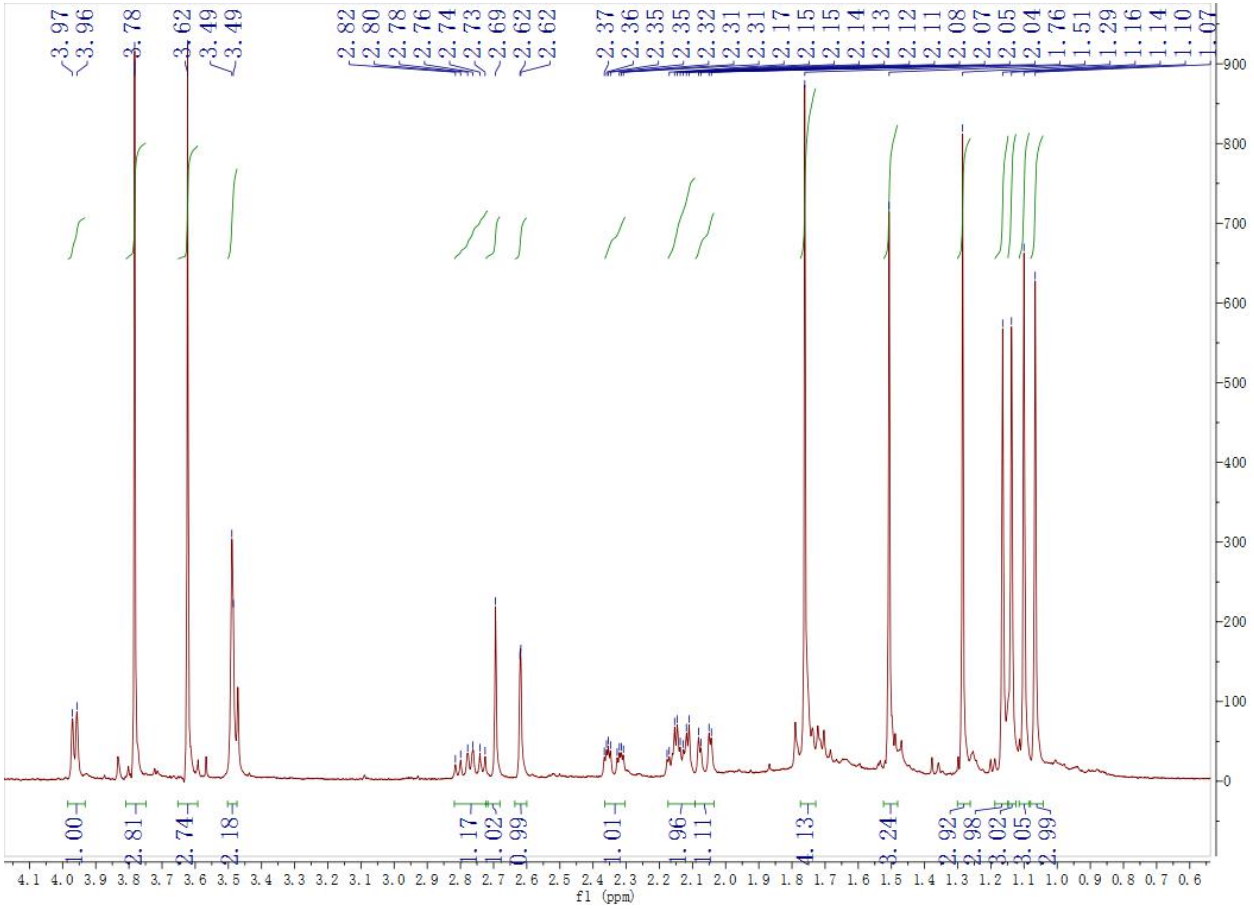
UV of compound **1**



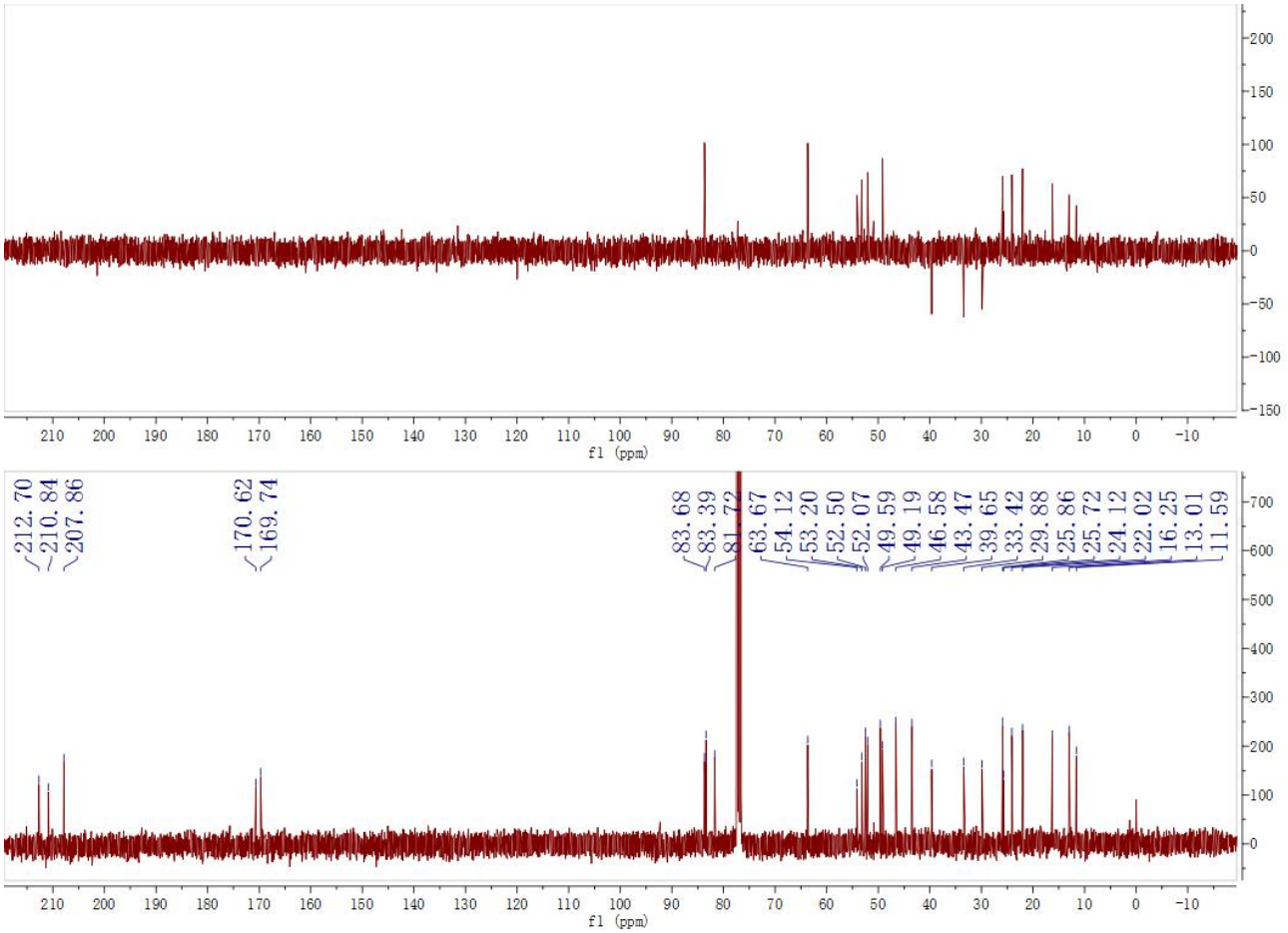
CD of compound **1**



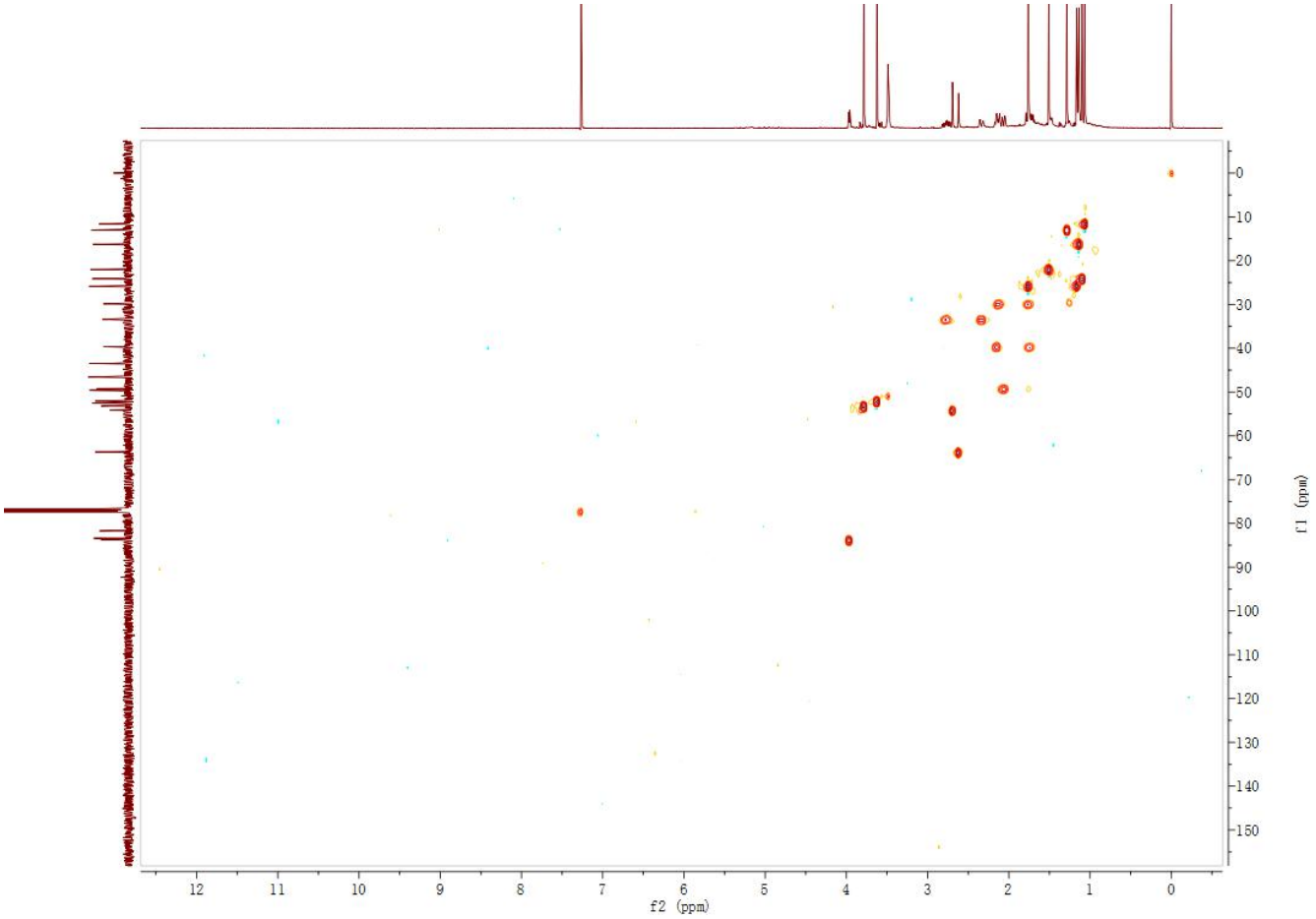
^{1}H NMR of compound **1** (in $CDCl_3$)



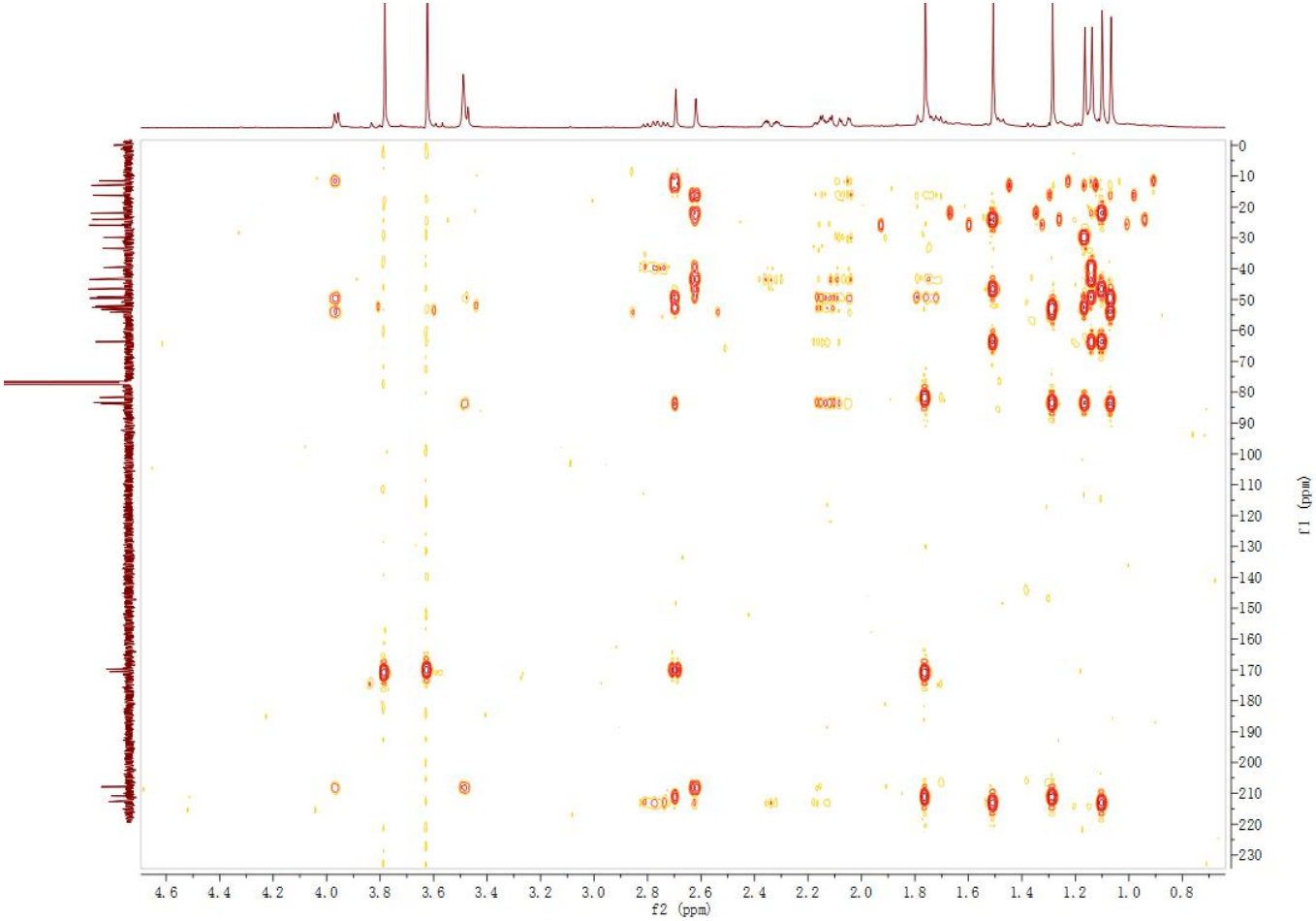
^{13}C NMR of compound **1** (in $CDCl_3$)



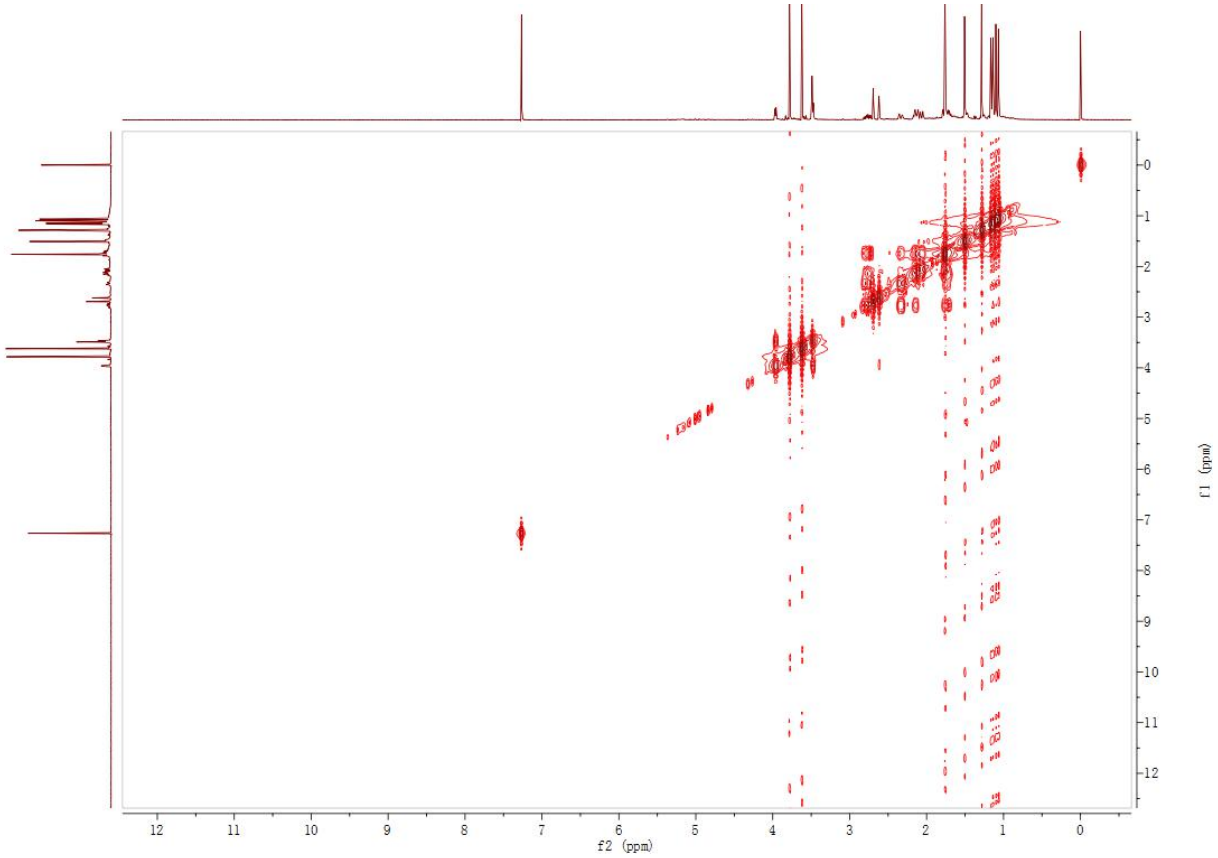
HSQC of compound **1** (in $CDCl_3$)



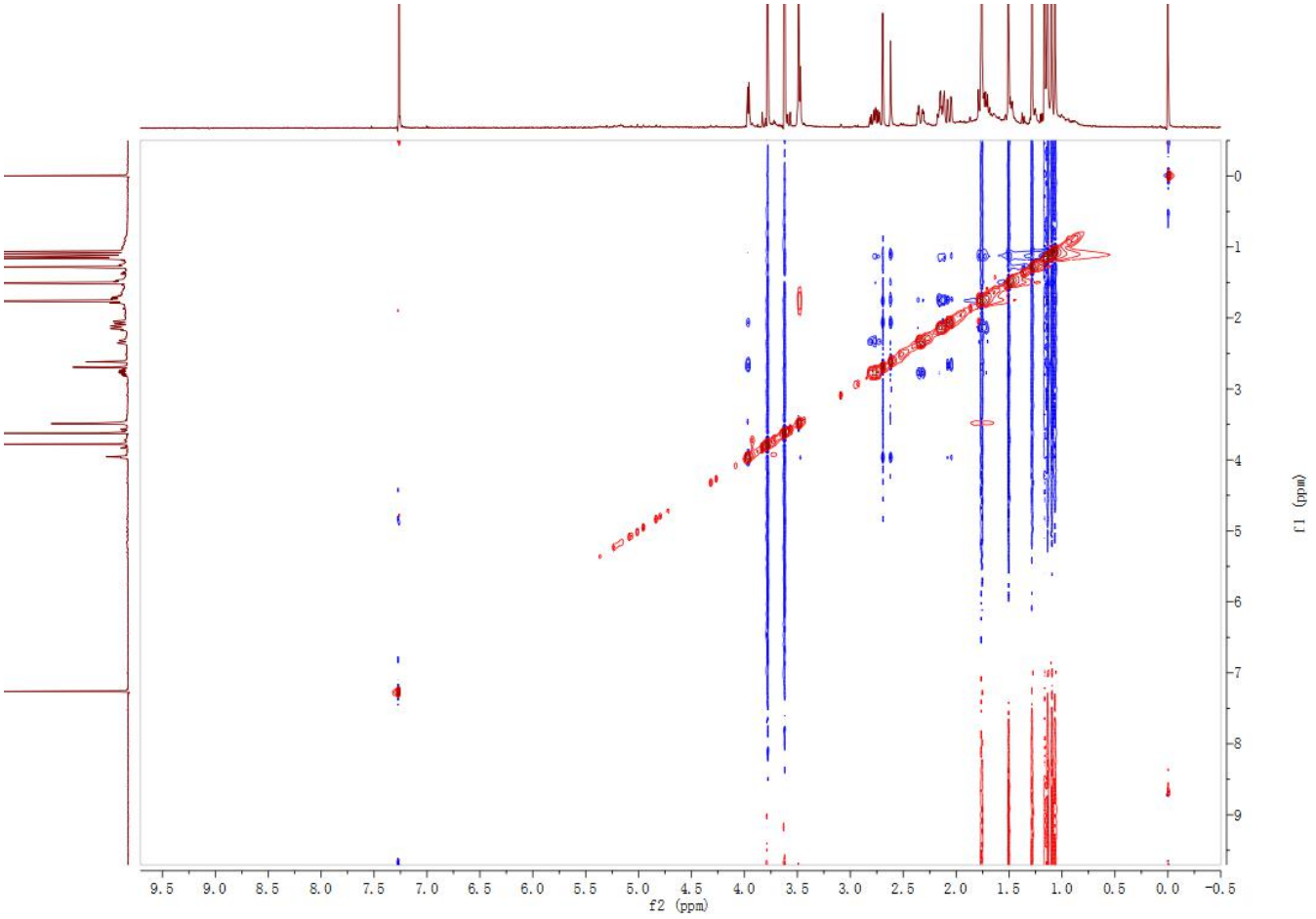
HMBC of compound **1** (in $CDCl_3$)



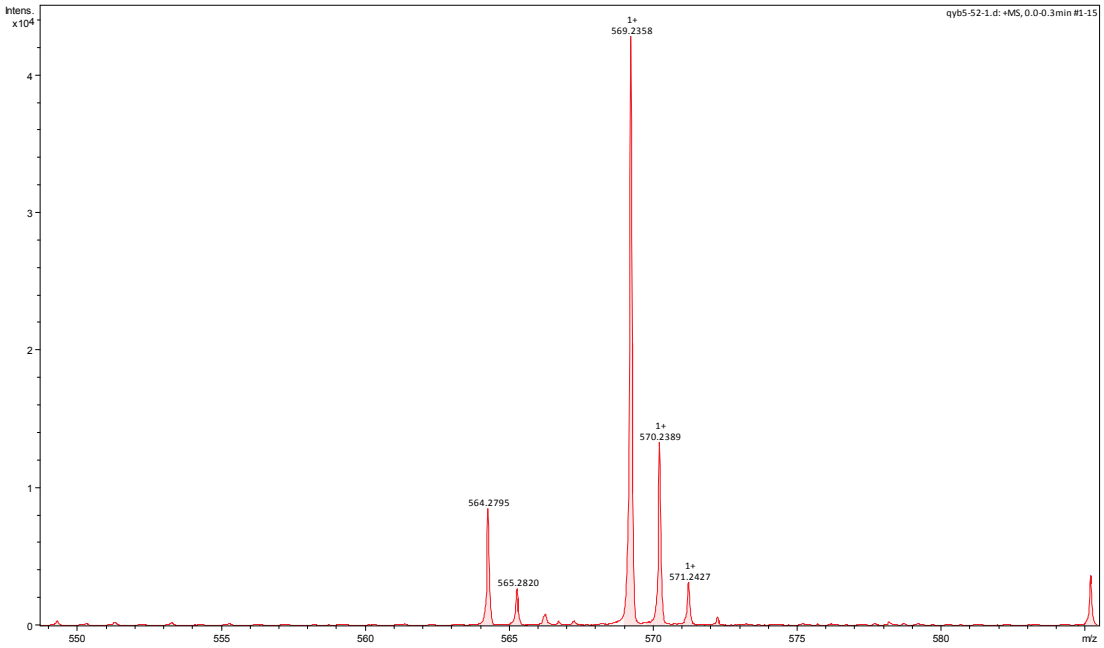
^{1}H–^{1}H COSY of compound **1** (in $CDCl_3$)



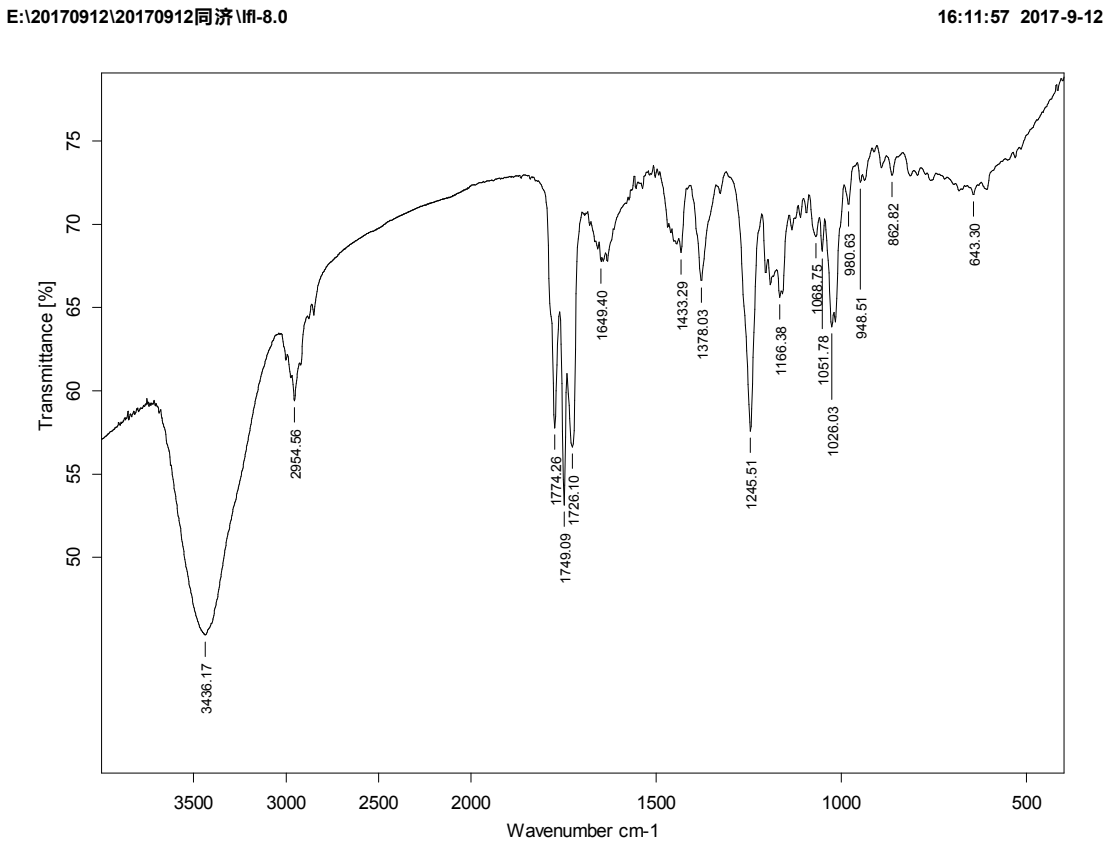
NOESY of compound **1** (in $CDCl_3$)



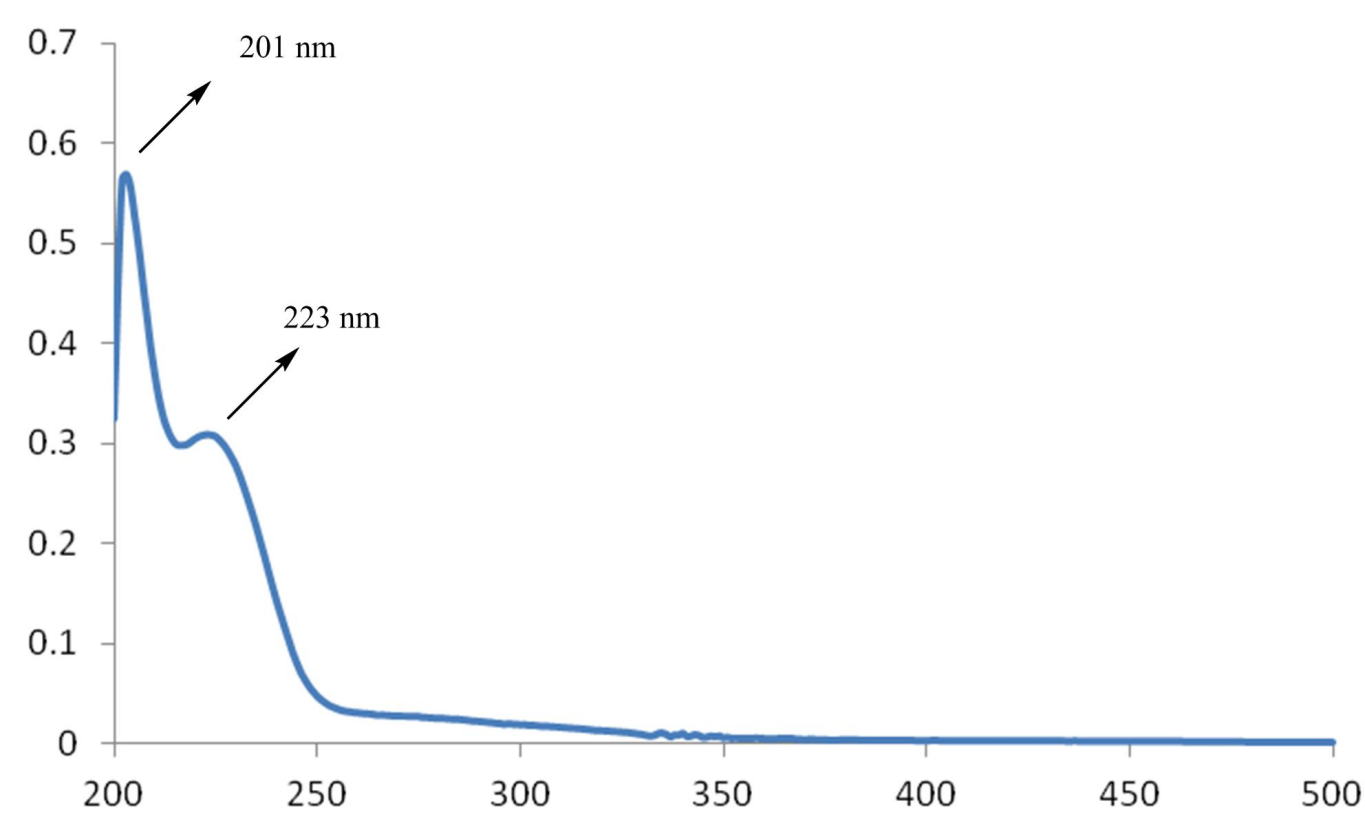
HRESIMS of compound **2**



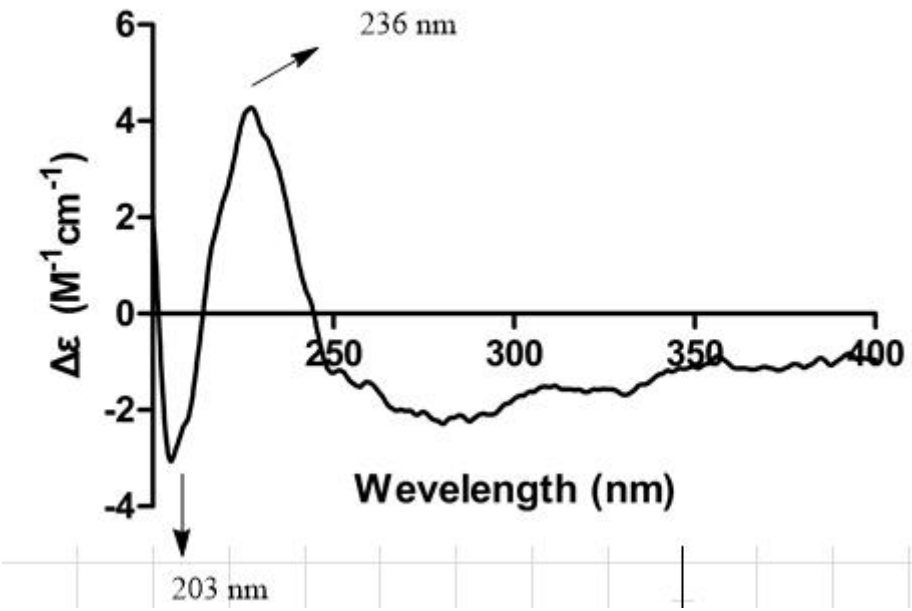
IR of compound **2**



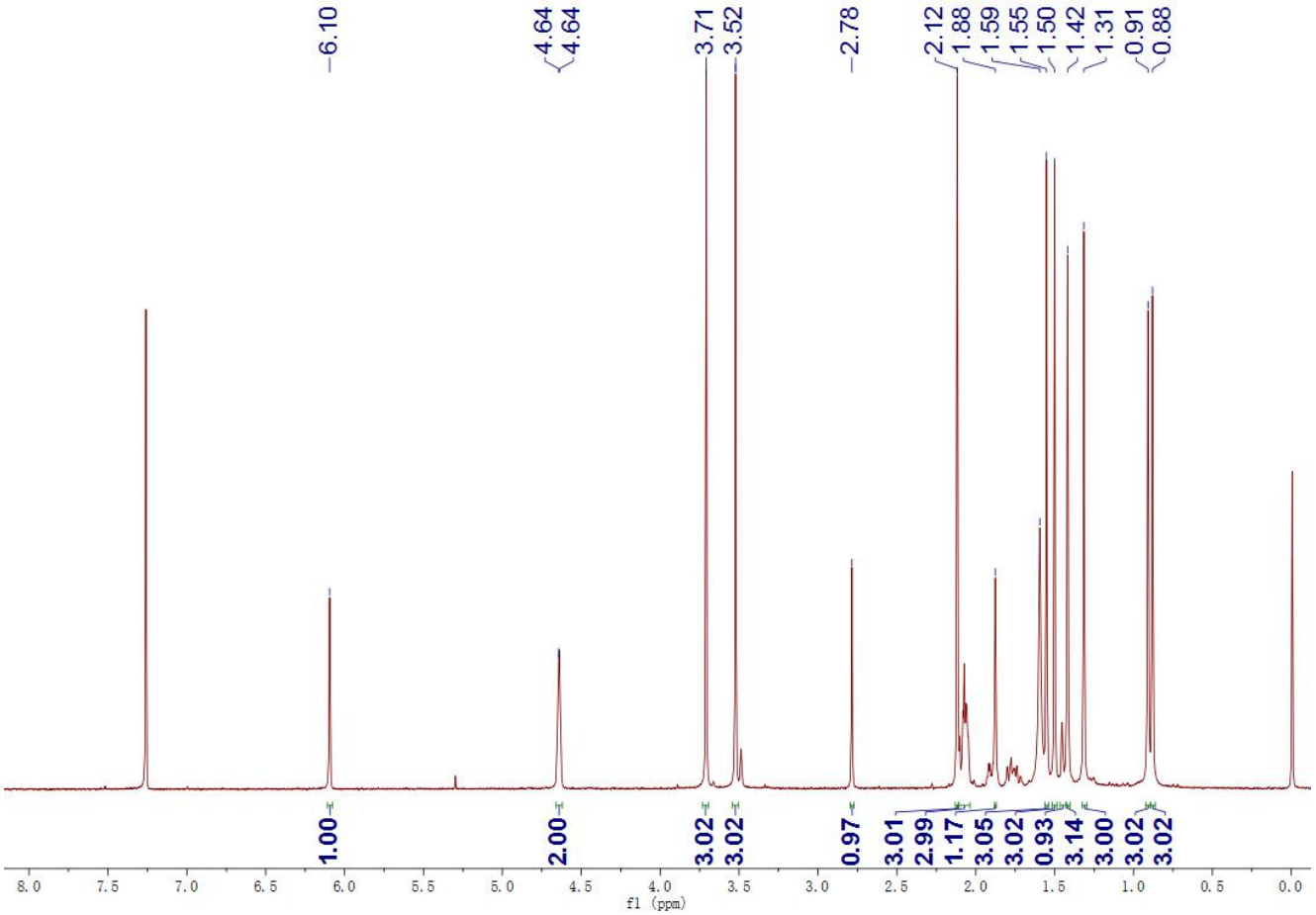
UV of compound **2**



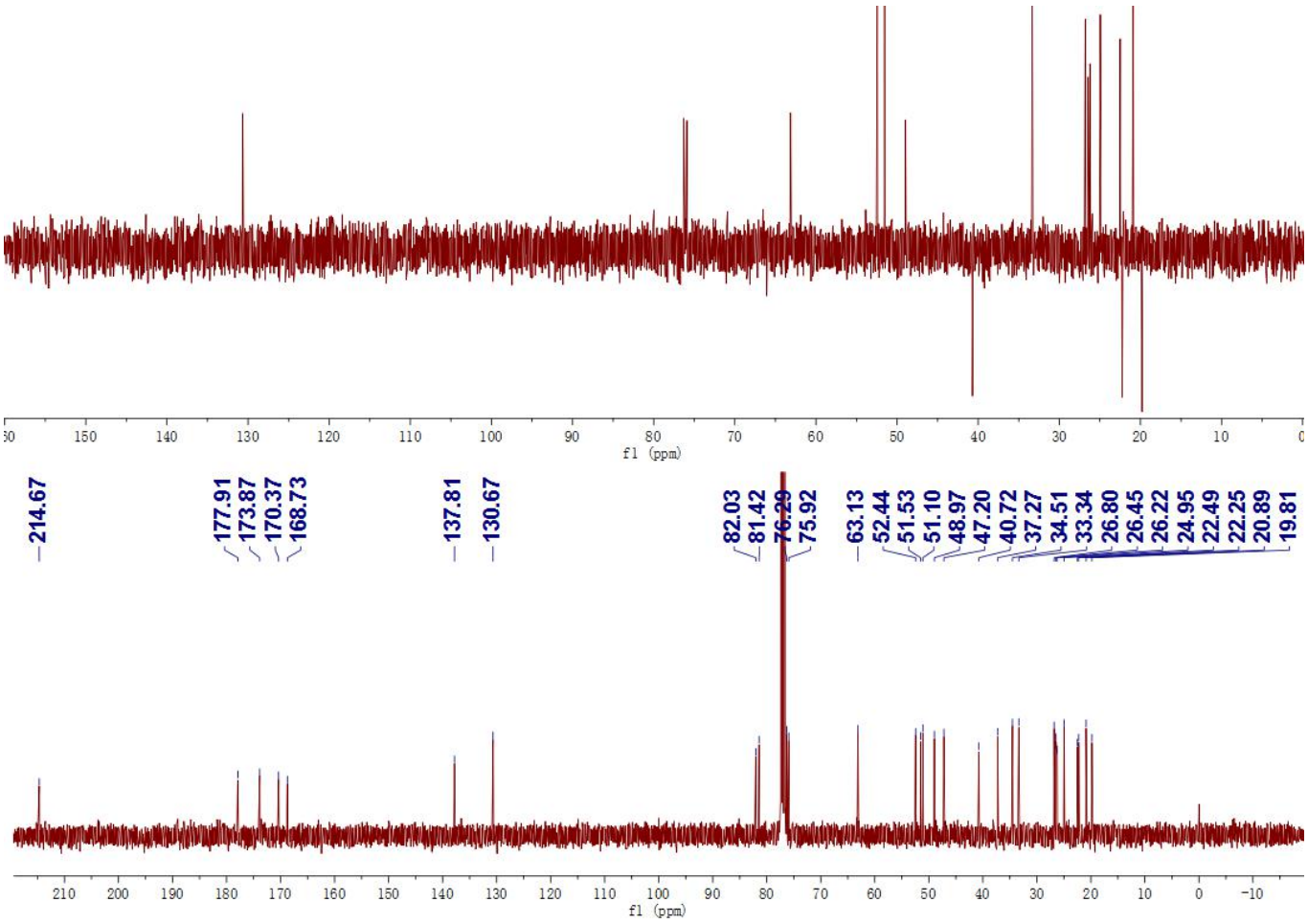
CD of compound **2**



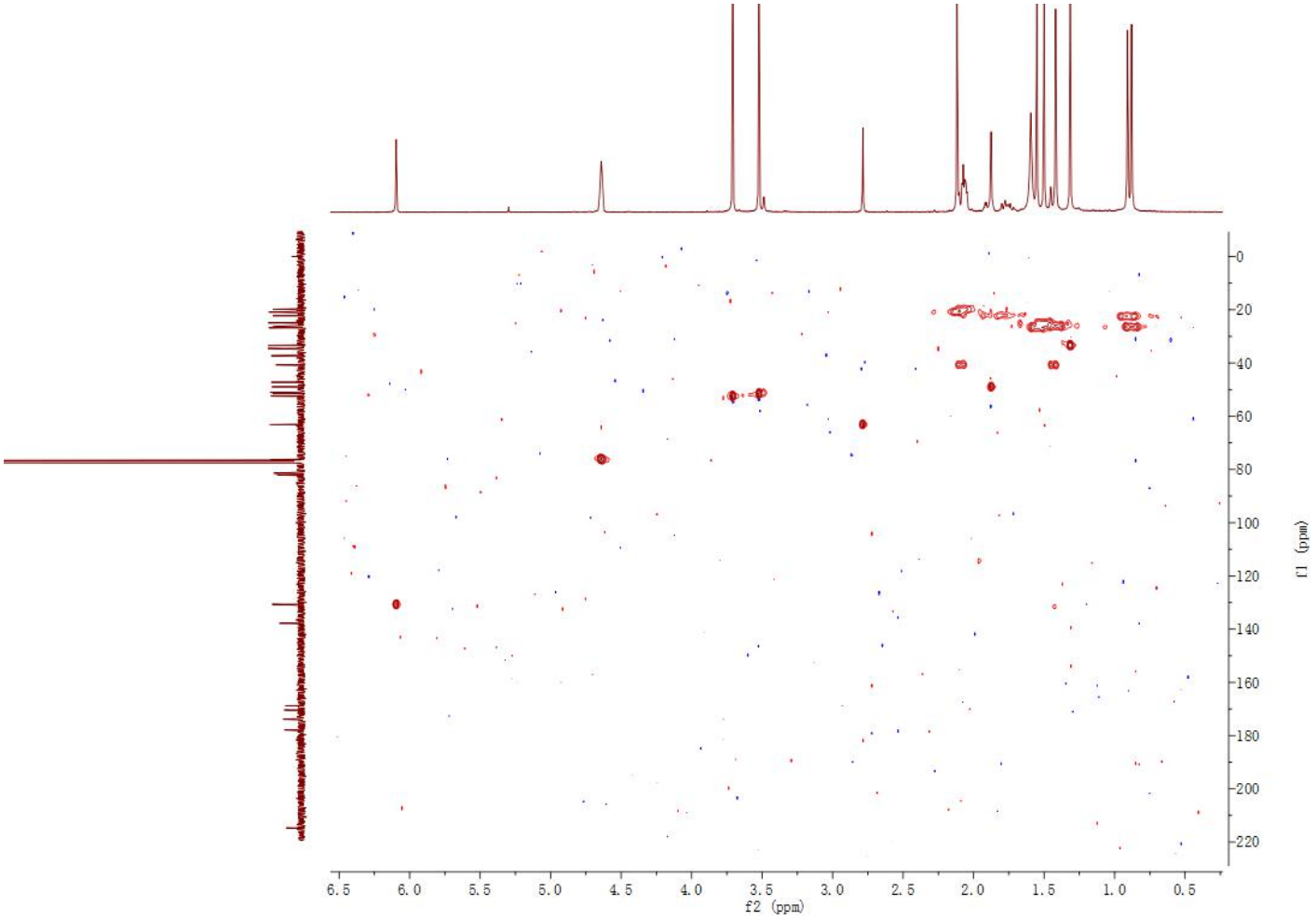
^{1}H NMR of compound **2** (in $CDCl_3$)



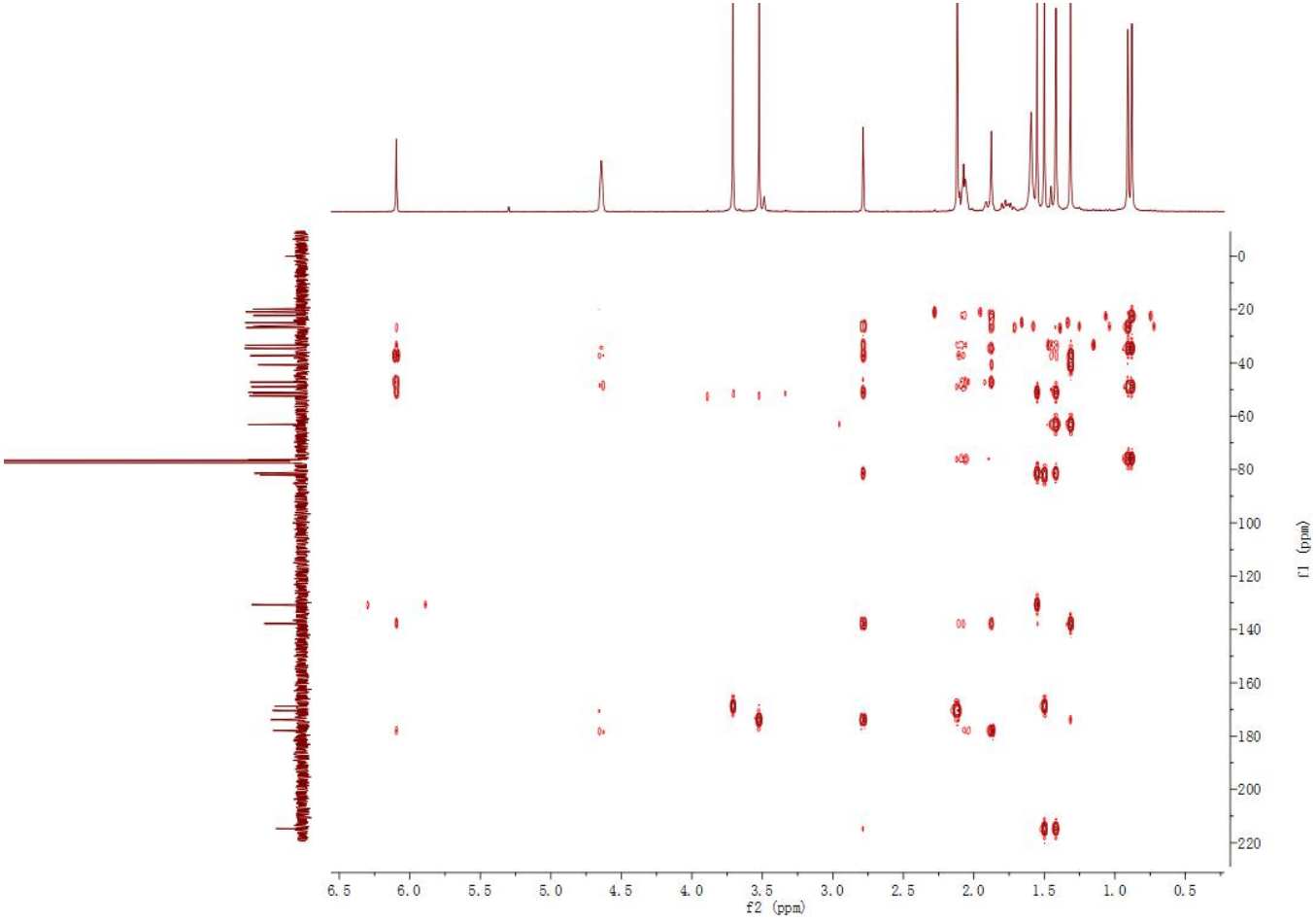
^{13}C NMR of compound **2** (in $CDCl_3$)



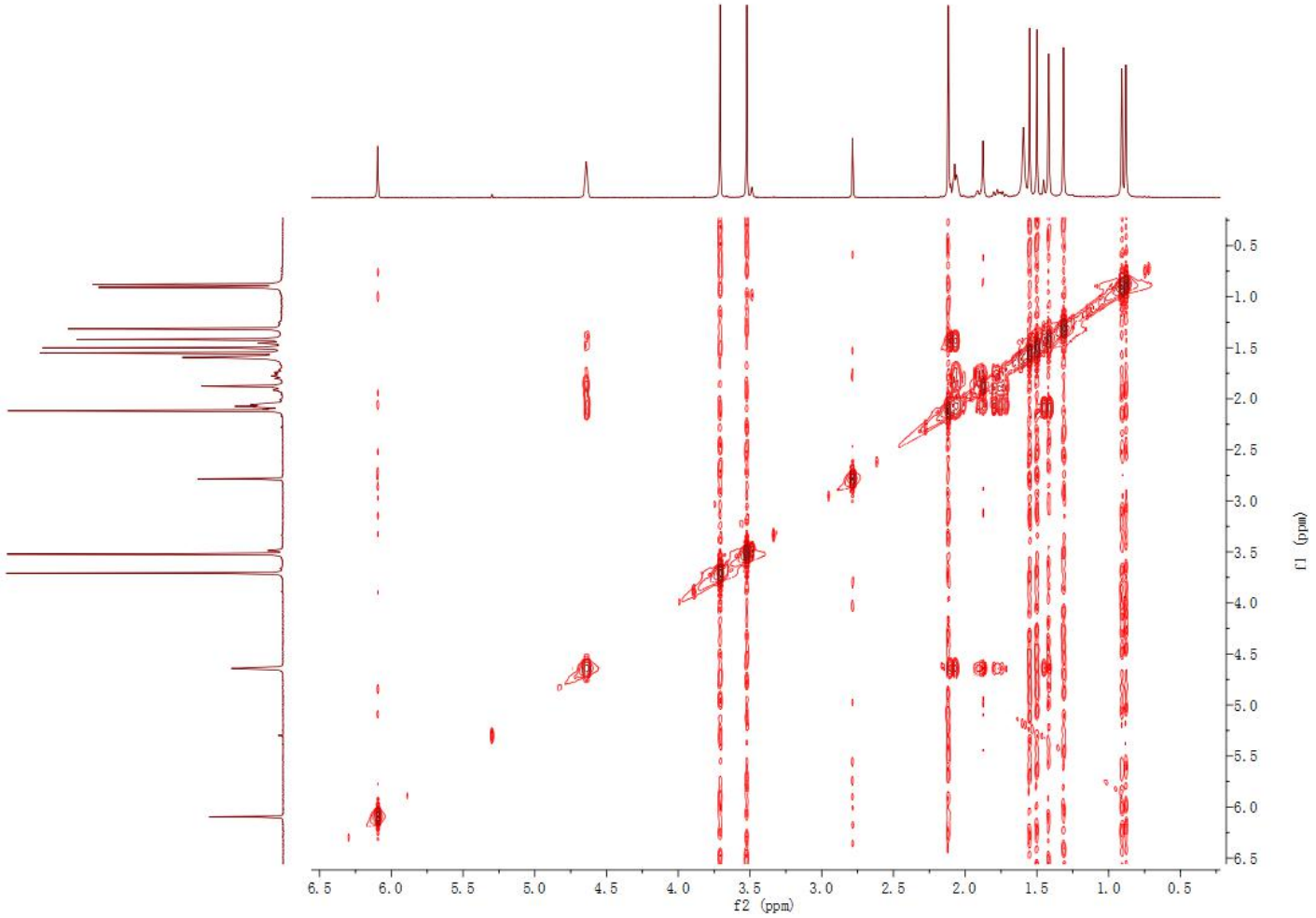
HSQC of compound **2** (in $CDCl_3$)



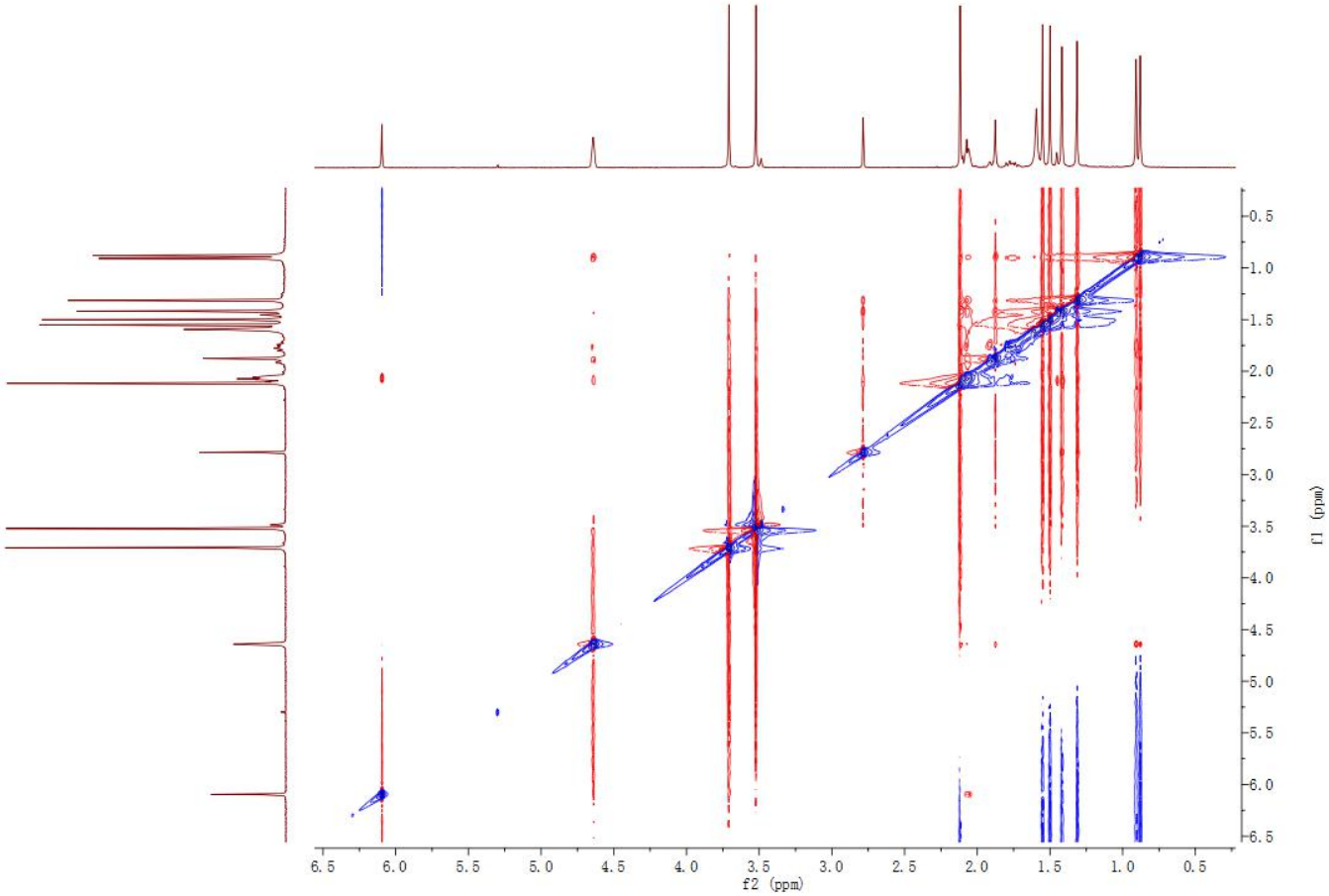
HMBC of compound **2** (in $CDCl_3$)



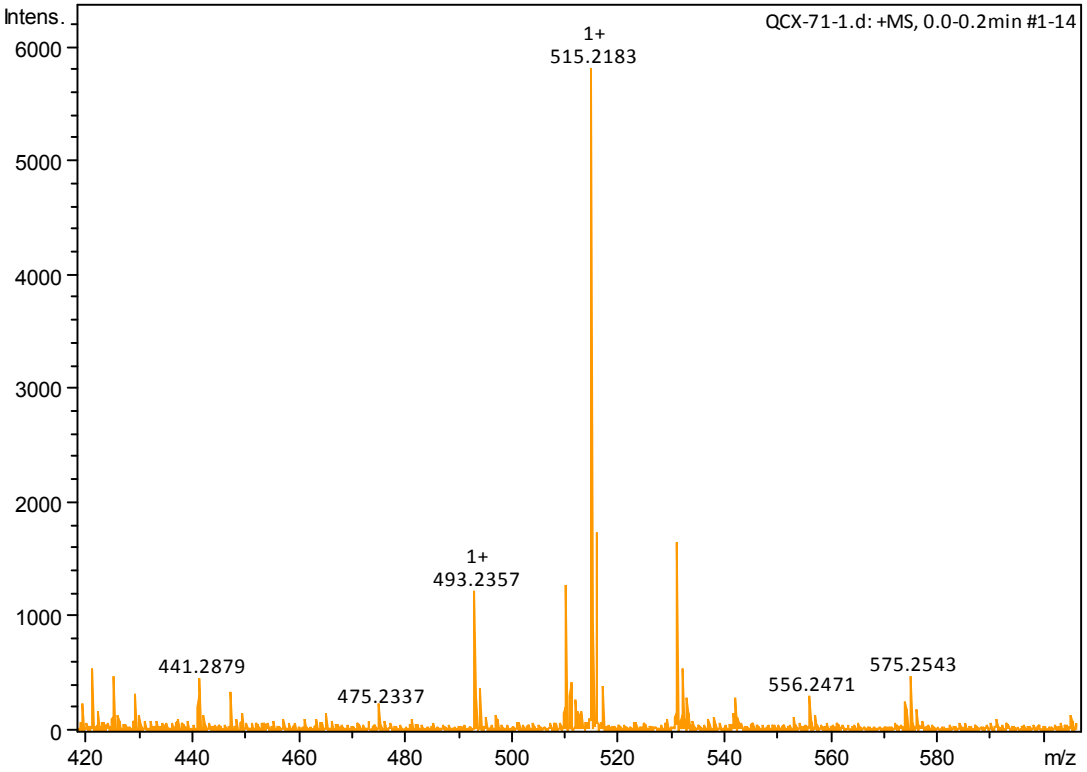
^{1}H–^{1}H COSY of compound **2** (in $CDCl_3$)



NOESY of compound **2** (in $CDCl_3$)



HRESIMS of compound **3**



IR of compound **3**

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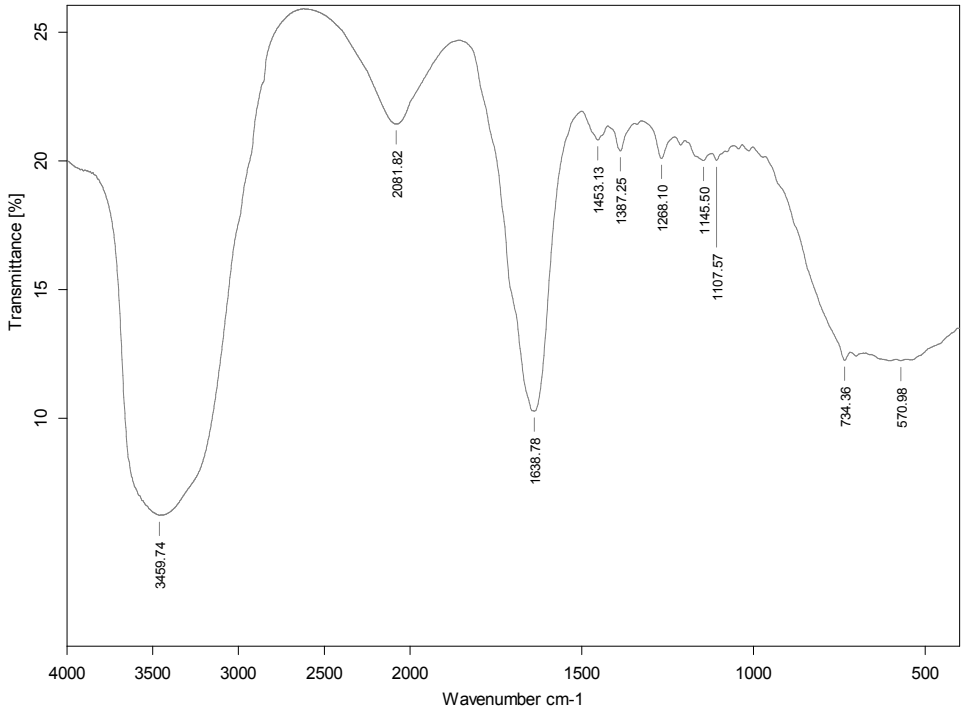
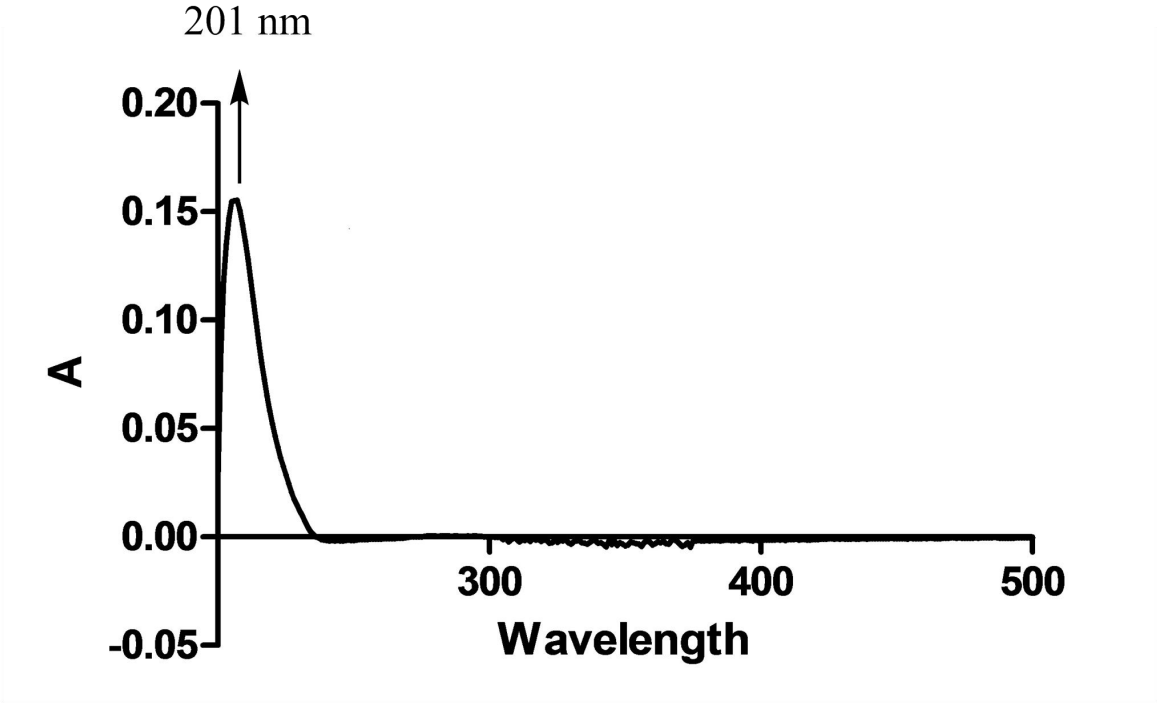
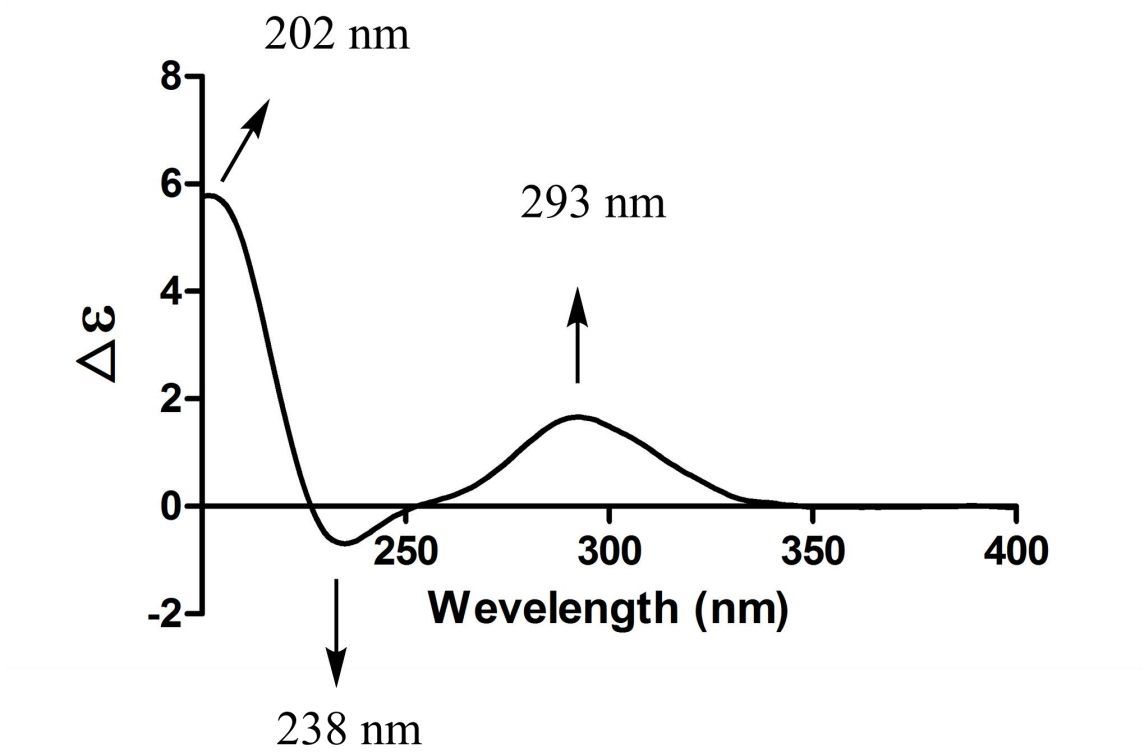


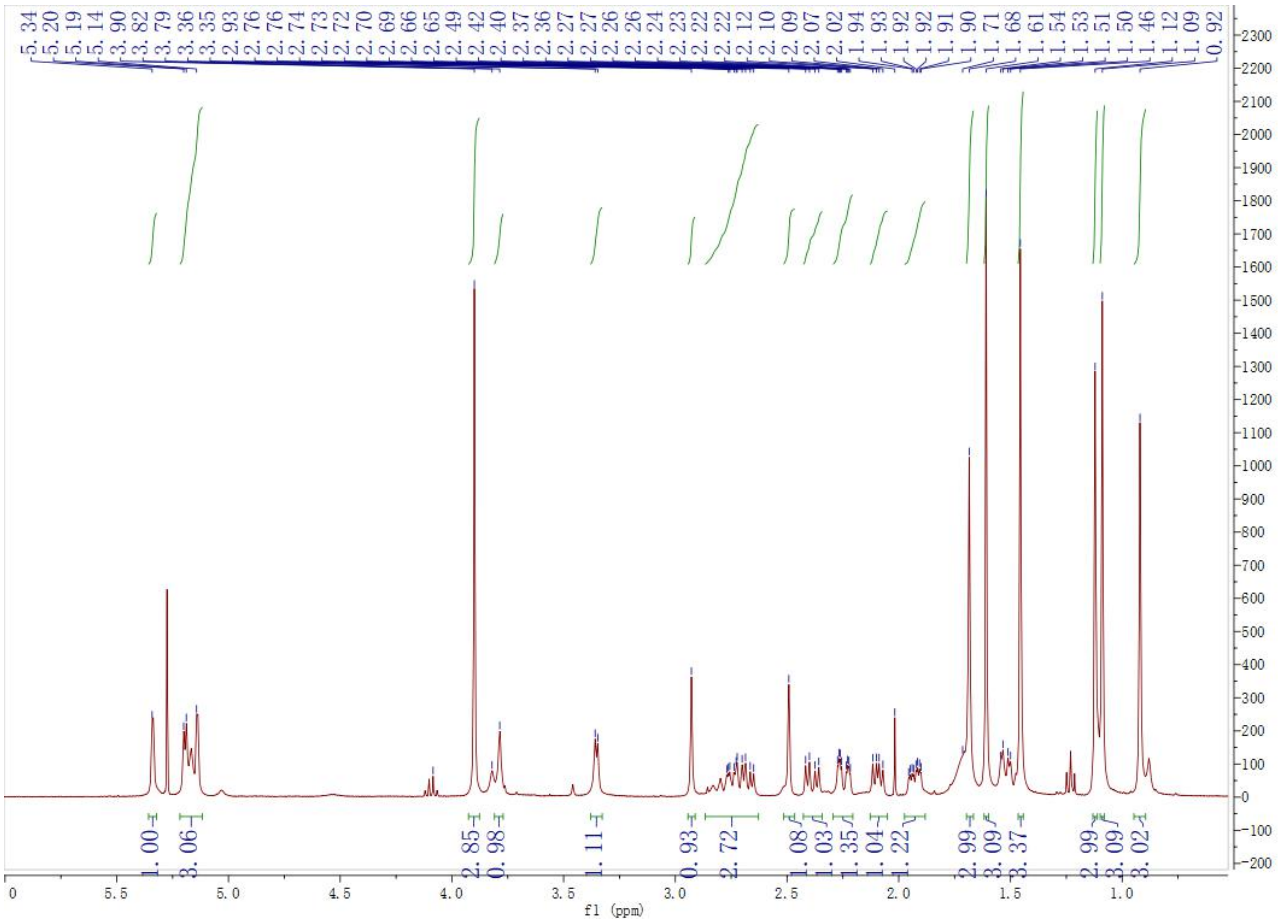
UV of compound **3**



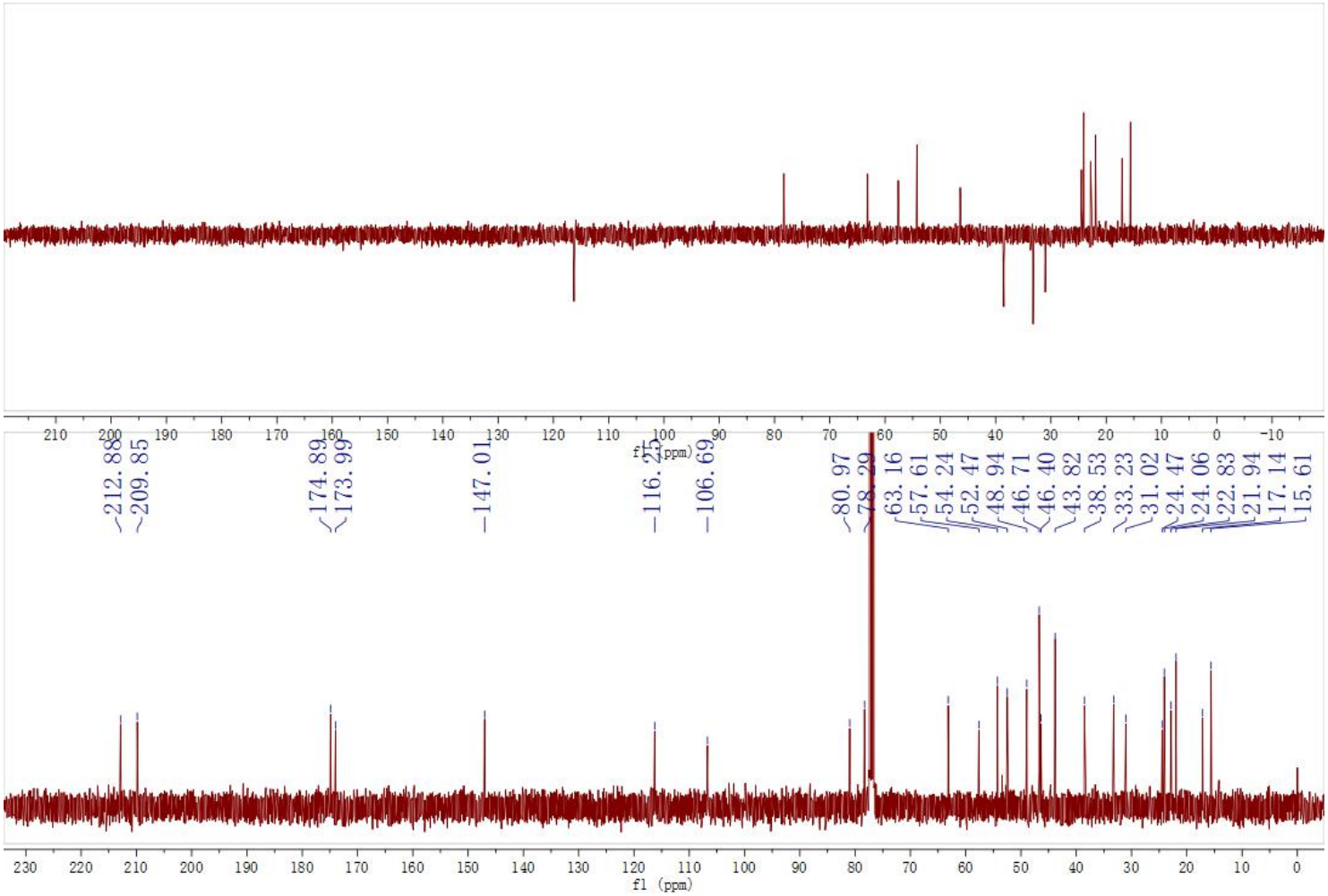
CD of compound **3**



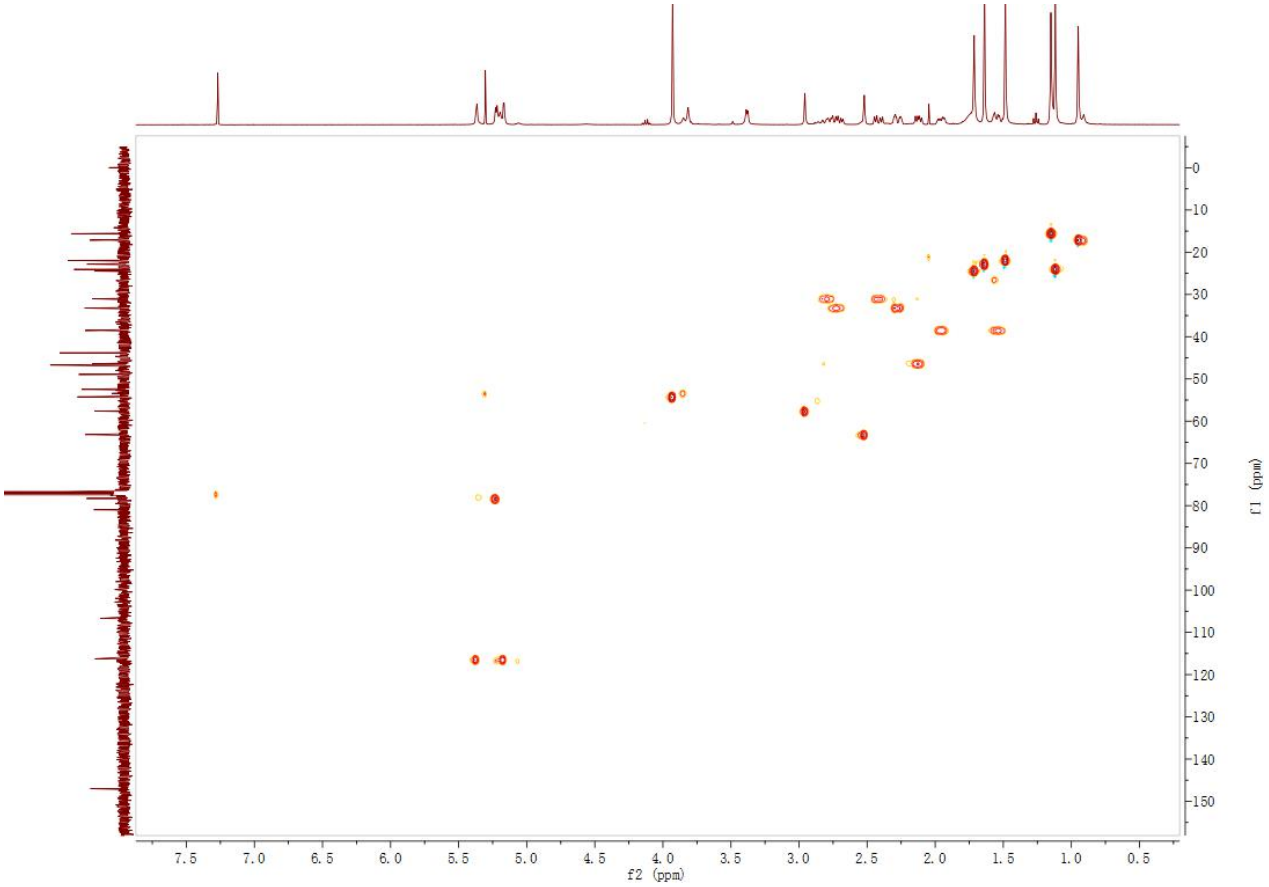
^{1}H NMR of compound **3** (in $CDCl_3$)



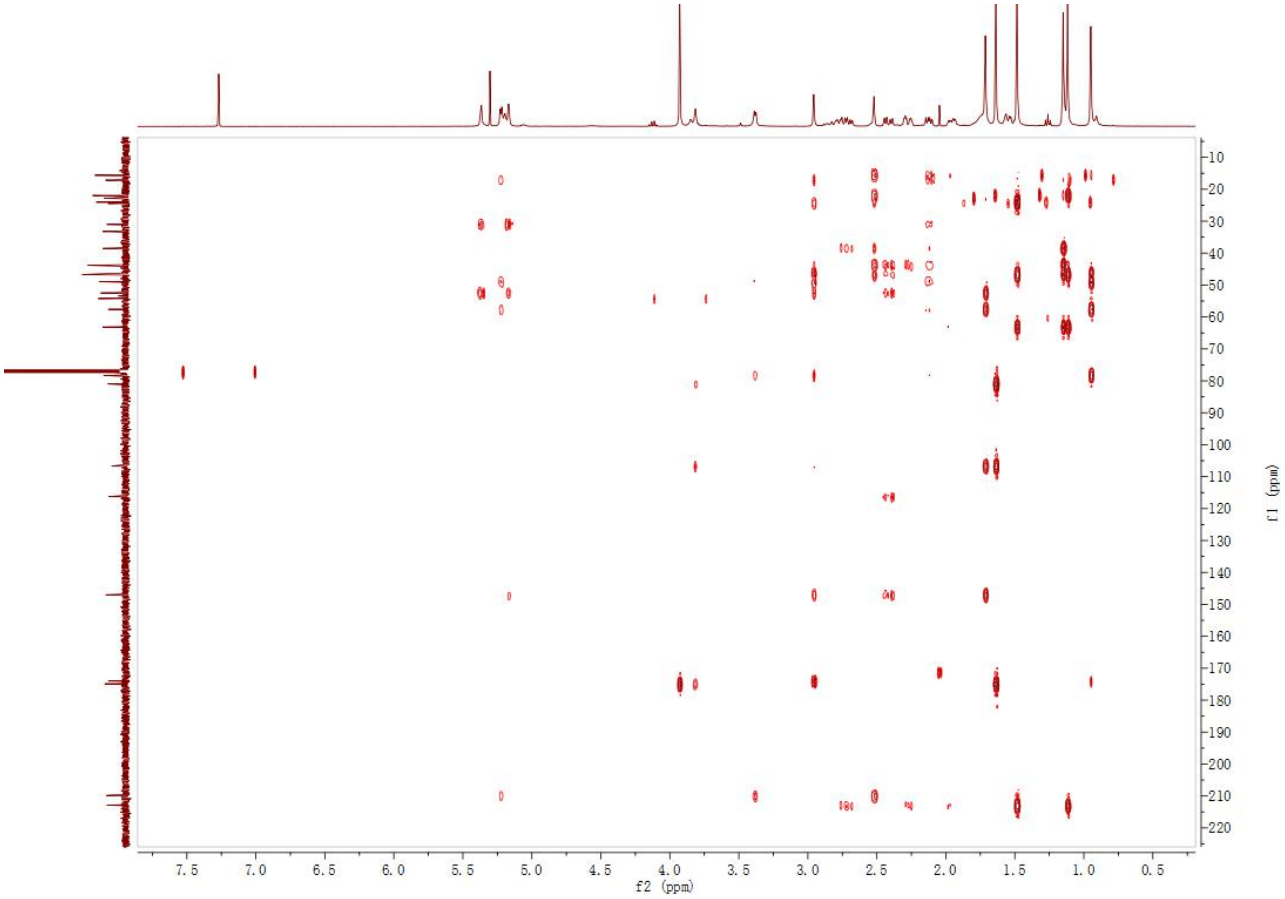
^{13}C NMR of compound **3** (in $CDCl_3$)



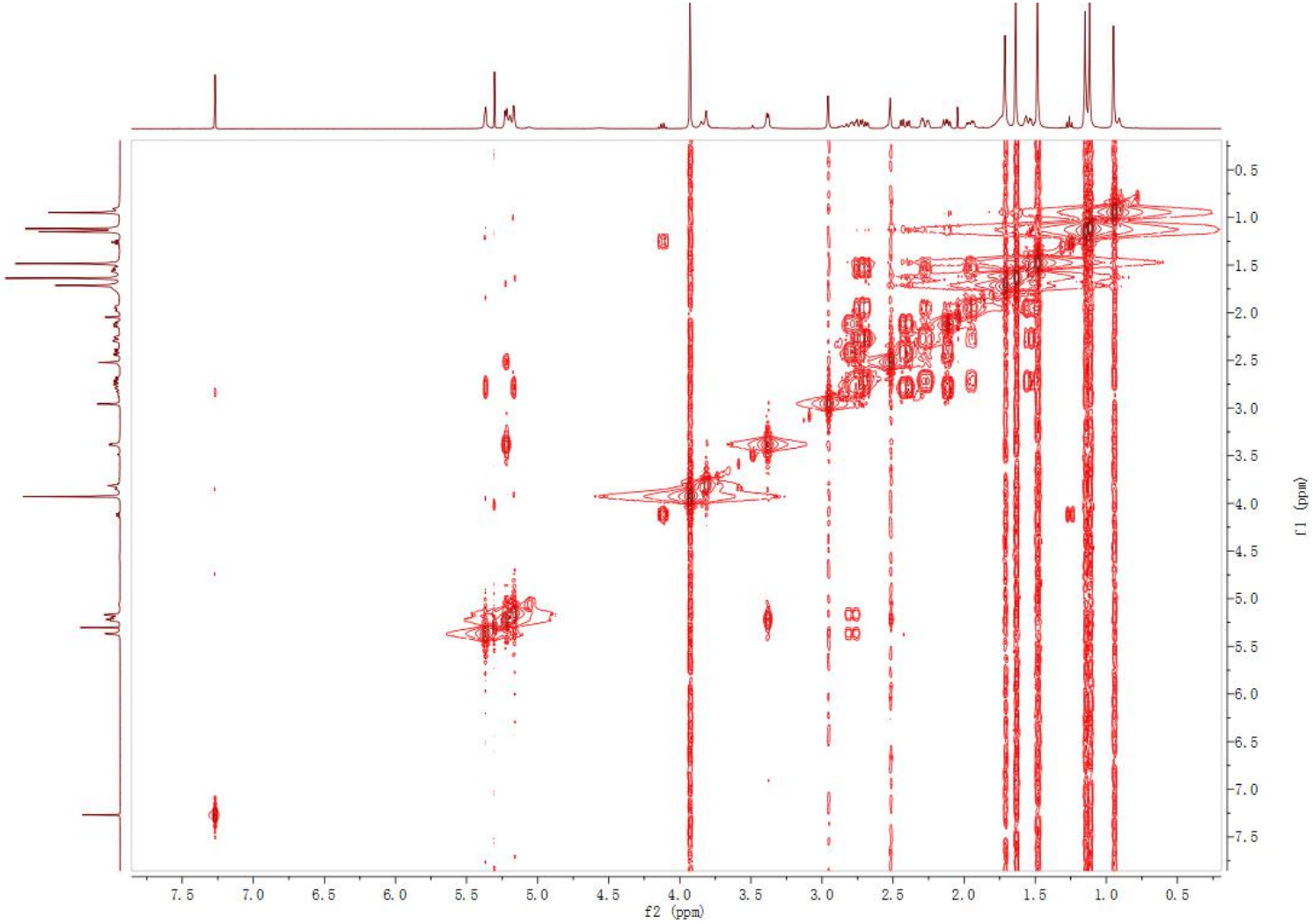
HSQC of compound **3** (in $CDCl_3$)



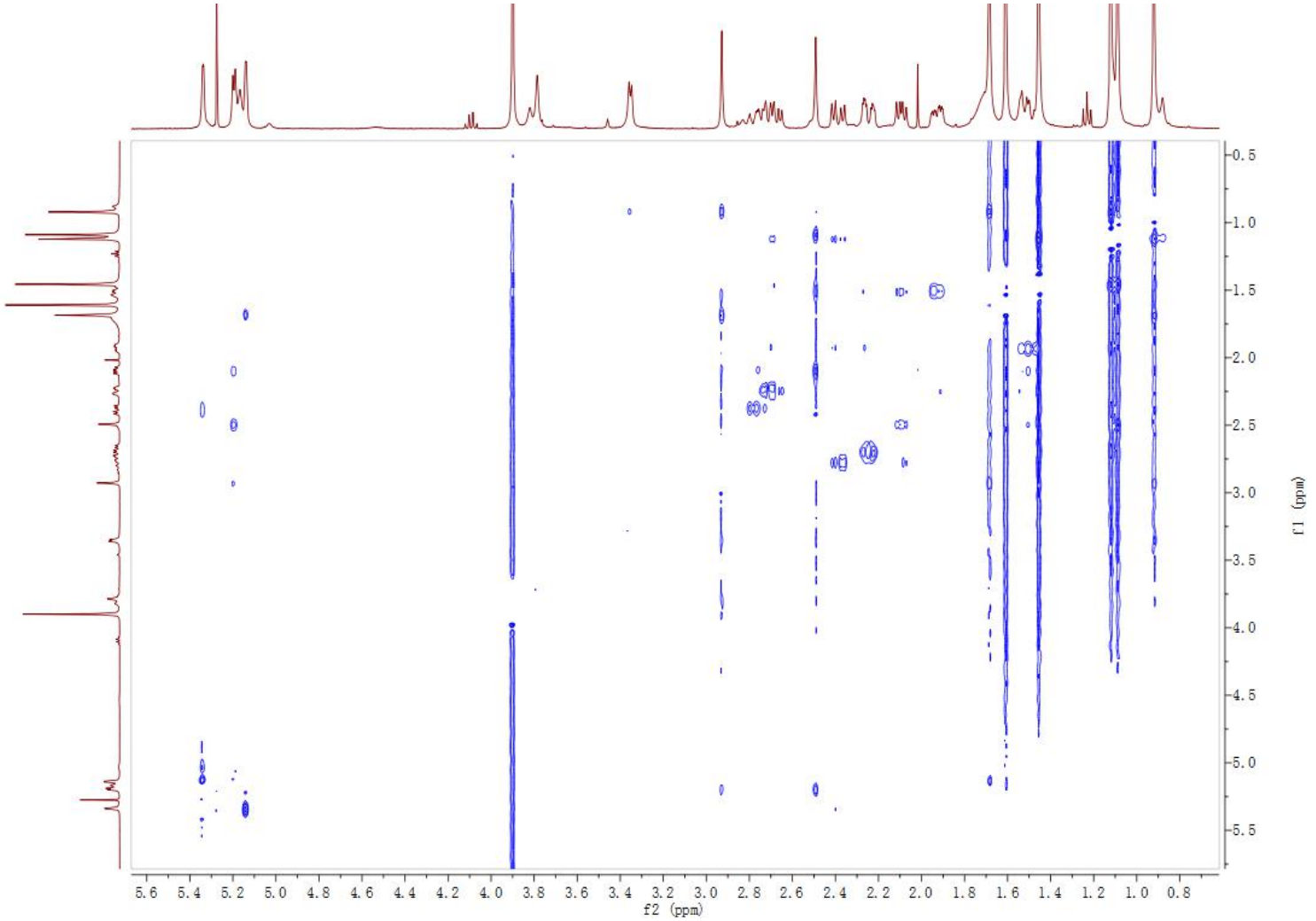
HMBC of compound **3** (in $CDCl_3$)



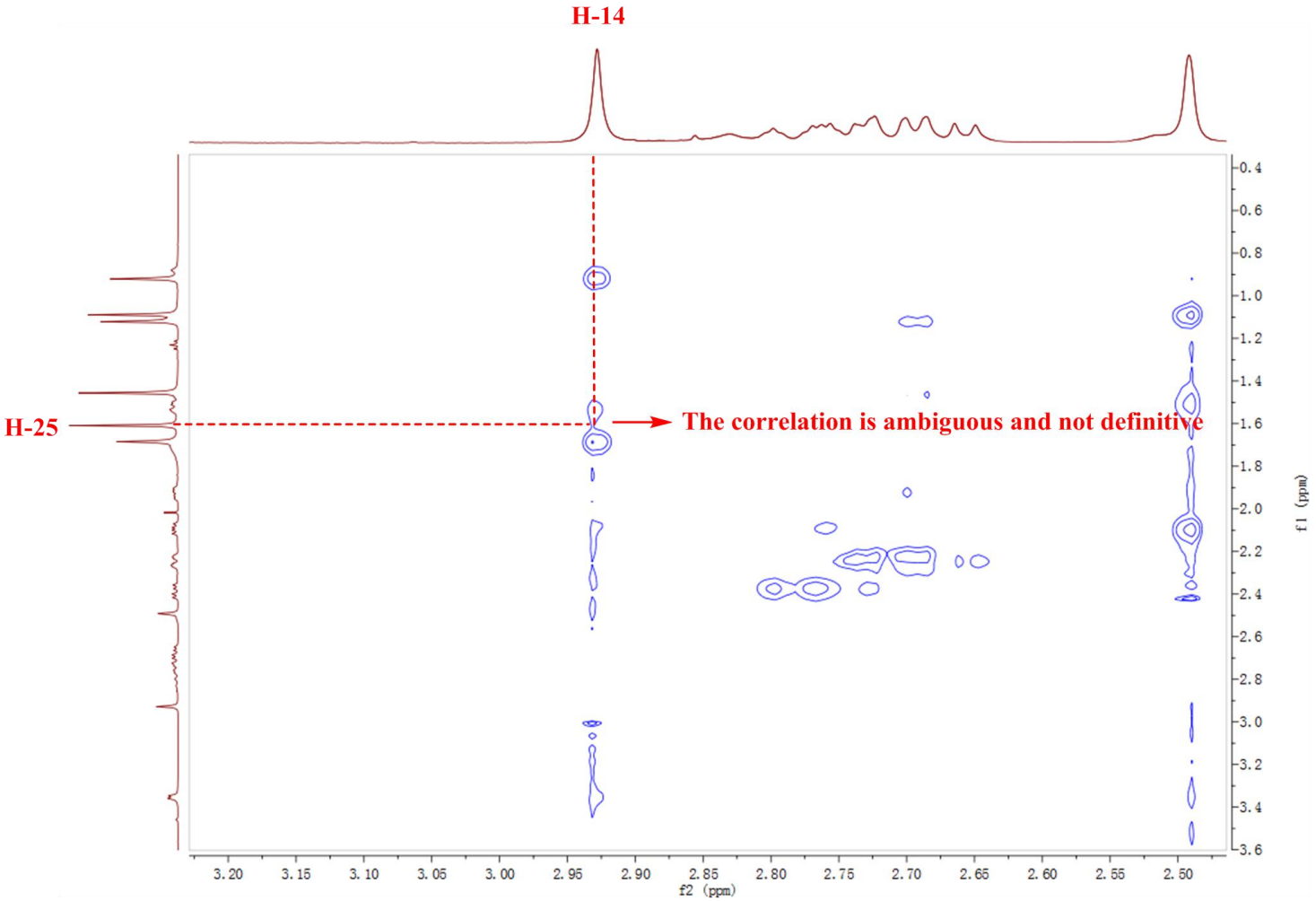
^{1}H–^{1}H COSY of compound **3** (in $CDCl_3$)



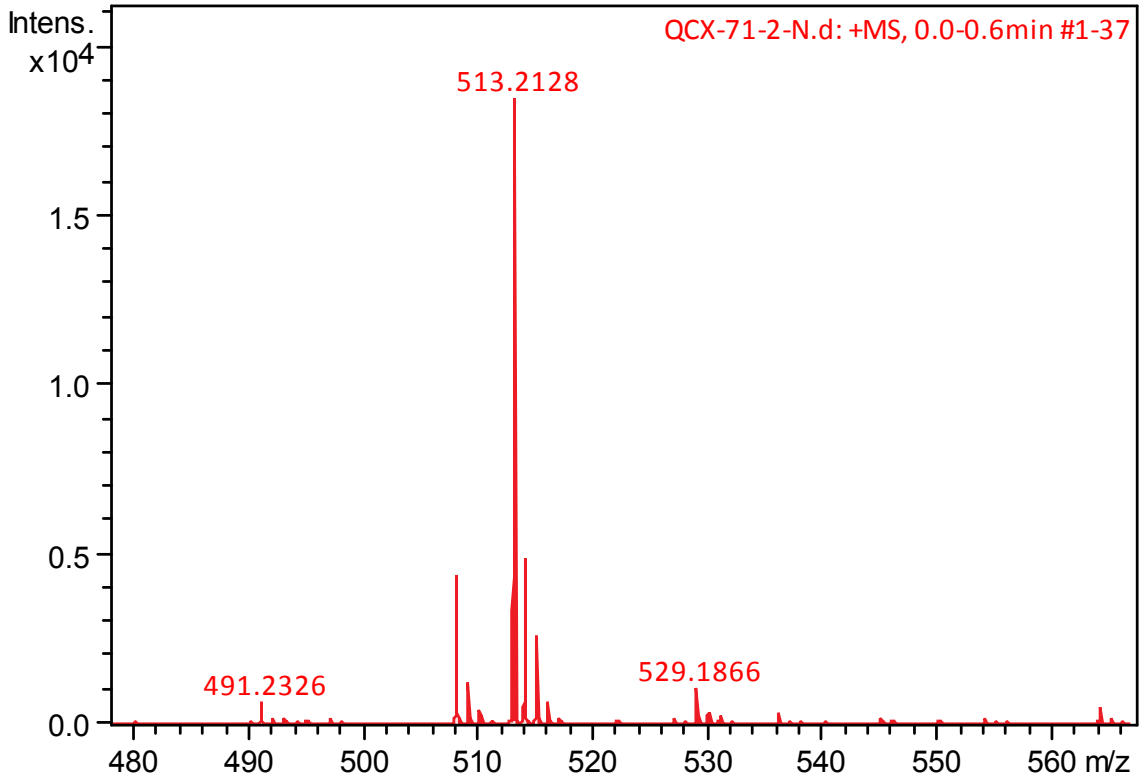
NOESY of compound **3** (in $CDCl_3$)



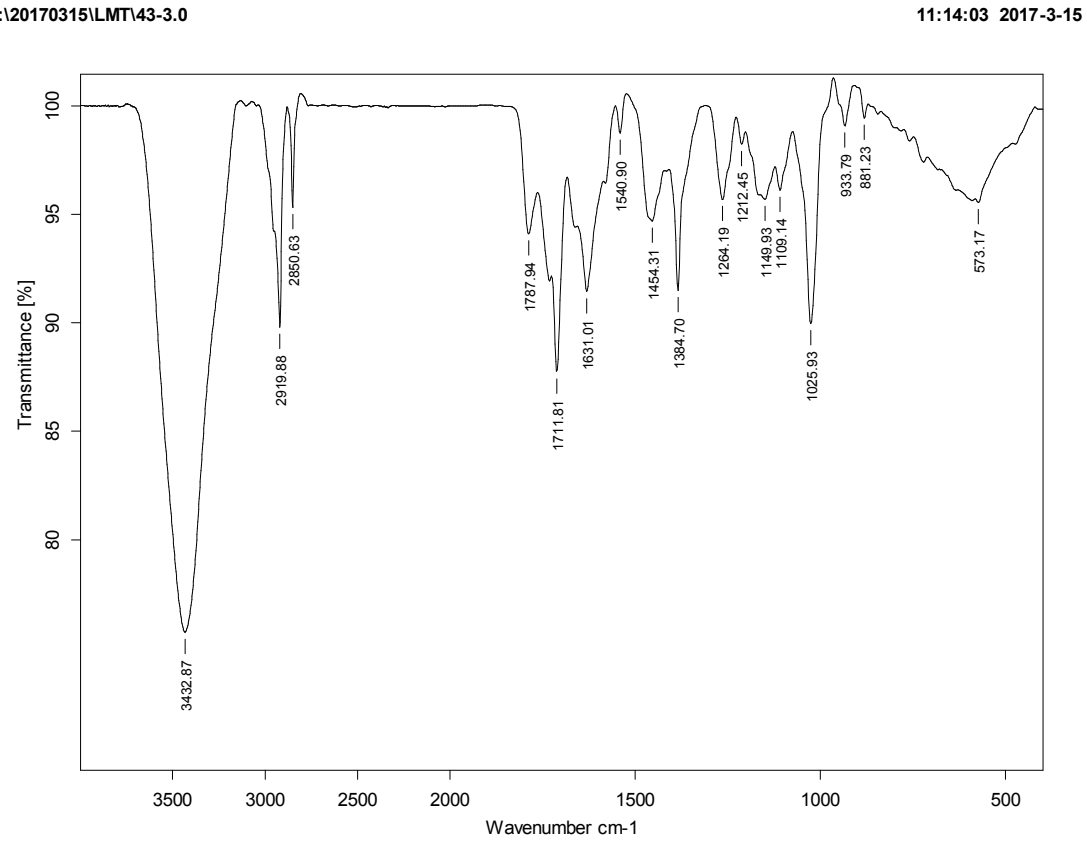
Enlarged NOESY of compound **3** (in $CDCl_3$)



HRESIMS of compound **4**

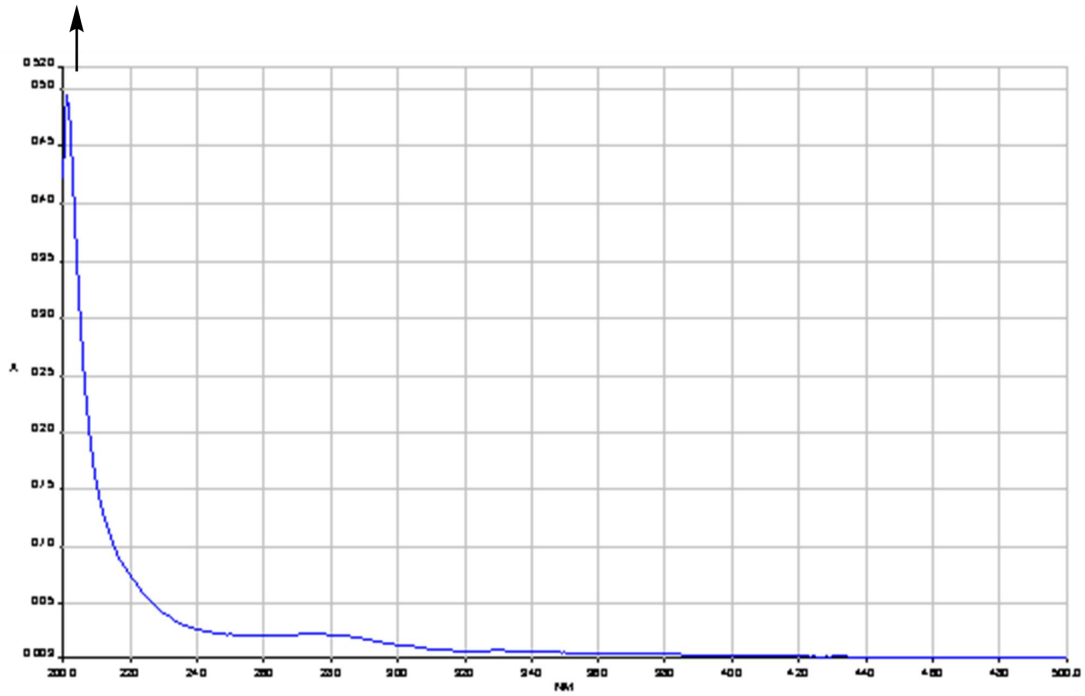


IR of compound **4**

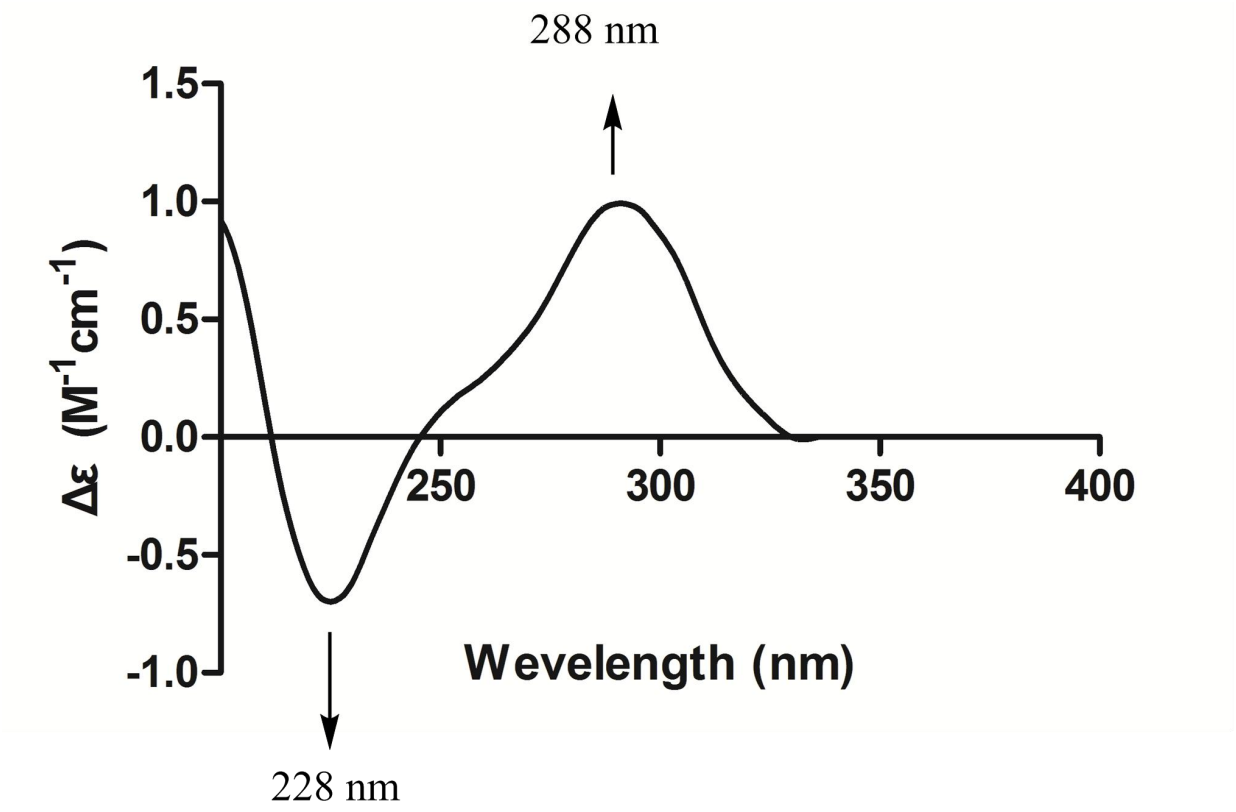


UV of compound **4**

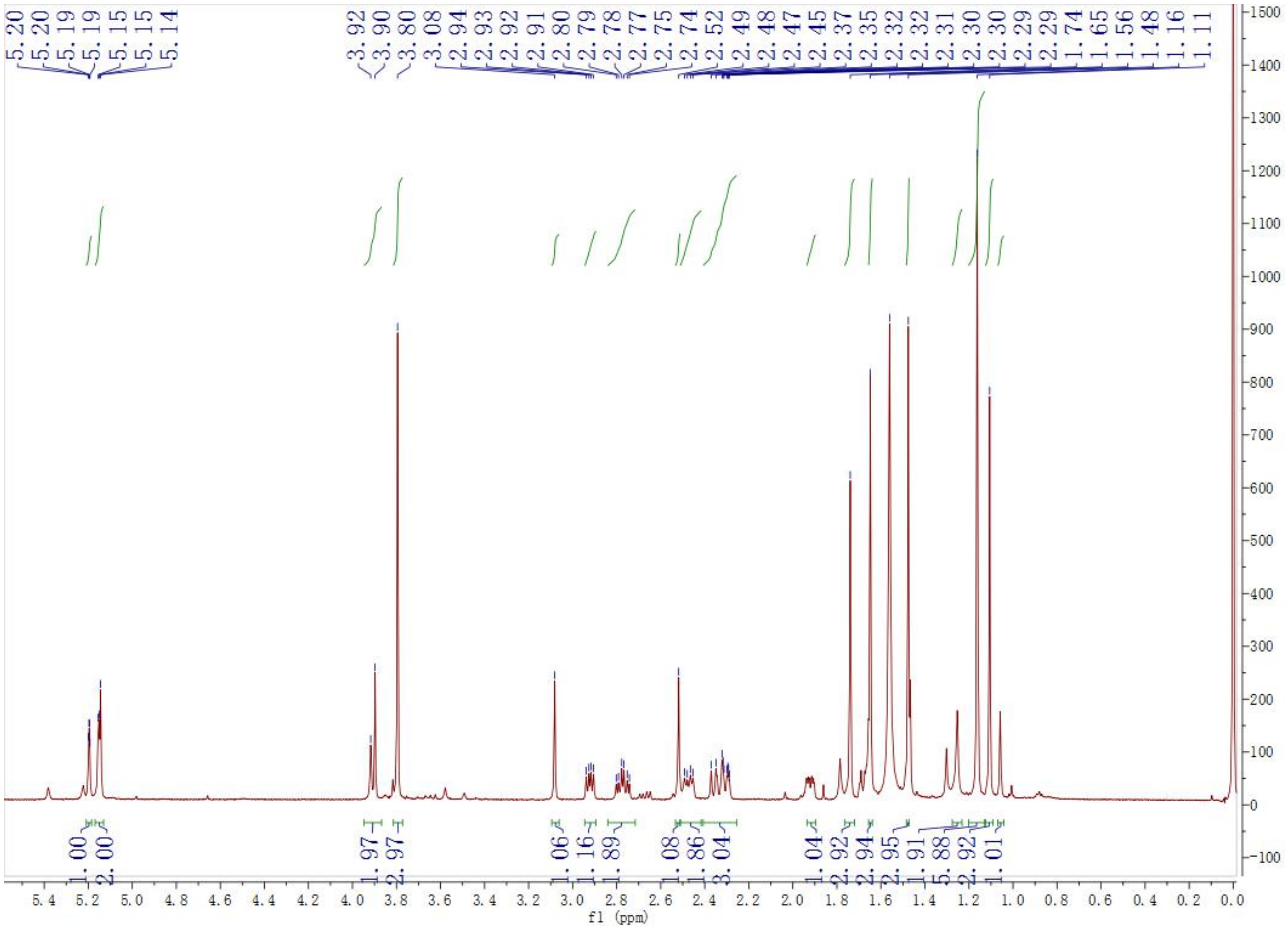
201 nm



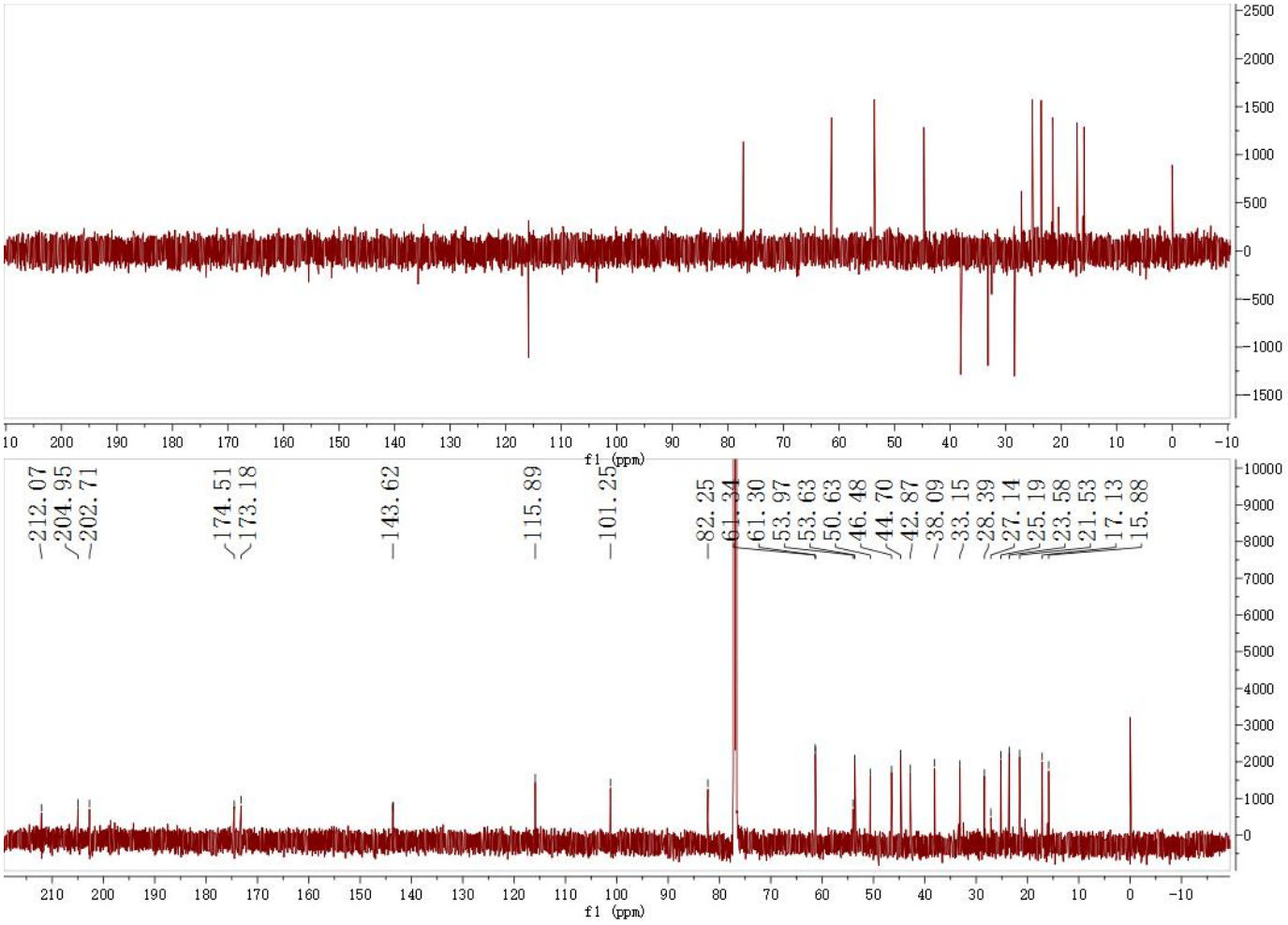
CD of compound **4**



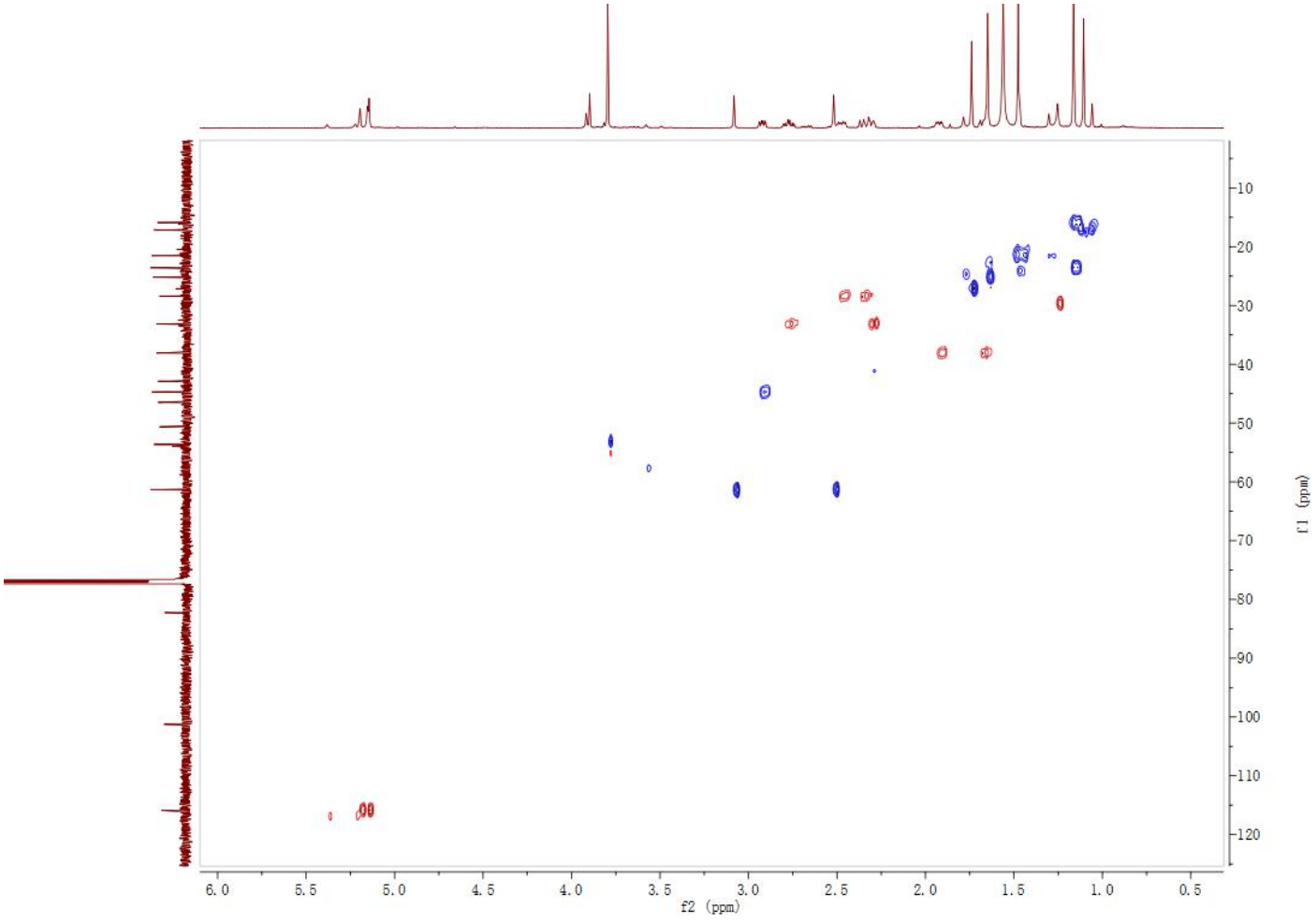
^{1}H NMR of compound **4** (in $CDCl_3$)



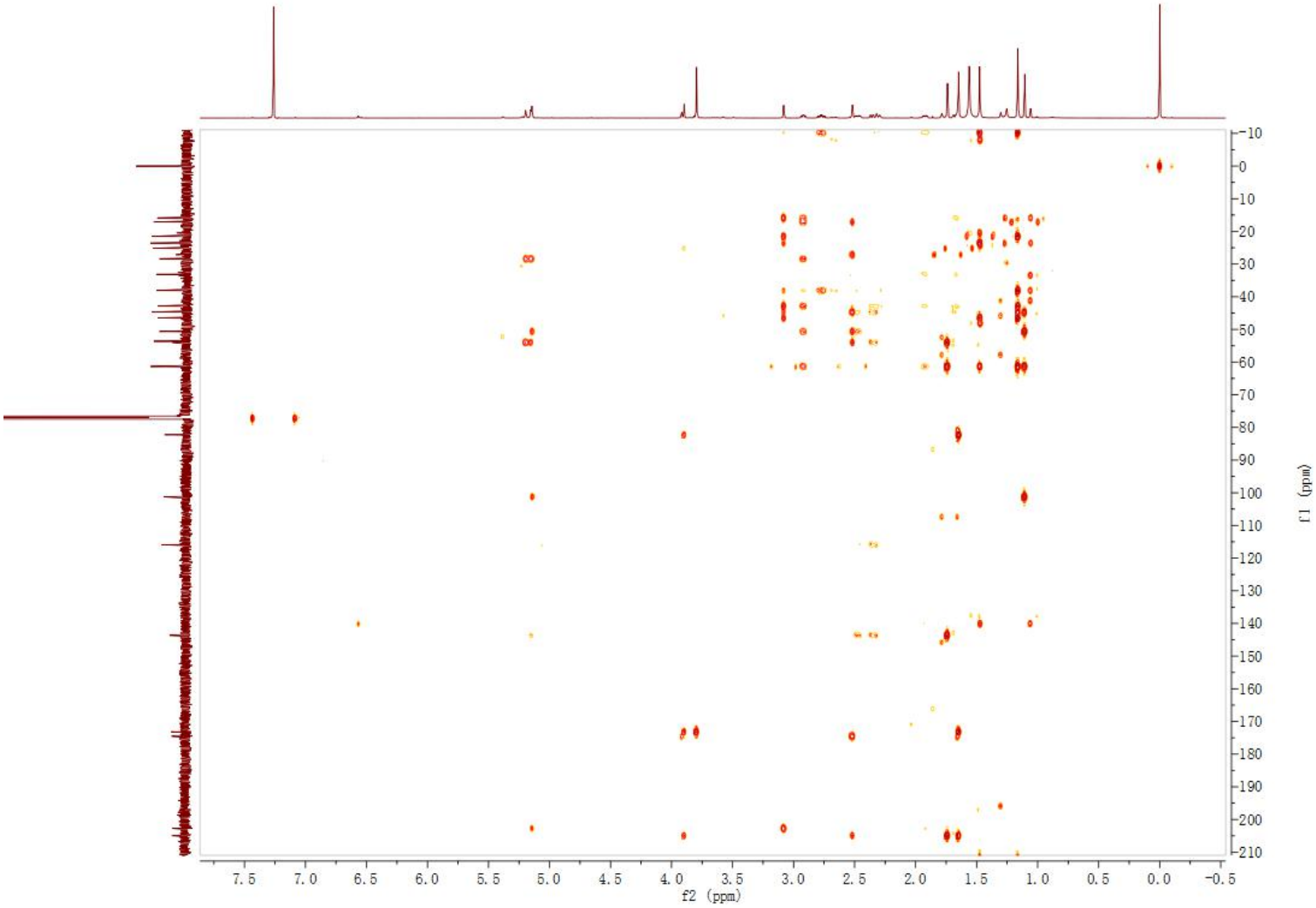
^{13}C NMR of compound **4** (in $CDCl_3$)



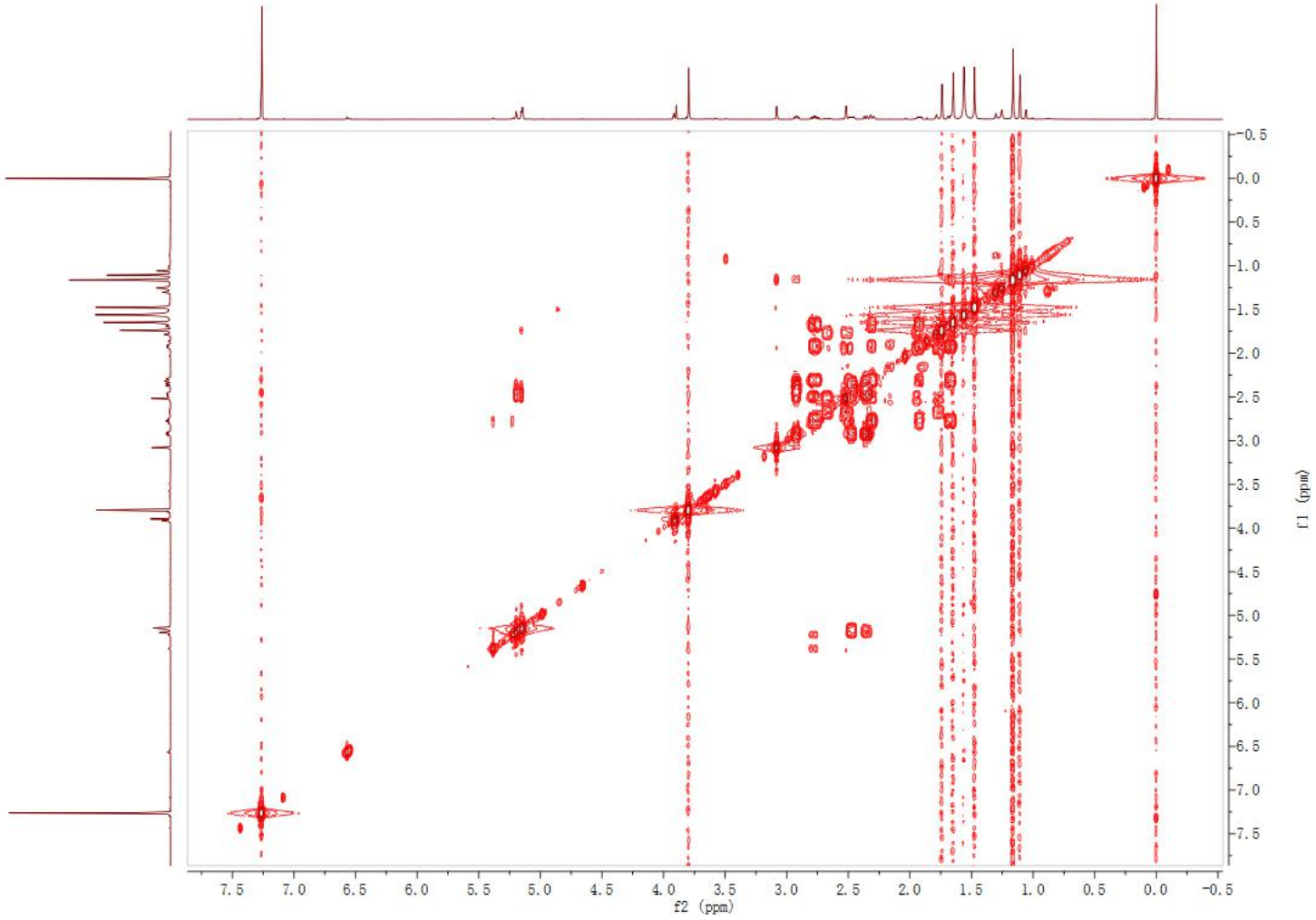
HSQC of compound **4** (in $CDCl_3$)



HMBC of compound **4** (in $CDCl_3$)



^{1}H–^{1}H COSY of compound **4** (in $CDCl_3$)



NOESY of compound **4** (in $CDCl_3$)