

Secondary Metabolites with Herbicidal and Antifungal Activities from Marine-Derived Fungus *Alternaria iridiauxalis*

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Table S1. Herbicidal spectrum of **9** against representative malignant weeds *D. sanguinalis*, *Portulaca oleracea*, and *Descurainia sophia*.

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Figure S1. HRESIMS spectrum of compound **1**.

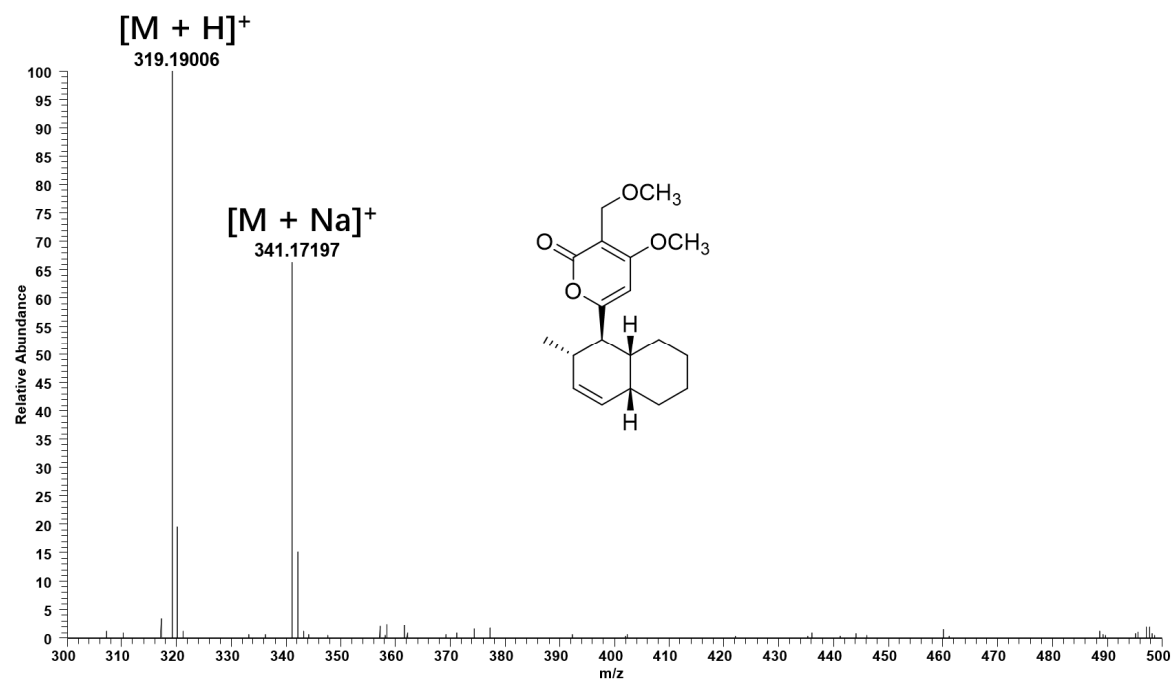


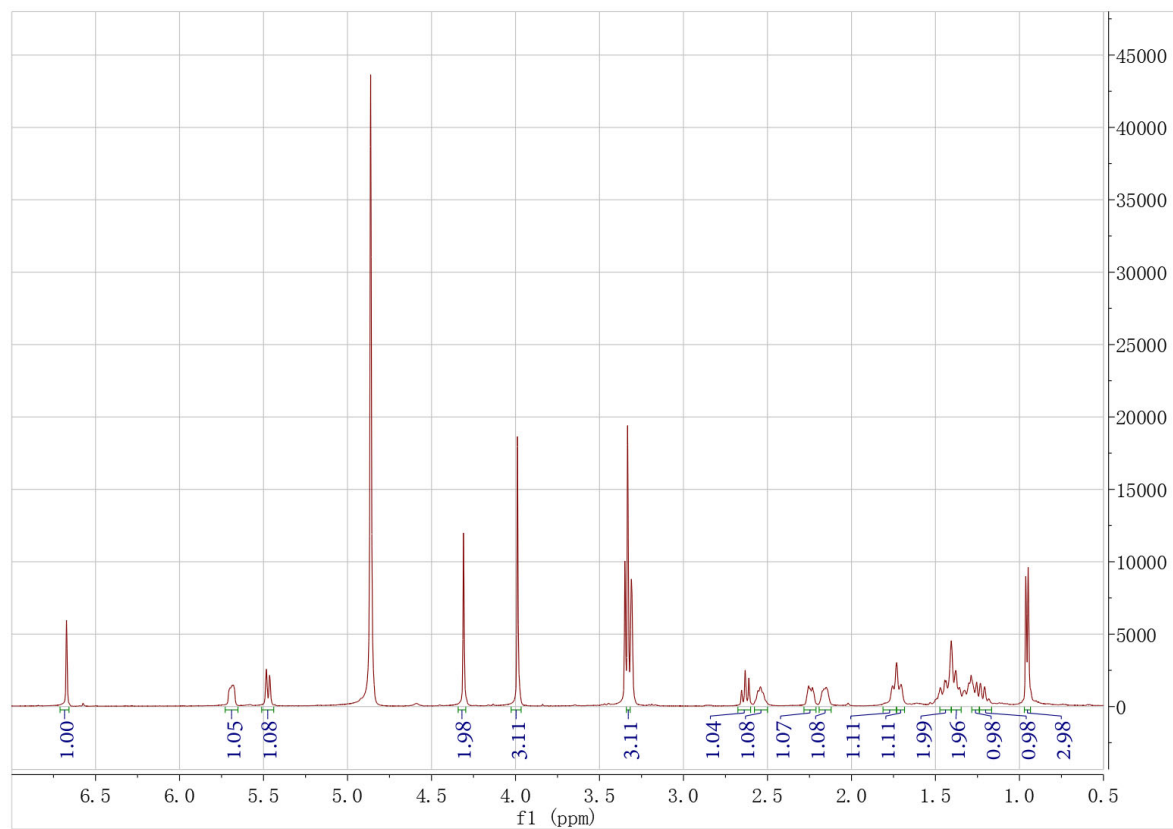
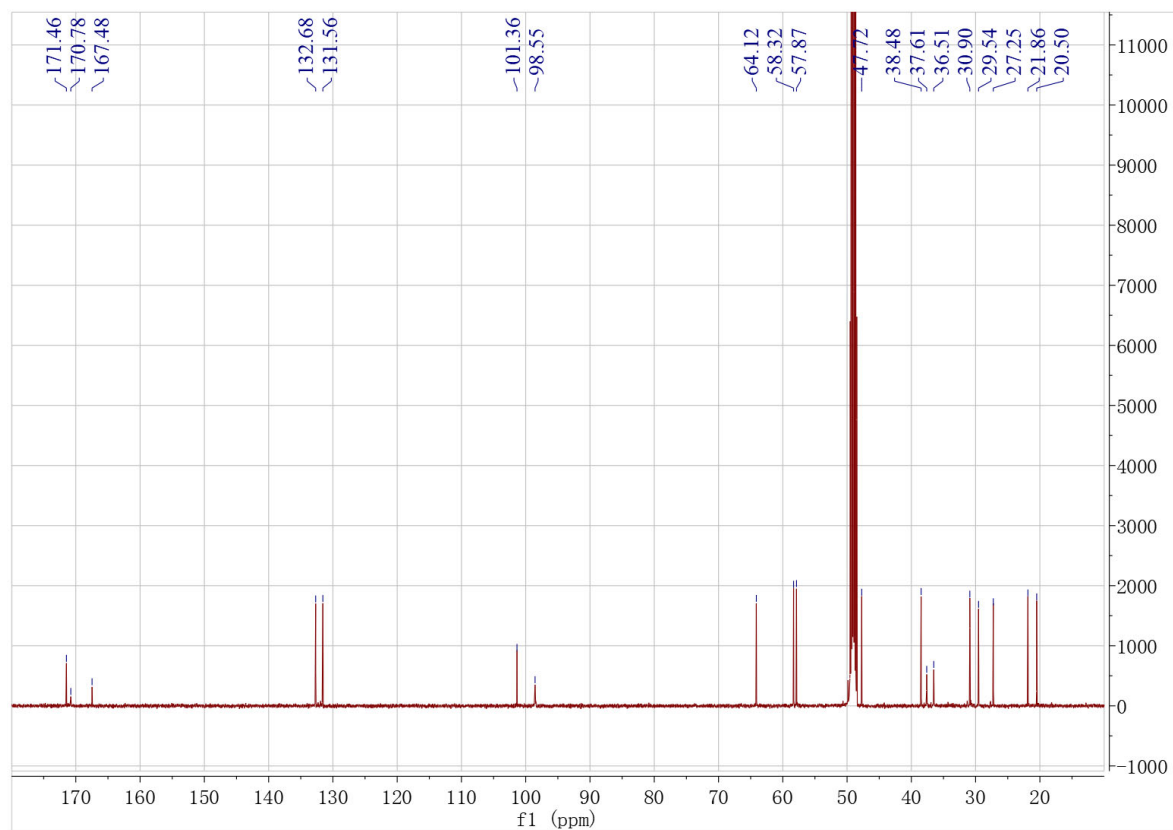
Figure S2. ^1H NMR (500 MHz, CD_3OD) spectrum of compound 1.**Figure S3.** ^{13}C NMR spectrum of compound 1.

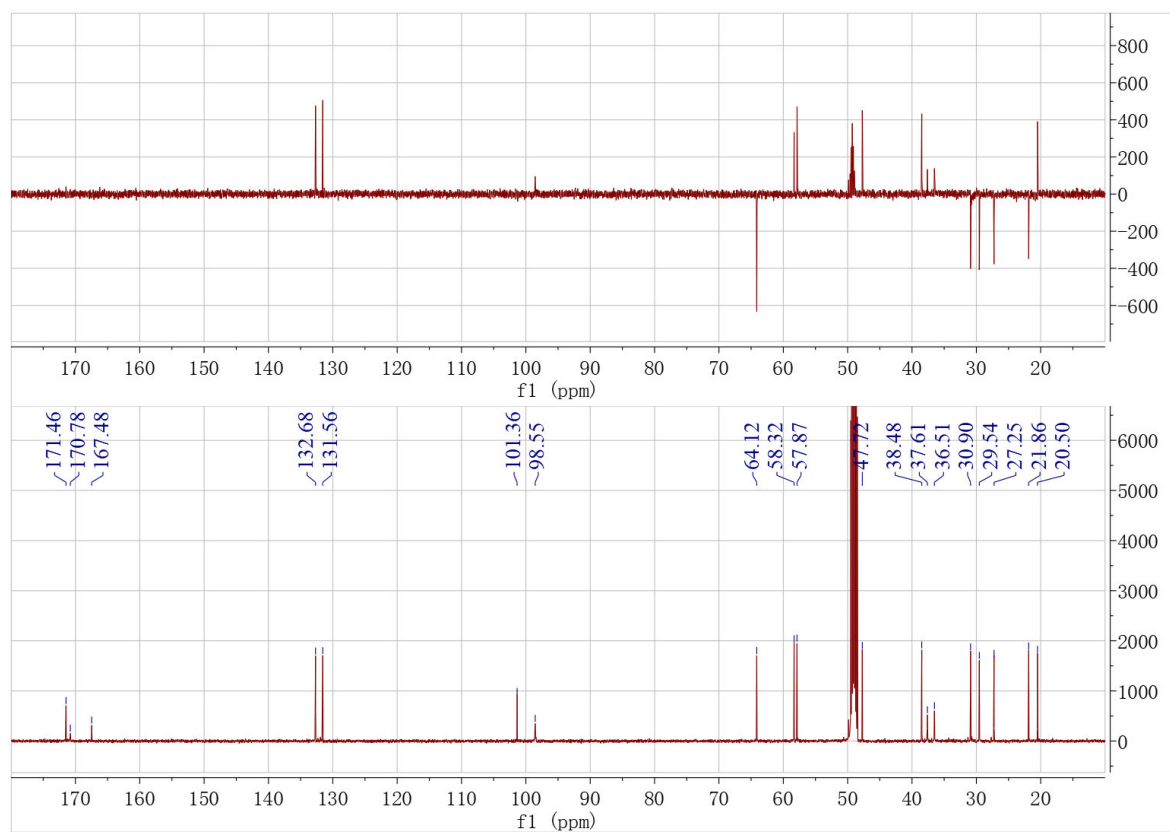
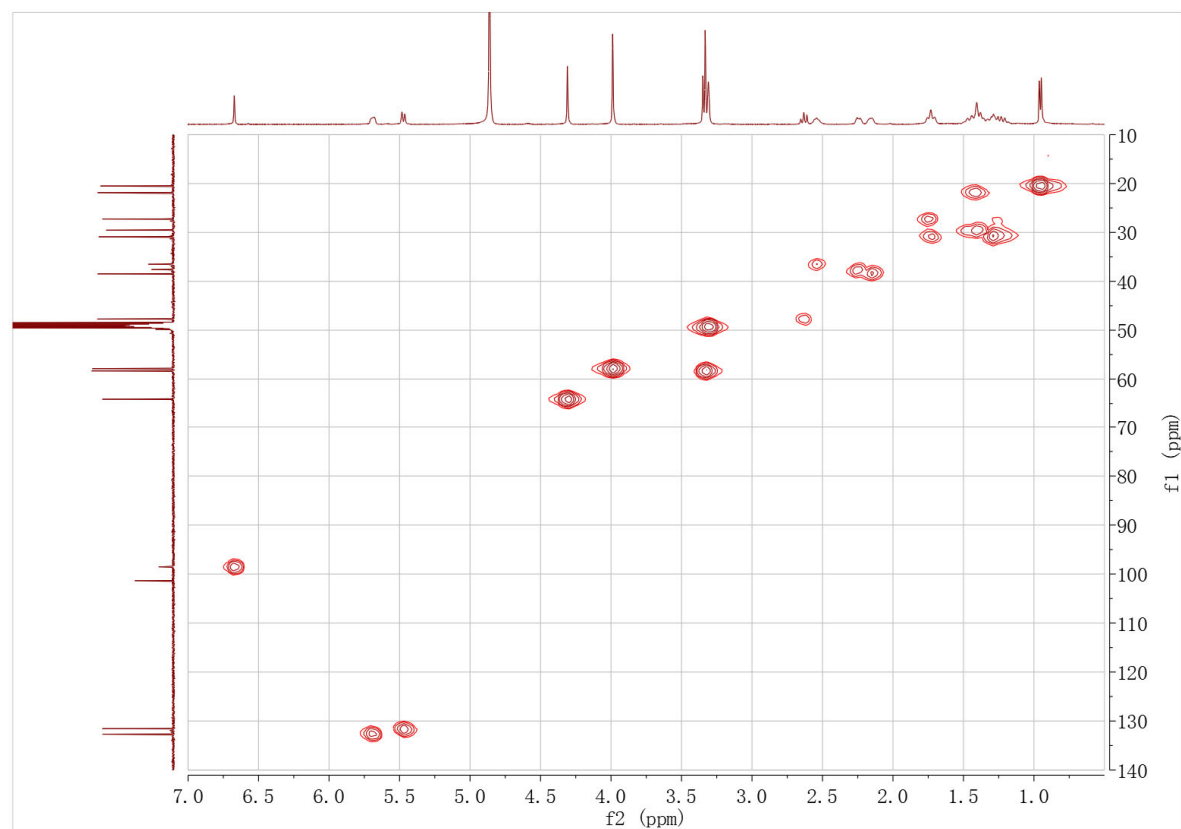
Figure S4. DEPT-135 spectrum of compound 1.**Figure S5.** HSQC spectrum of compound 1.

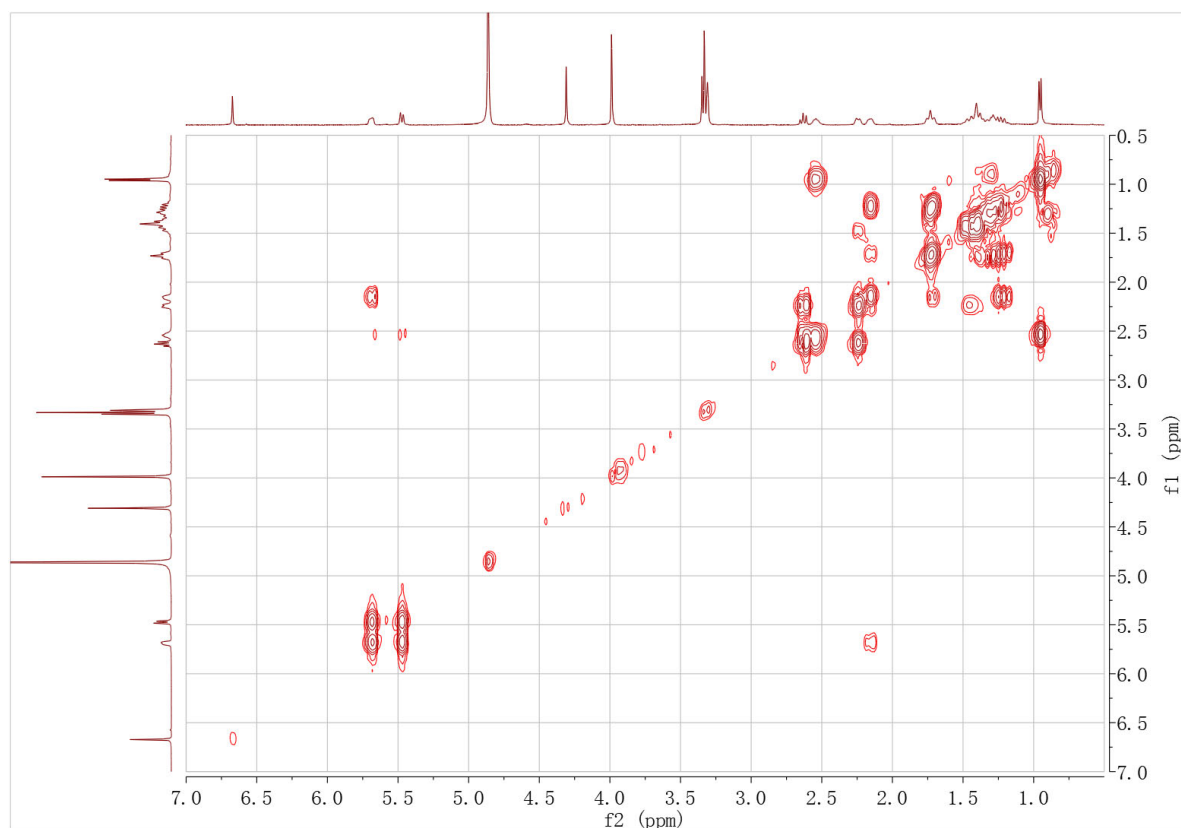
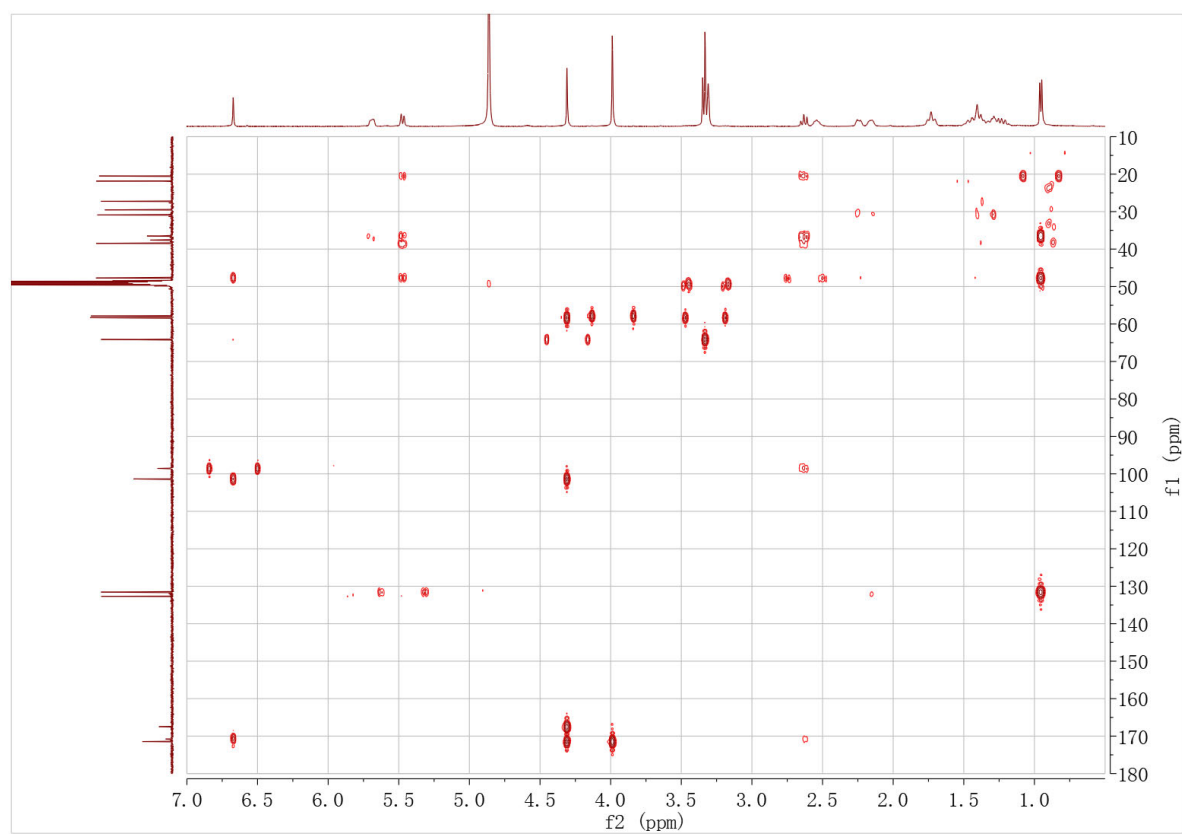
Figure S6. ^1H - ^1H COSY spectrum of compound 1.**Figure S7.** HMBC spectrum of compound 1.

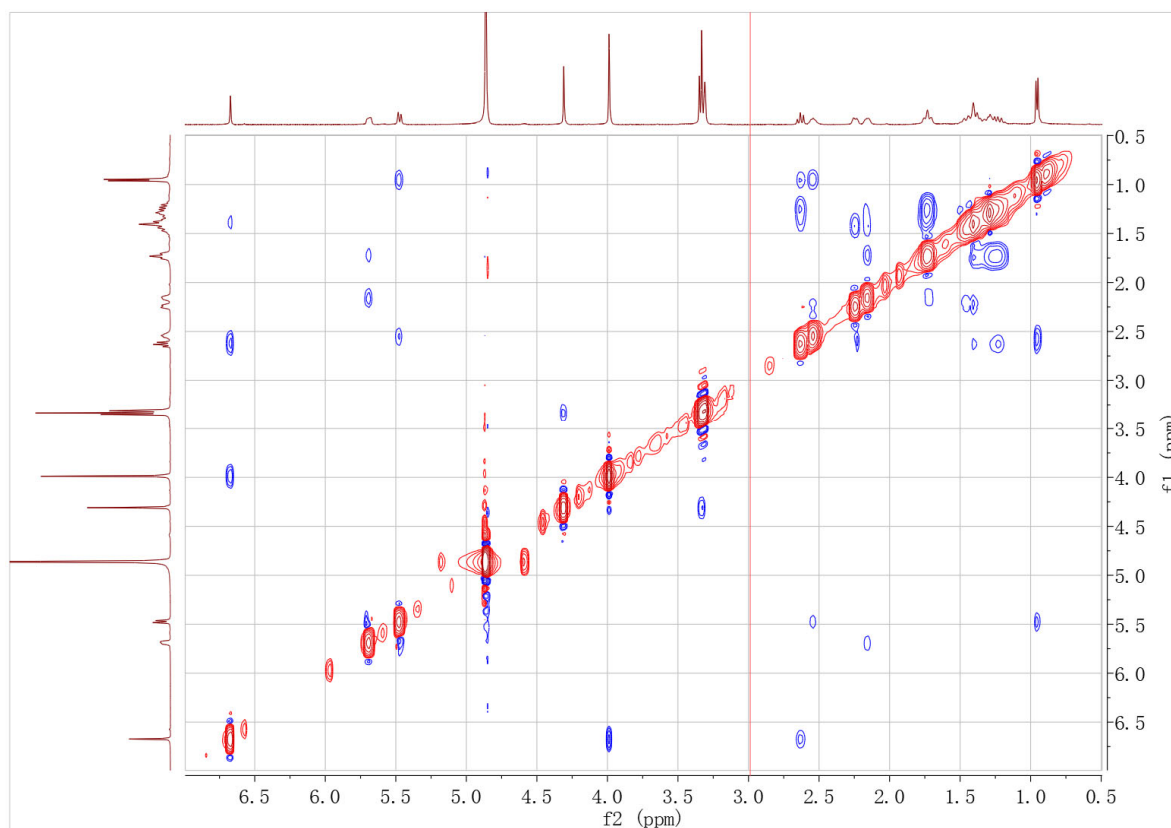
Figure S8. NOESY spectrum of compound 1.

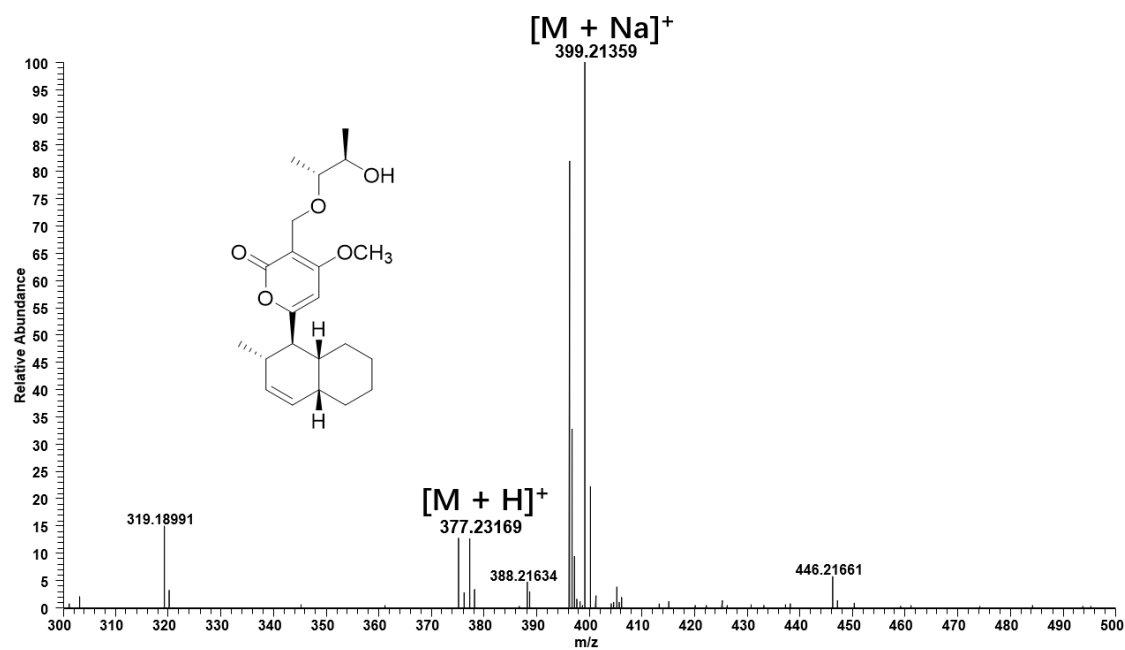
Figure S9. HRESIMS spectrum of compound 3.

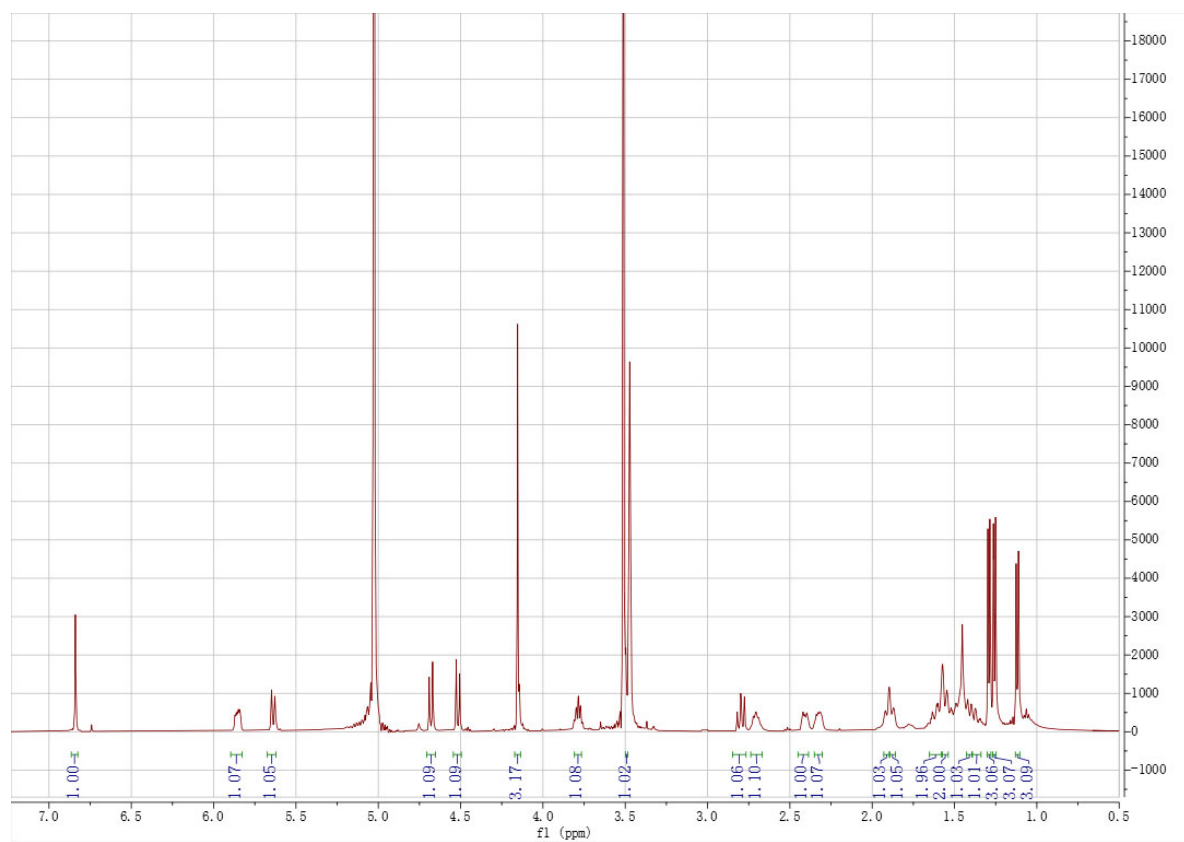
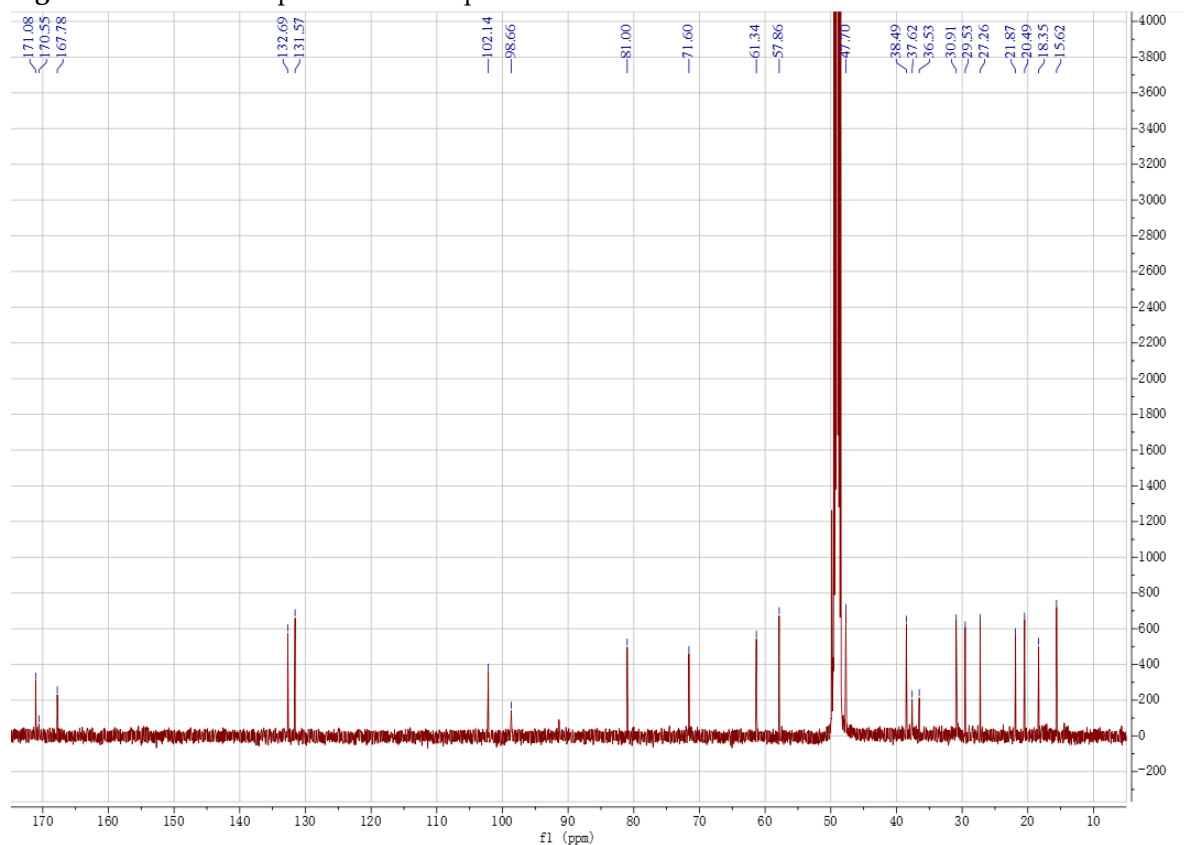
Figure S10. ^1H NMR (500 MHz, MeOD) spectrum of compound 3.**Figure S11.** ^{13}C NMR spectrum of compound 3.

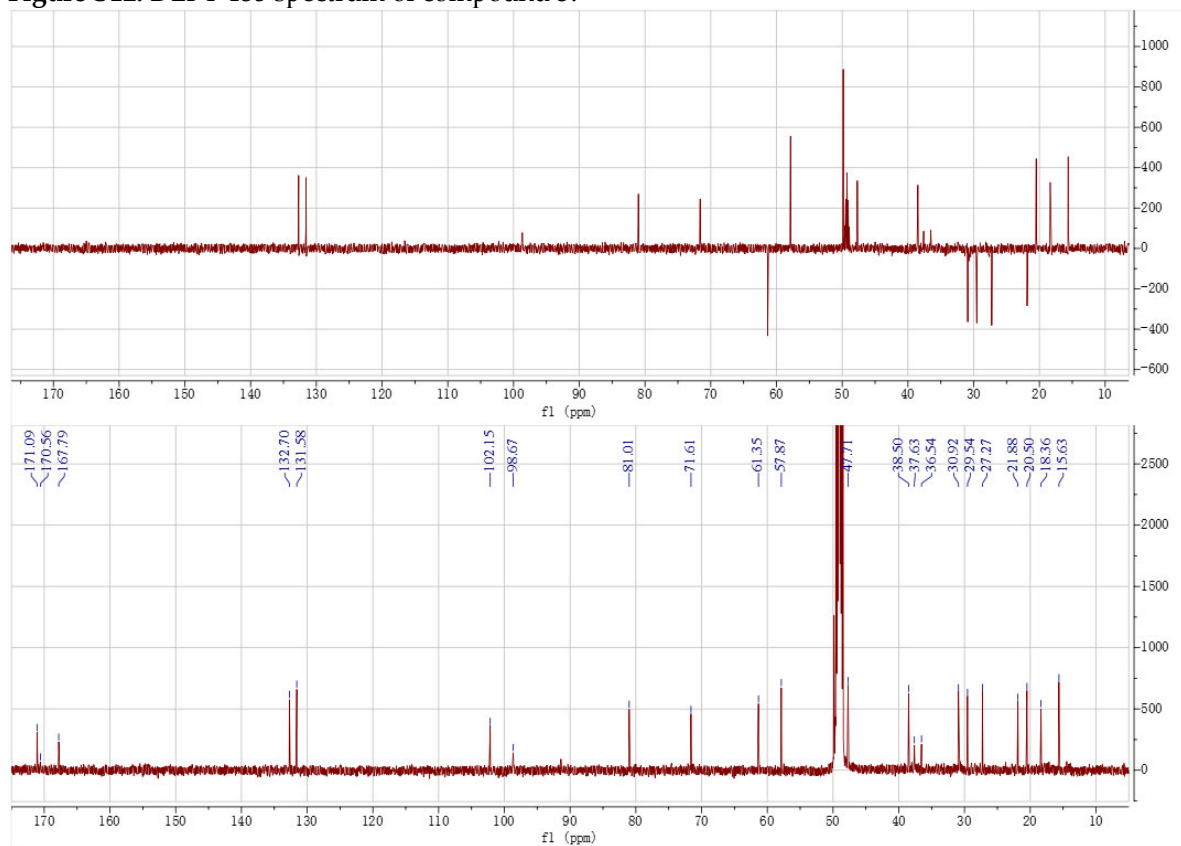
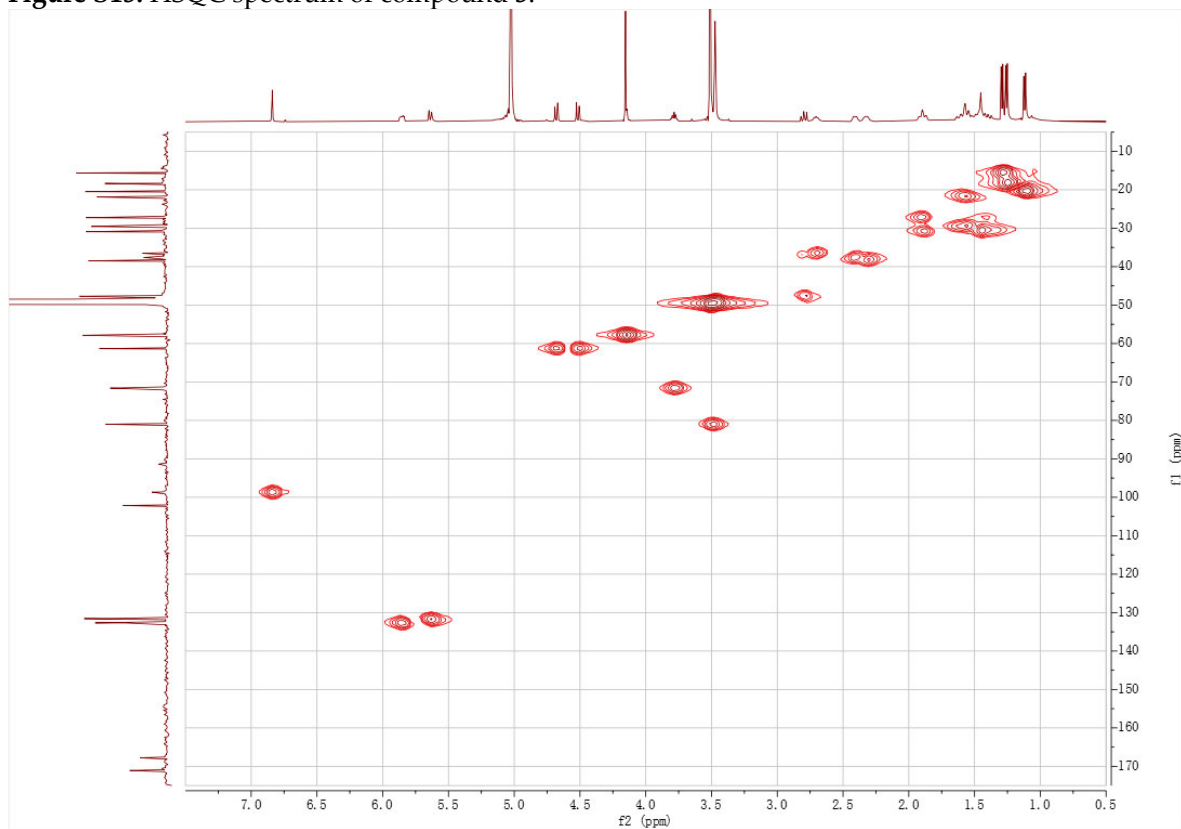
Figure S12. DEPT-135 spectrum of compound 3.**Figure S13.** HSQC spectrum of compound 3.

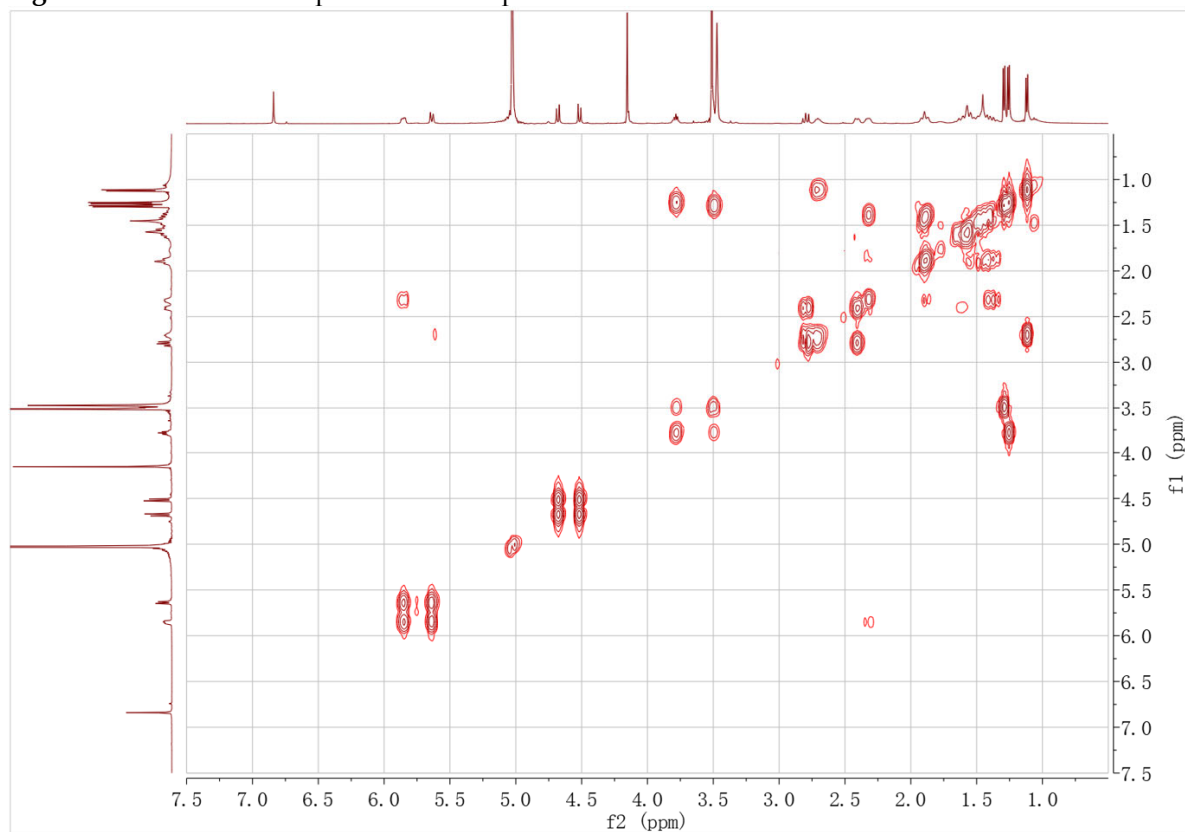
Figure S14. ^1H - ^1H COSY spectrum of compound 3.**Figure S15.** HMBC spectrum of compound 3.

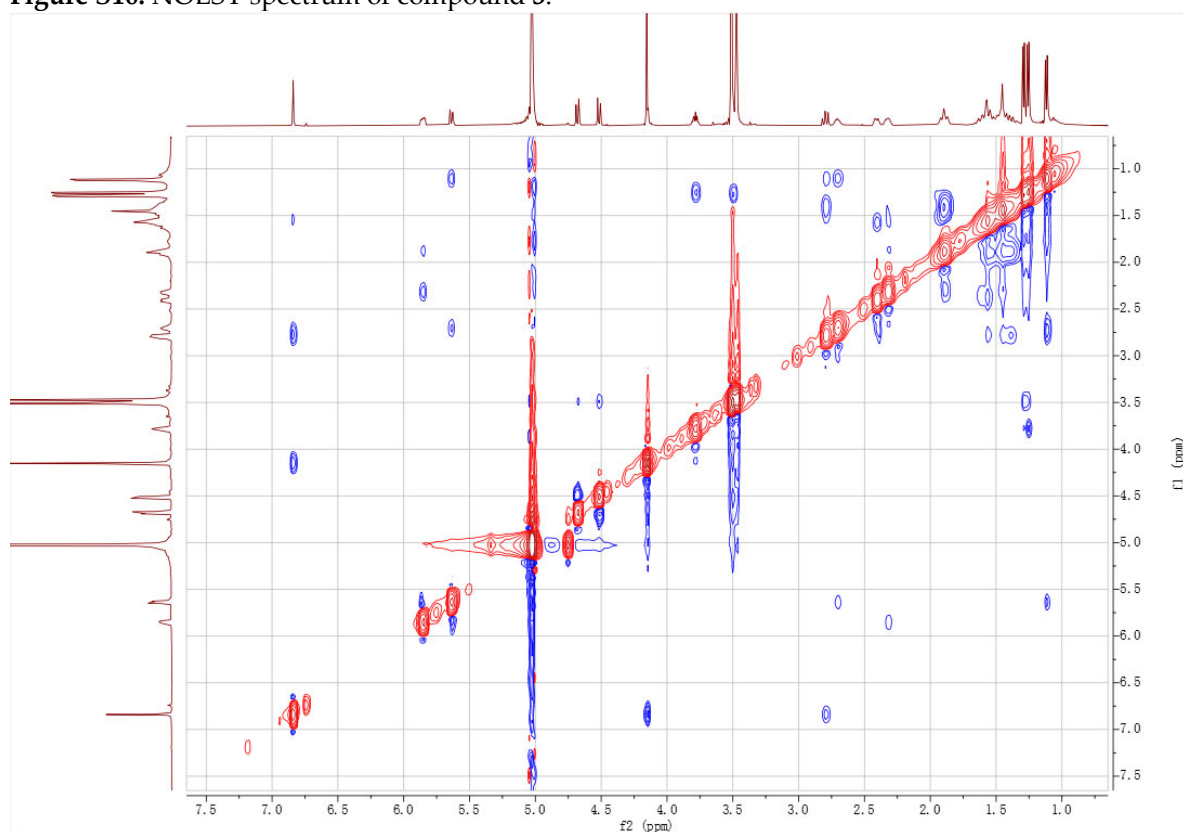
Figure S16. NOESY spectrum of compound 3.

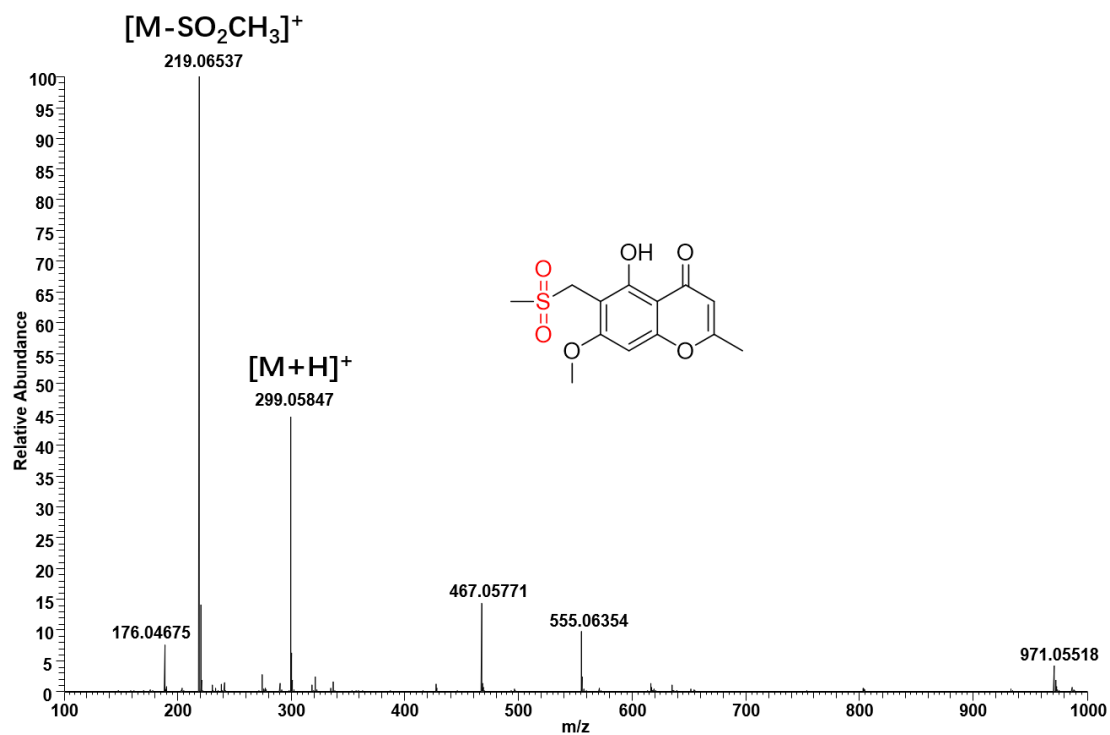
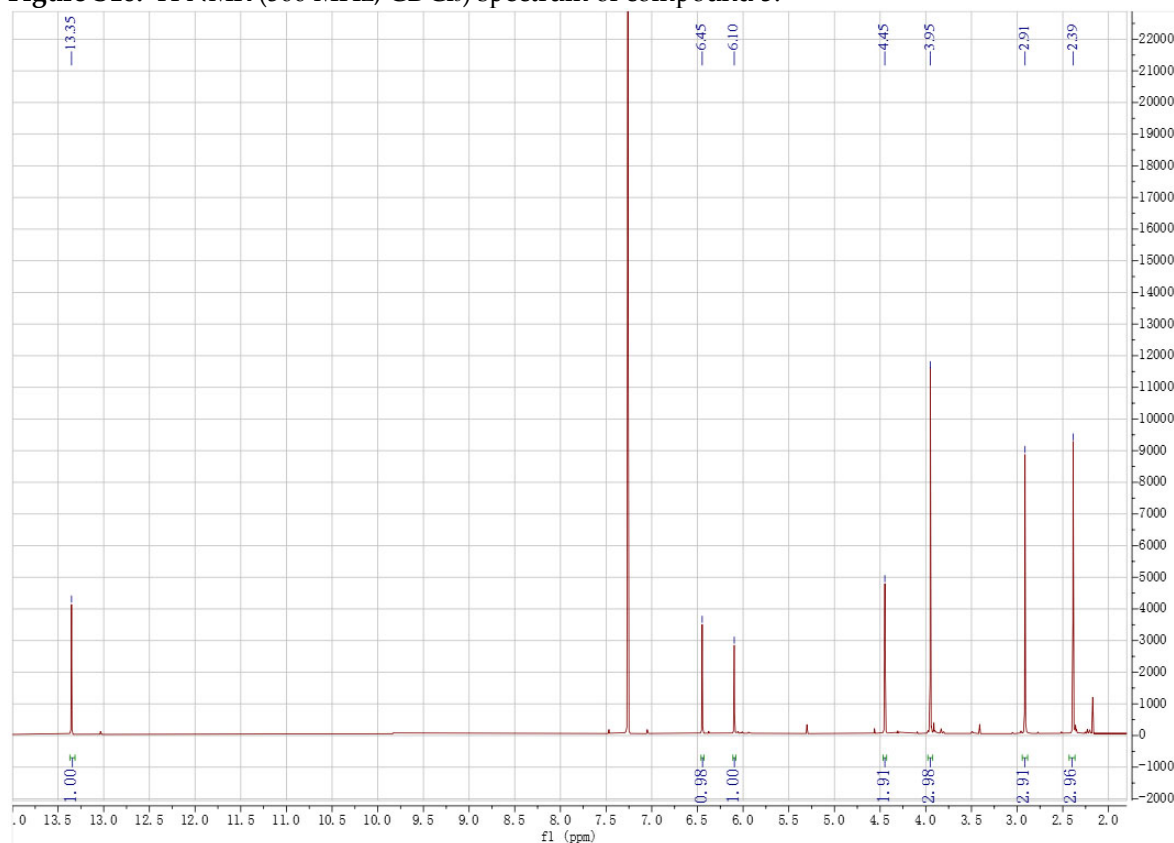
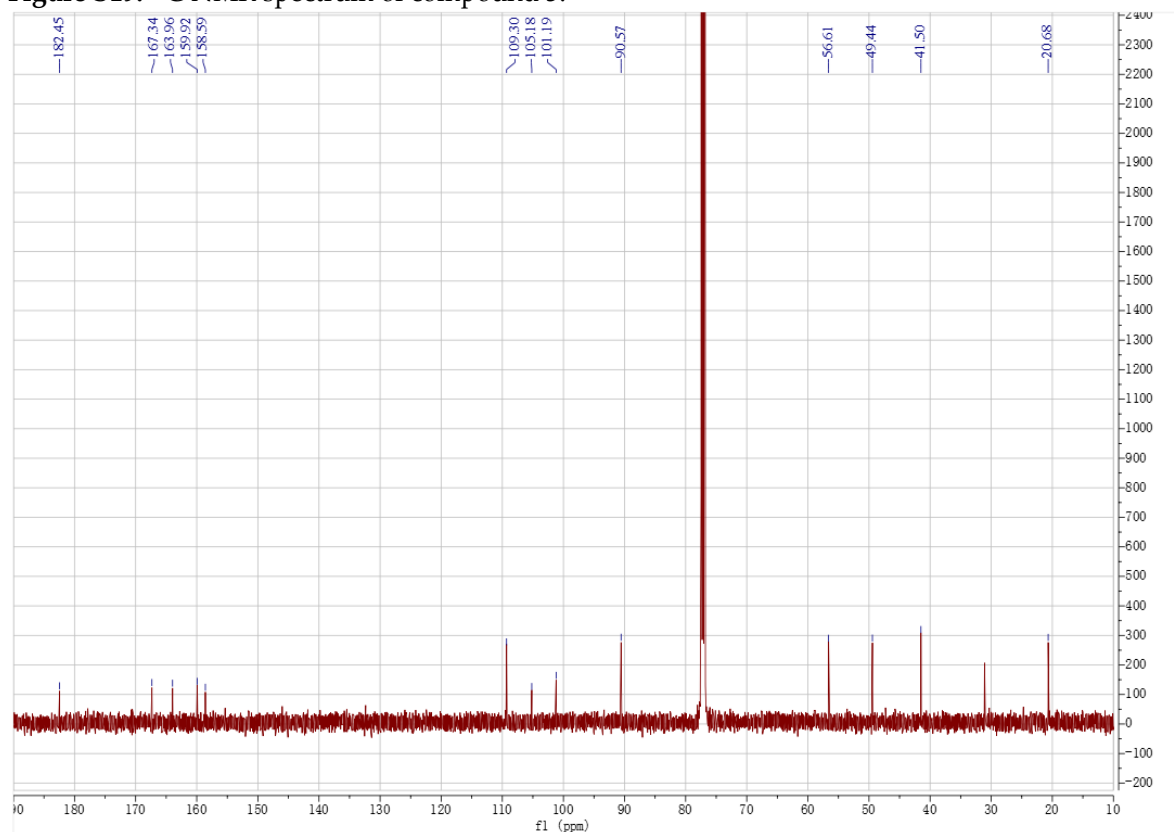
Figure S17. HRESIMS spectrum of compound 5.

Figure S18. ^1H NMR (500 MHz, CDCl_3) spectrum of compound 5.**Figure S19.** ^{13}C NMR spectrum of compound 5.**Figure S20.** DEPT-135 spectrum of compound 5.

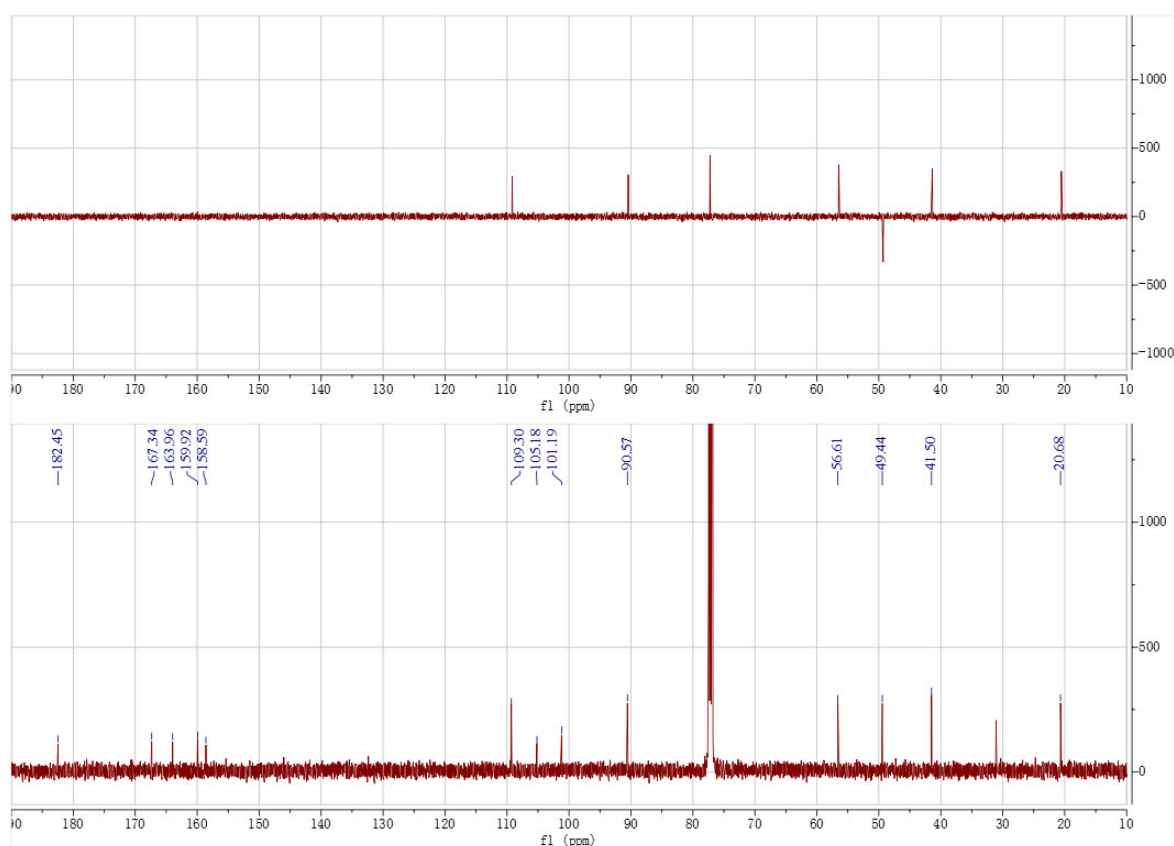


Figure S21. HSQC spectrum of compound 5.

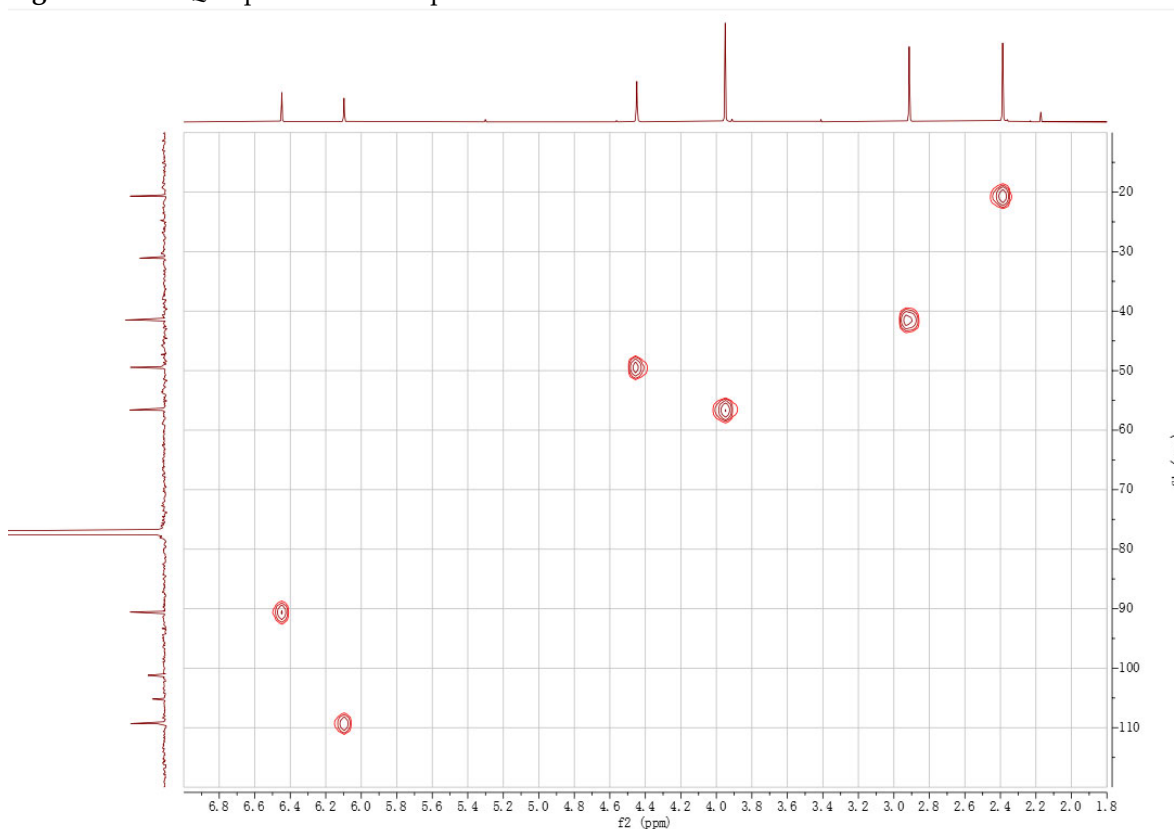


Figure S22. HMBC spectrum of compound 5.

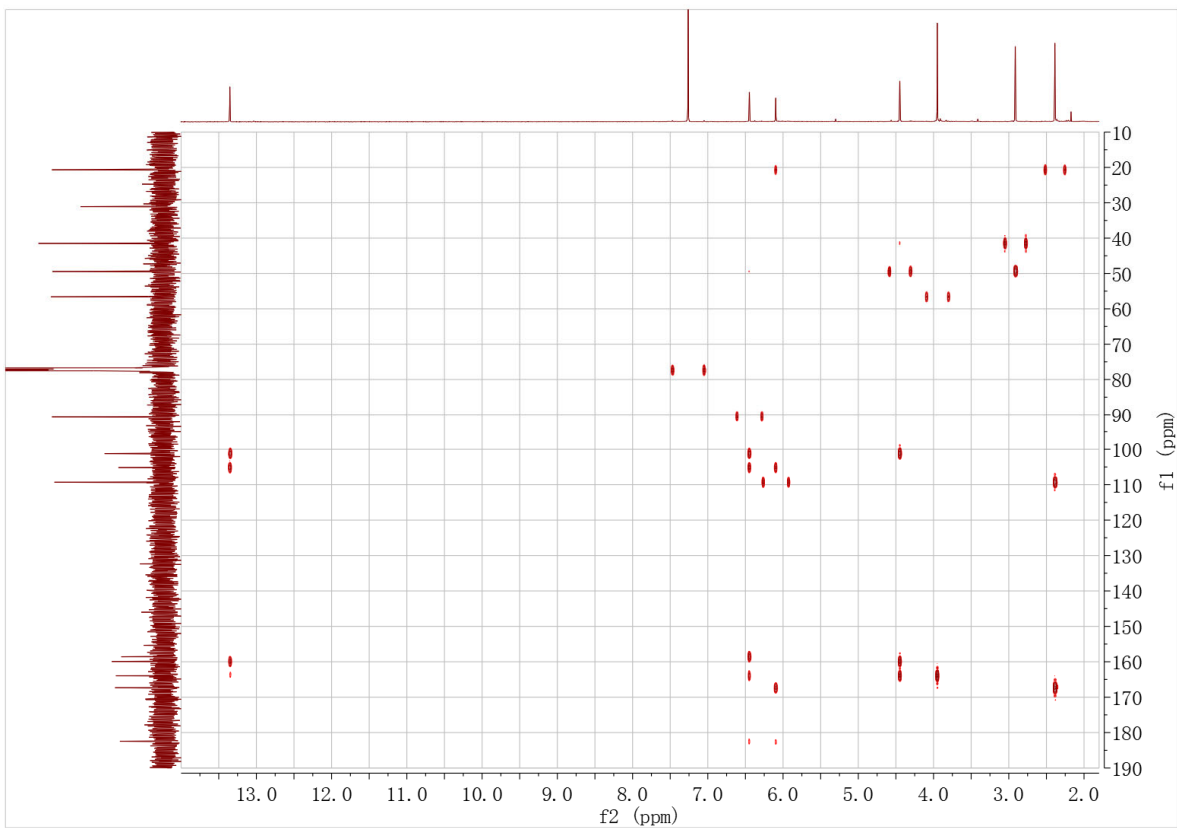


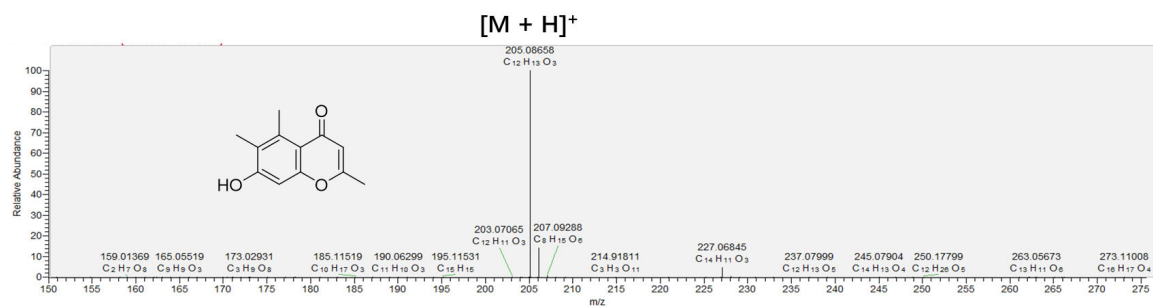
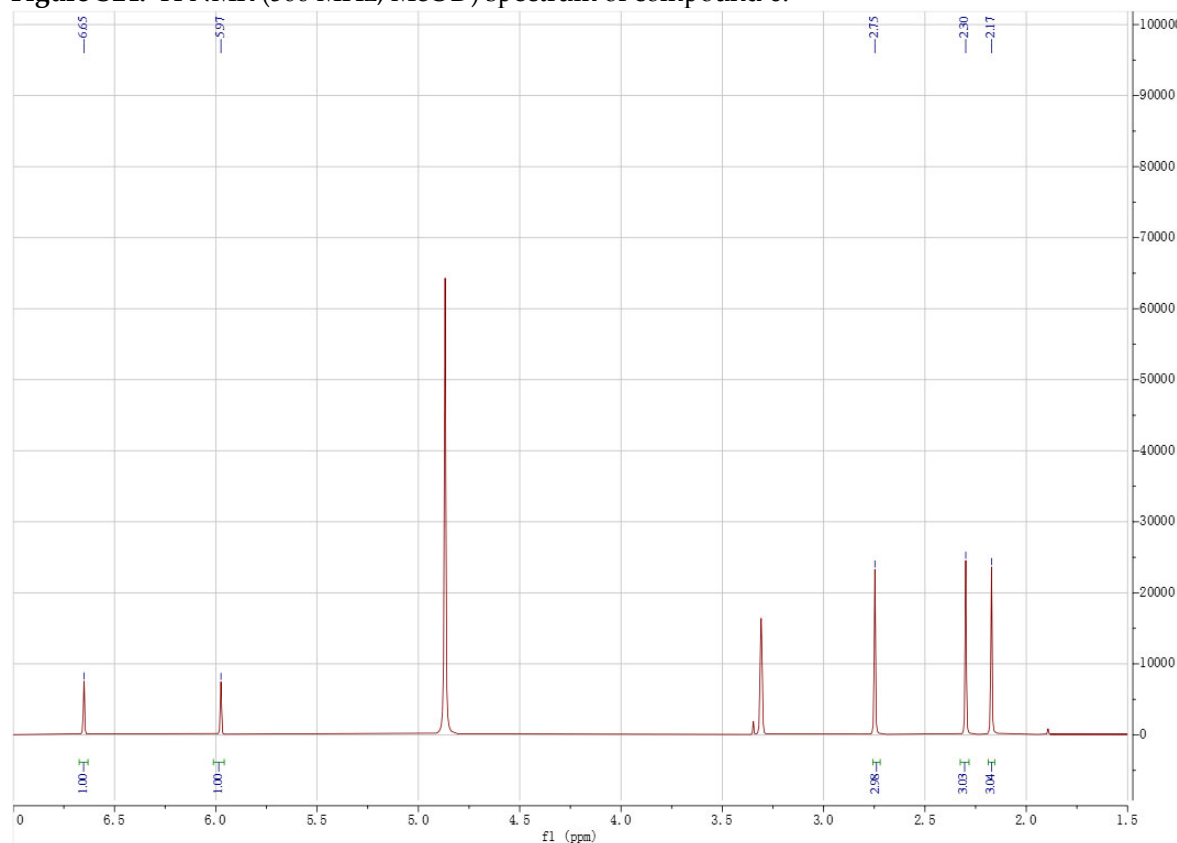
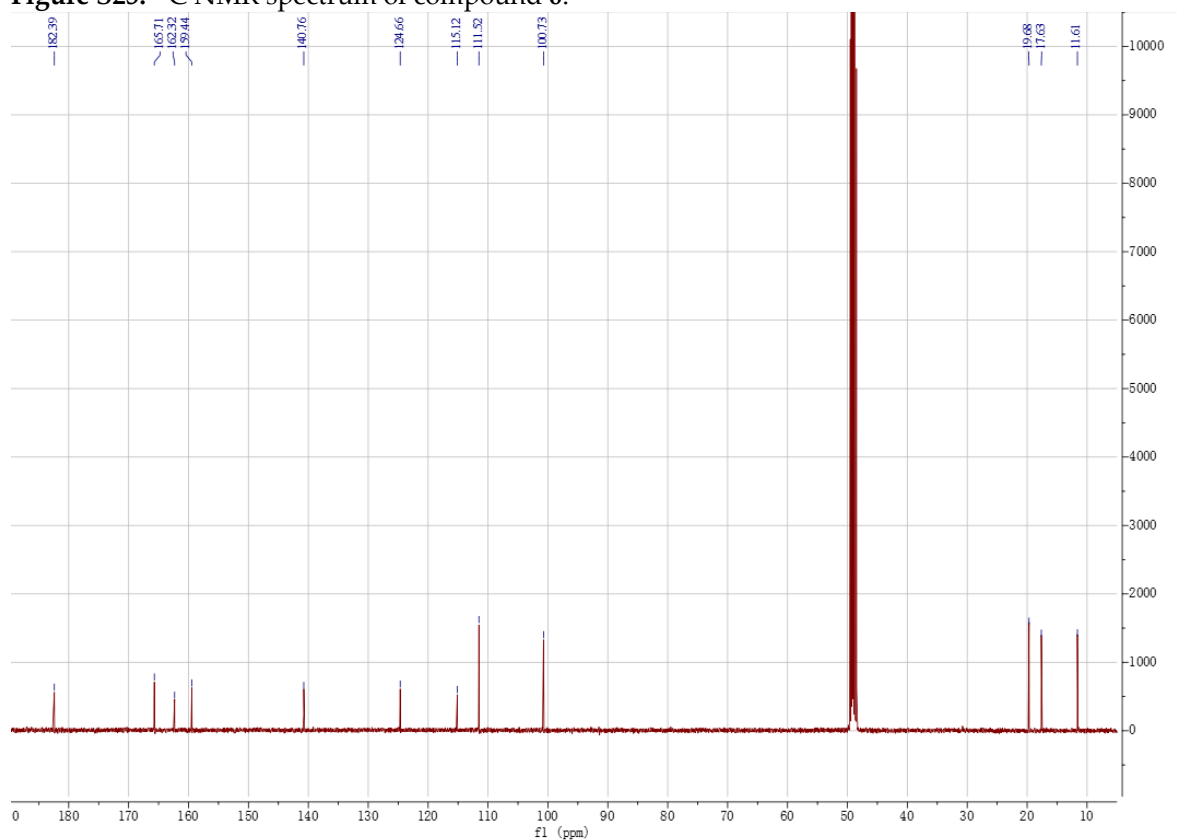
Figure S23. HRESIMS spectrum of compound 6.

Figure S24. ^1H NMR (500 MHz, MeOD) spectrum of compound 6.**Figure S25.** ^{13}C NMR spectrum of compound 6.**Figure S26.** HSQC spectrum of compound 6.

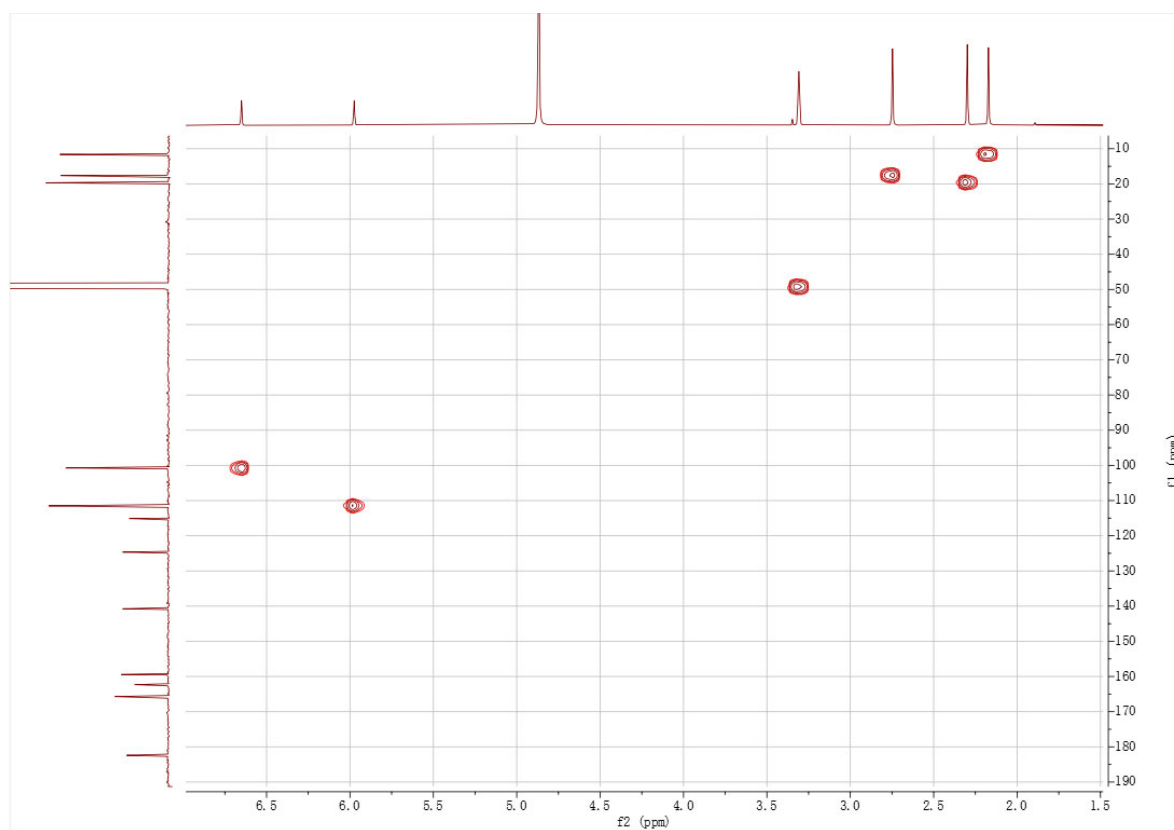


Figure S27. HMBC spectrum of compound 6.

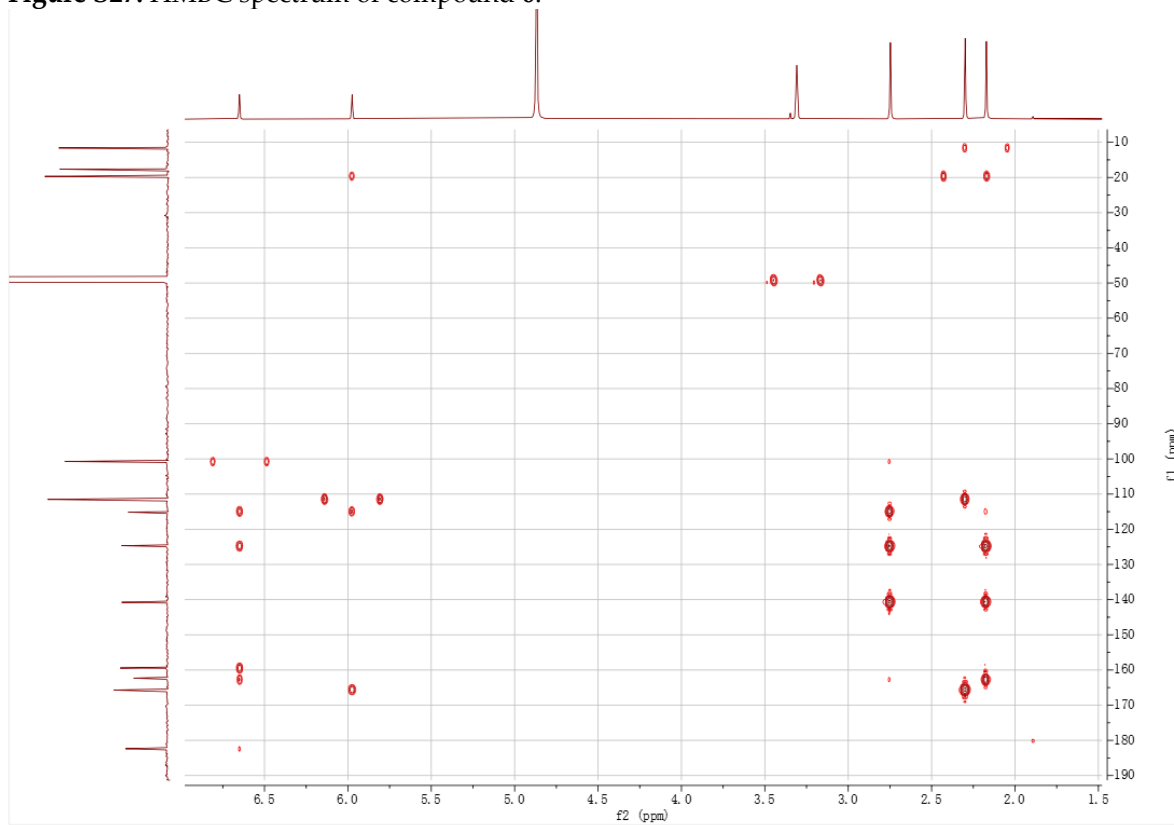


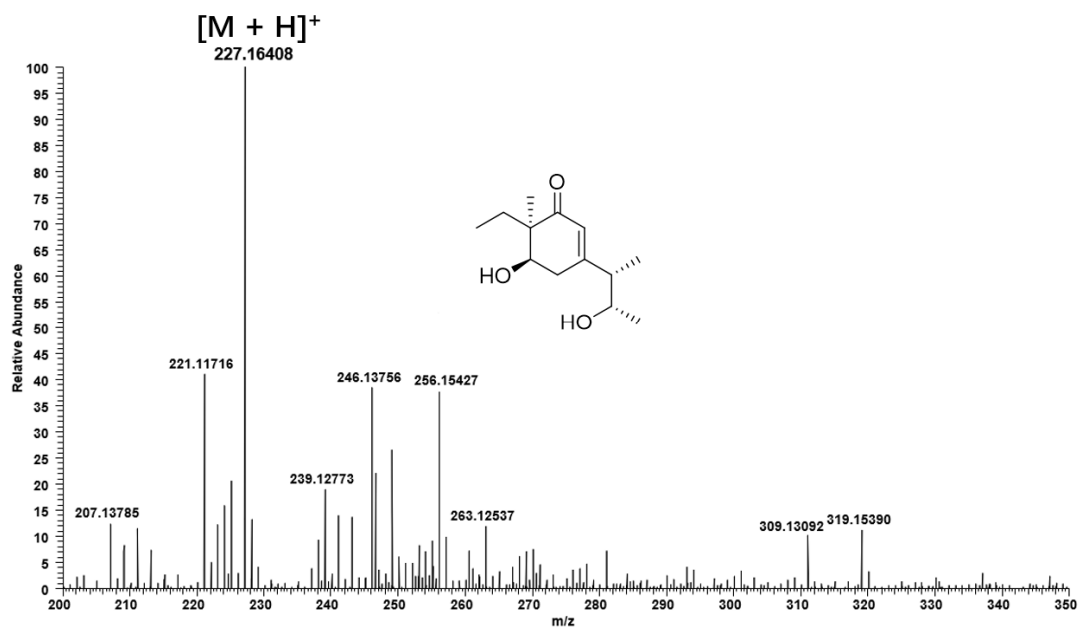
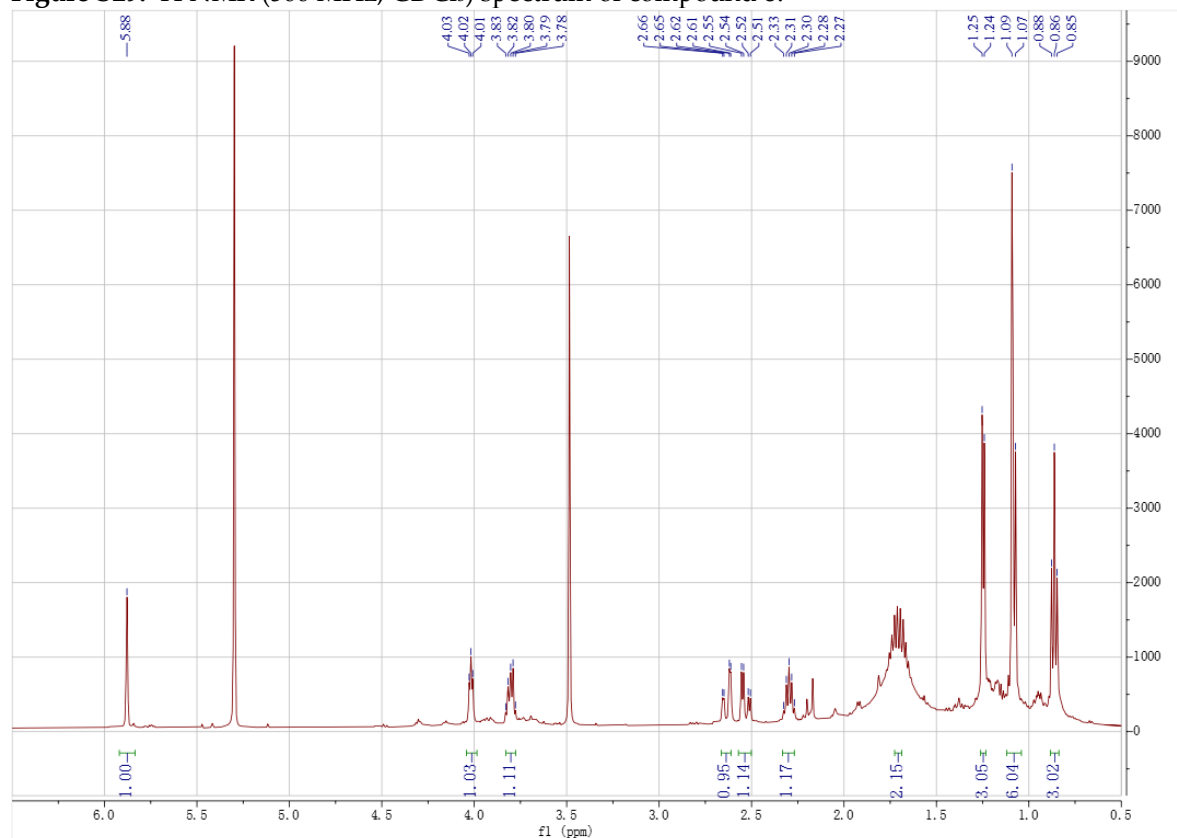
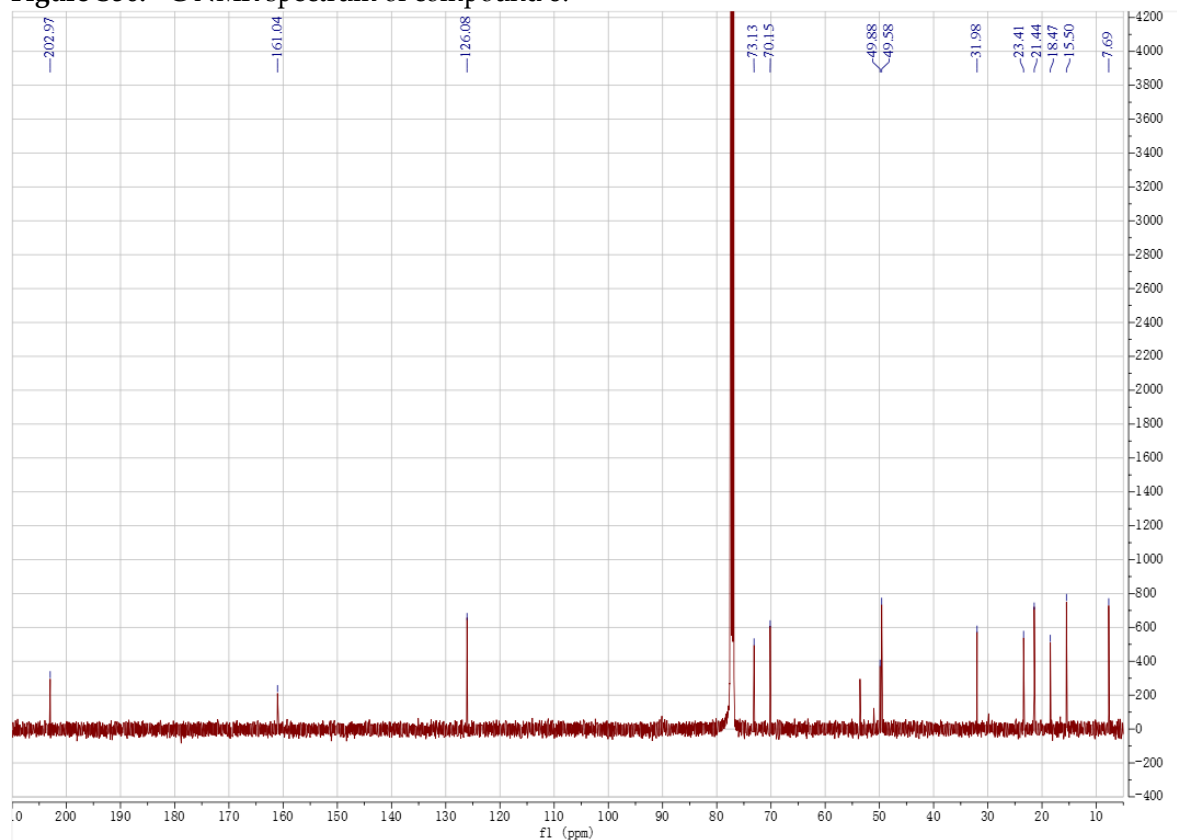
Figure S28. HRESIMS spectrum of compound 8.

Figure S29. ^1H NMR (500 MHz, CDCl_3) spectrum of compound 8.**Figure S30.** ^{13}C NMR spectrum of compound 8.**Figure S31.** DEPT-135 spectrum of compound 8.

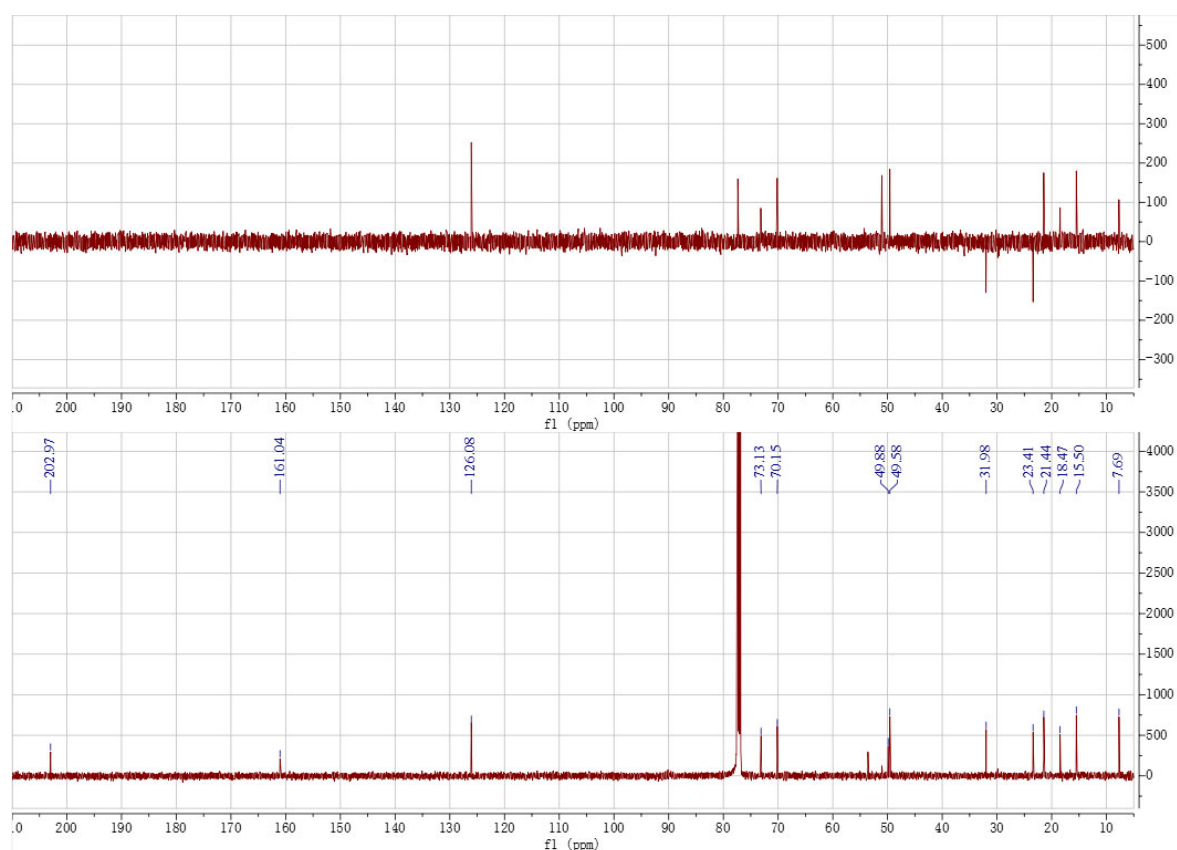


Figure S32. HSQC spectrum of compound 8.

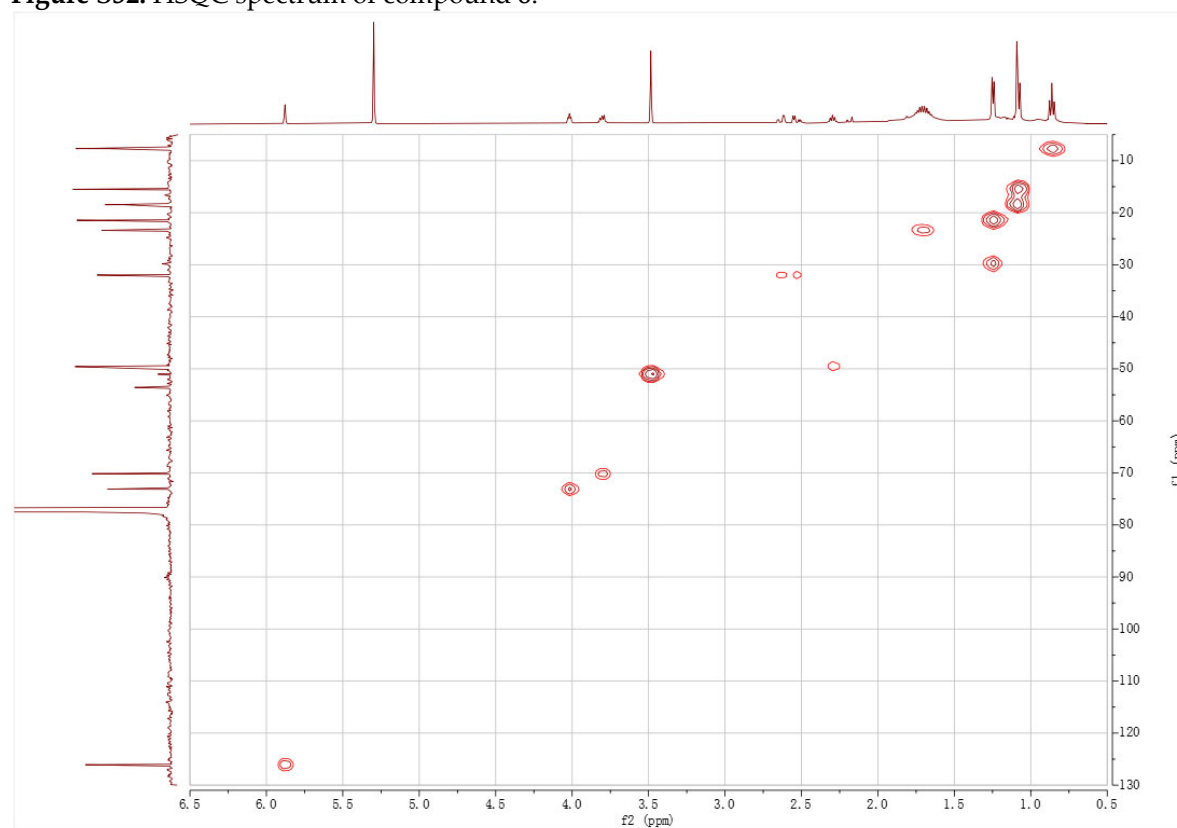


Figure S33. ^1H - ^1H COSY spectrum of compound 8.

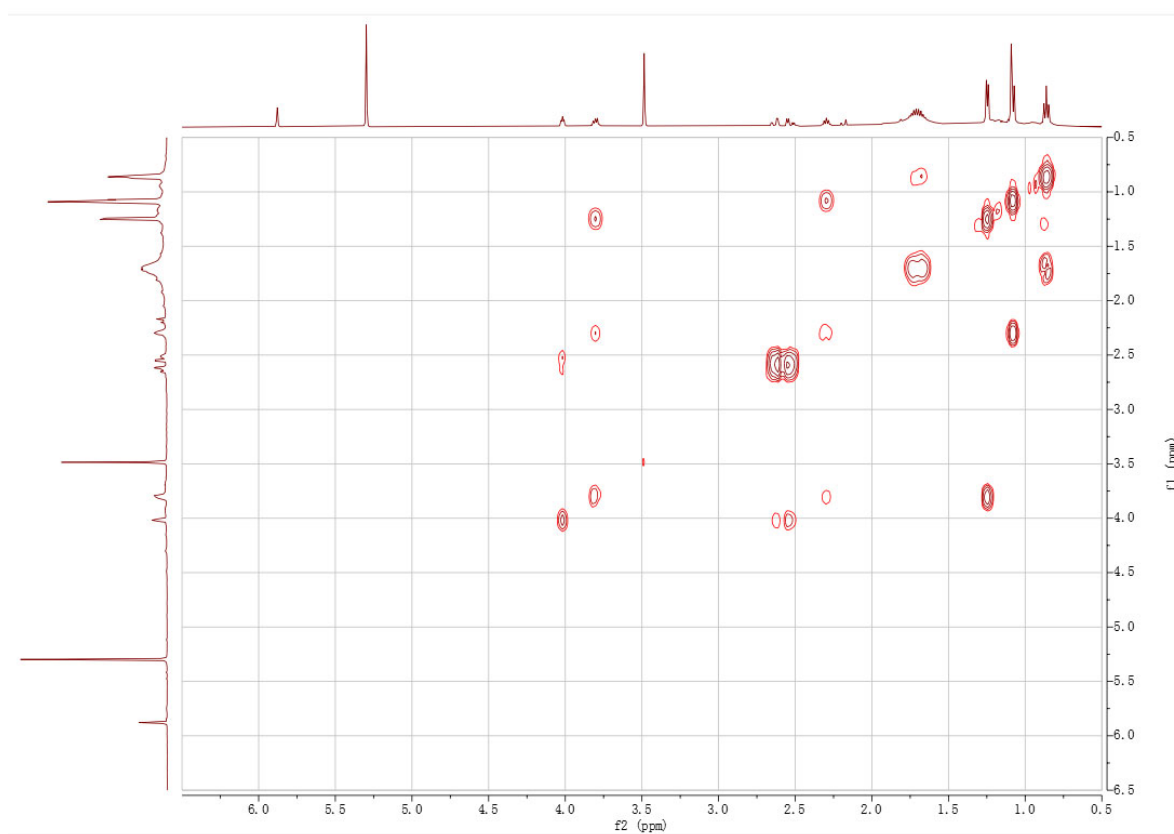


Figure S34. HMBC spectrum of compound 8.

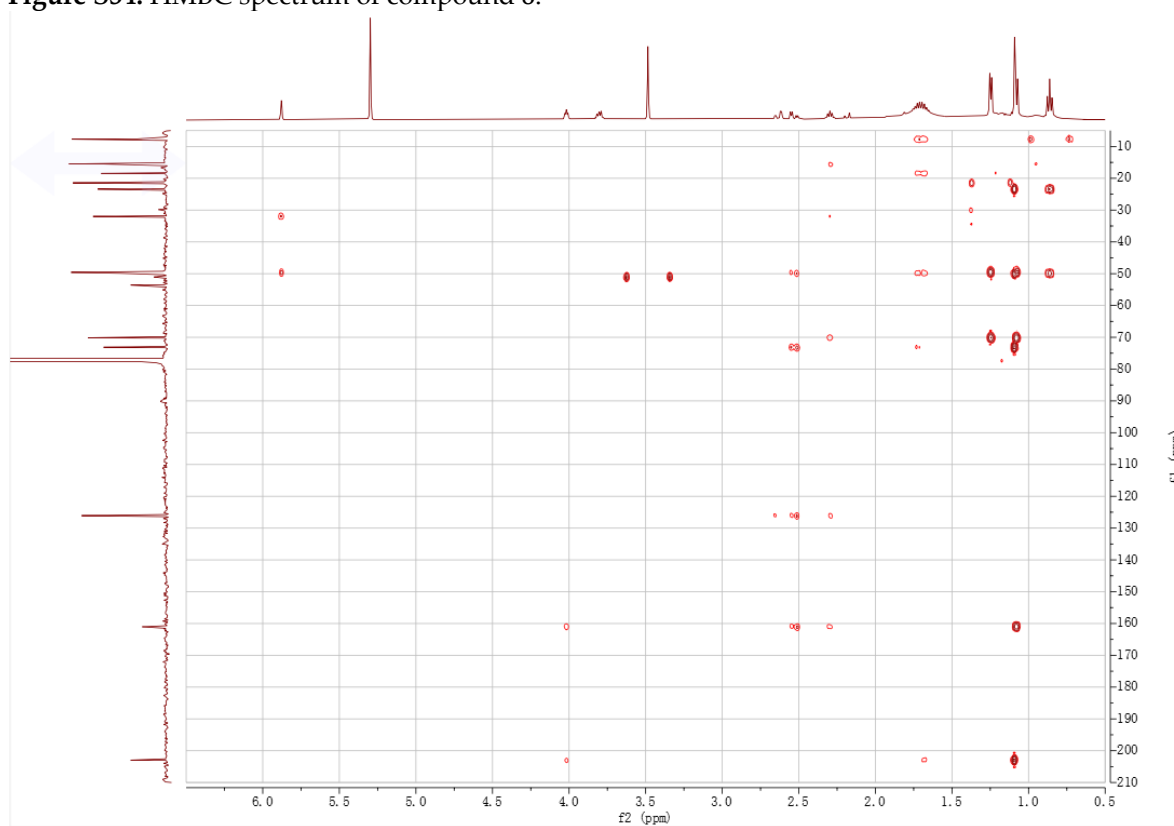


Figure S35. NOESY spectrum of compound 8.

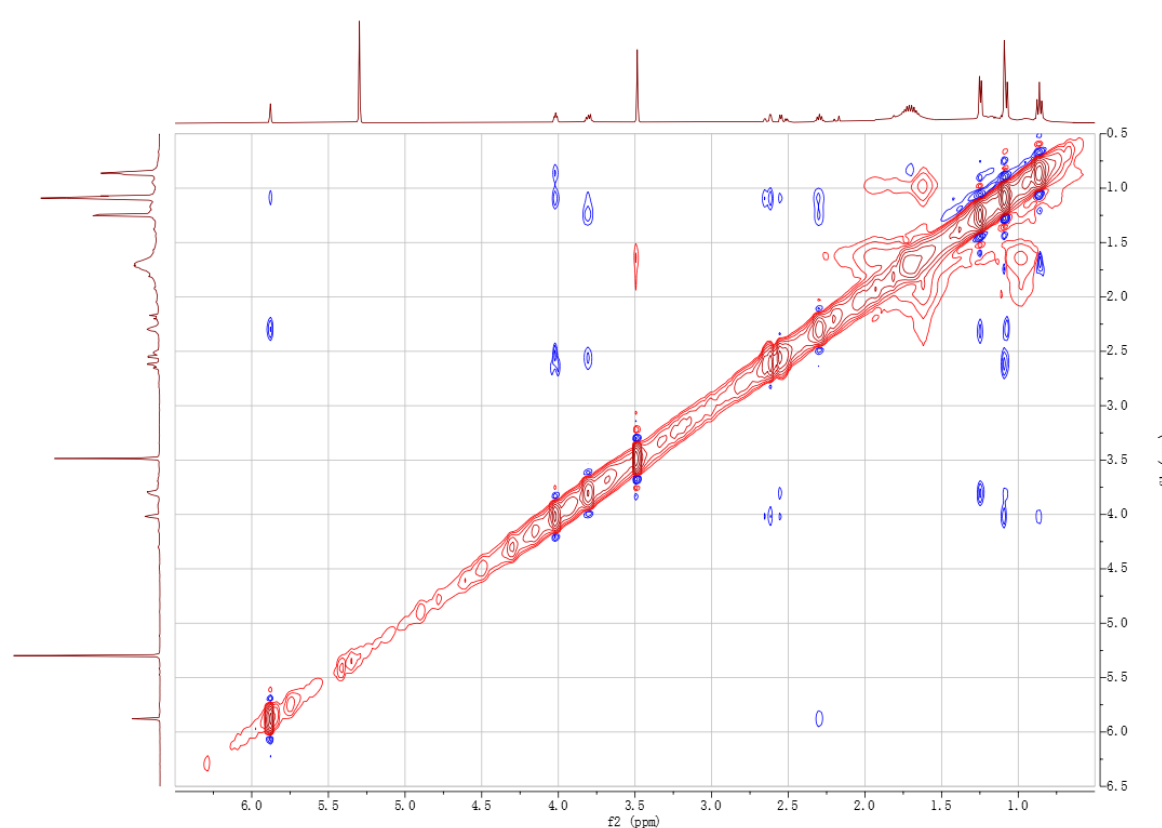


Figure S36. Optimized geometries of predominant conformers (weighting factors) for compound **1** at the B3LYP/6-311++g(d, p) level above 1% population.

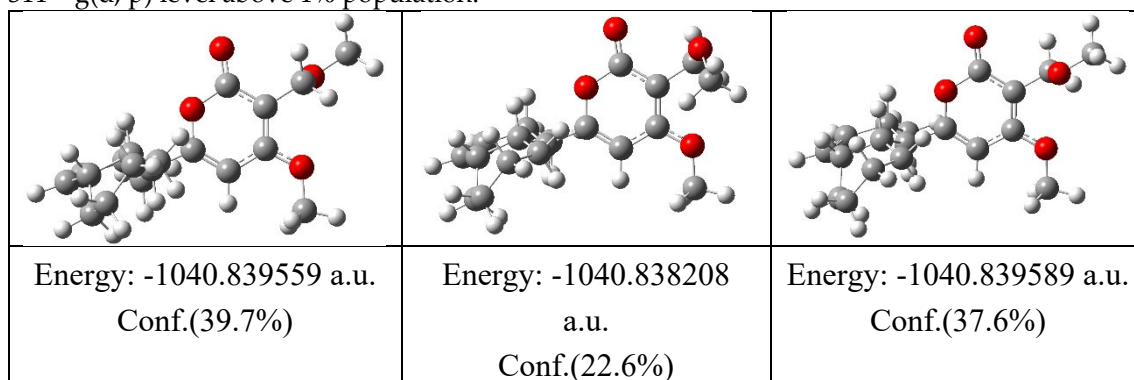


Figure S37. Optimized geometries of predominant conformers (weighting factors) for compound **3** at the B3LYP/6-311++g(d, p) level above 1% population.

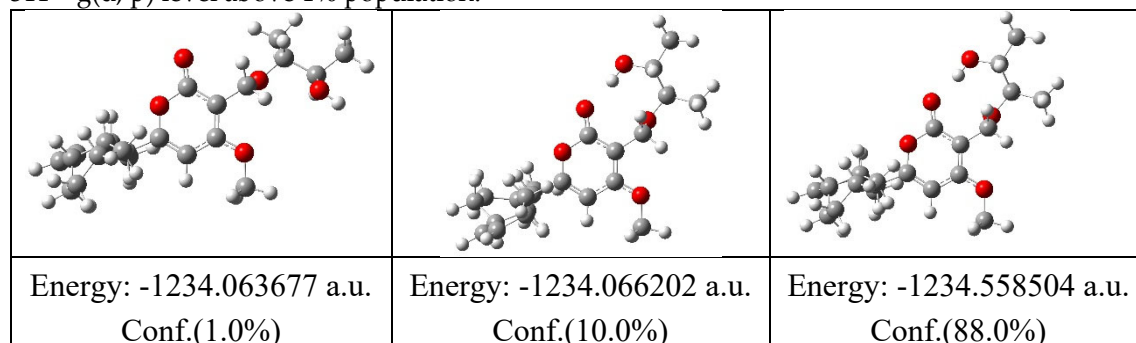


Figure S38. Optimized geometries of predominant conformers (weighting factors) for compound **8** at the B3LYP/6-311++g(d, p) level above 1% population.

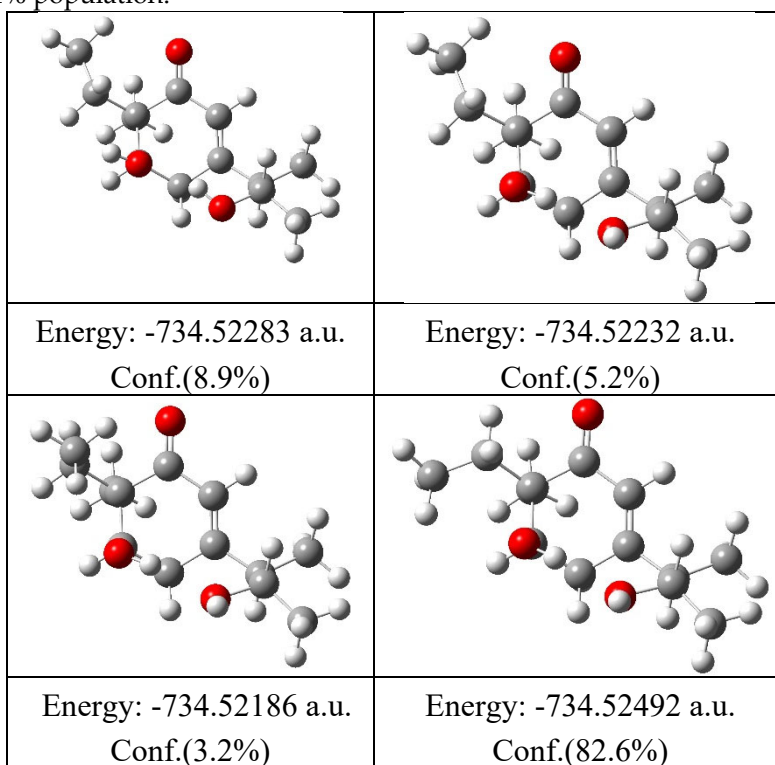


Figure S39. Regression analyses of experimental versus calculated ^{13}C NMR chemical shifts of compounds **1**, **3** and **8**.

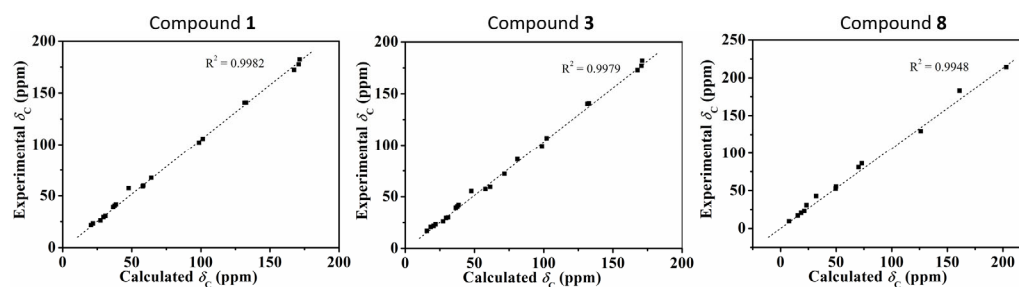
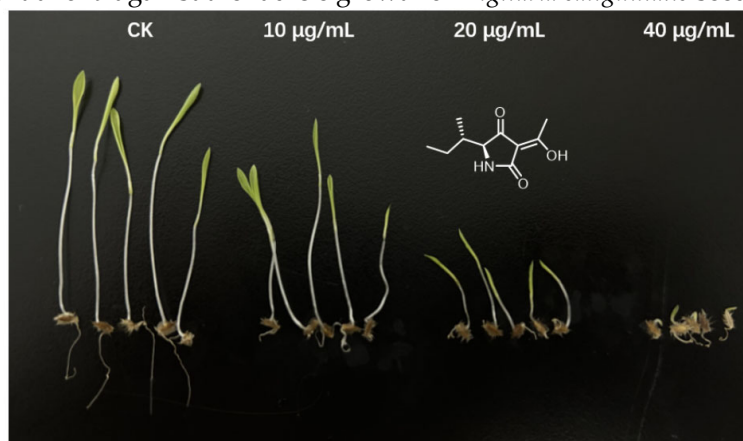


Figure S40. Herbicidal potential of **9** against the radicle growth of *Digitaria sanguinalis* seedlings.Table S1. Herbicidal spectrum of **9** against representative malignant weeds *D. sanguinalis*, *Portulaca oleracea*, and *Descurainia sophia*.

| Weeds | Compounds | 40 µg/mL | 20 | 10 |
|-----------------------|-----------------|----------|----------|----------|
| <i>D. sanguinalis</i> | 9 | 88.6±2.1 | 84.1±1.5 | 73.2±1.9 |
| | CK ^a | 90.5±1.8 | 85.7±3.2 | 76.1±2.3 |
| <i>P. oleracea</i> | 9 | 71.9±2.2 | 62.6±1.4 | n.d. |
| | CK ^a | 89.2±2.9 | 81.3±1.7 | n.d. |
| <i>D. sophia</i> | 9 | 69.2±1.6 | 55.8±2.4 | n.d. |
| | CK ^b | 86.7±1.3 | 74.8±1.1 | n.d. |

^{a,b} CK was chemical herbicide acetochlor ^a and tribenuron-methyl ^b, respectively. n.d.: not detected.