

Supporting Information for

Chemical and Biosynthetic Potential of *Penicillium shentong*

XL-F41

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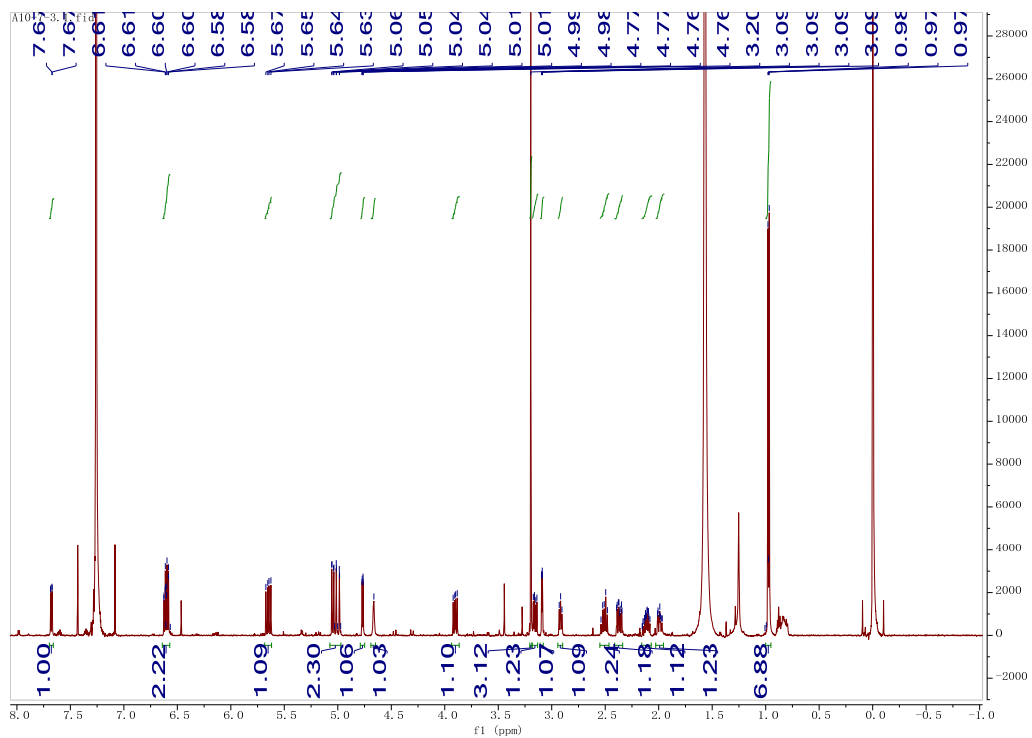


Figure S1. ^1H NMR spectrum (600 MHz, Chloroform-d) of **1**

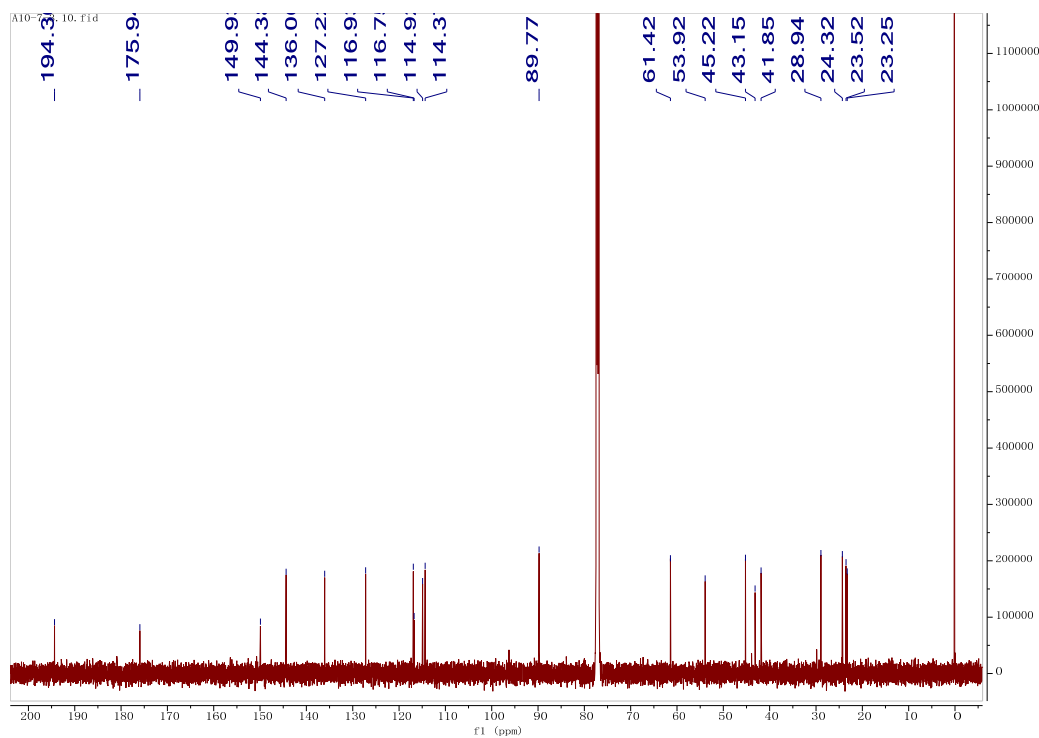


Figure S2. ^{13}C NMR spectrum (600 MHz, Chloroform-d) of **1**

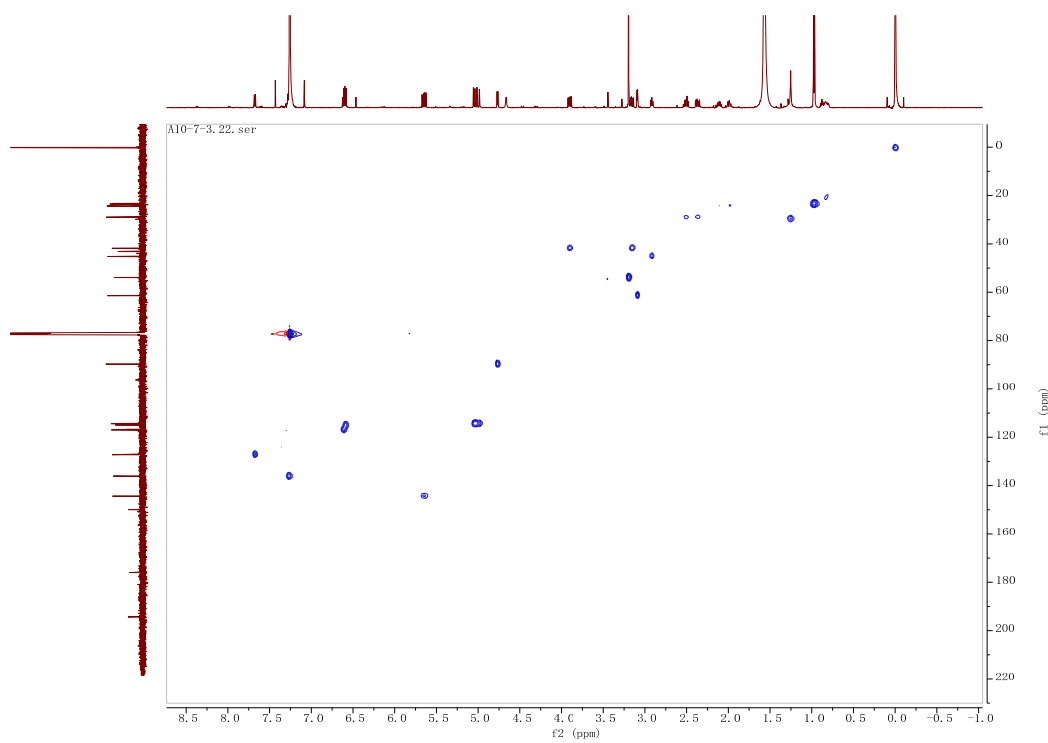


Figure S3. HSQC spectrum (600 MHz, Chloroform-d) of **1**

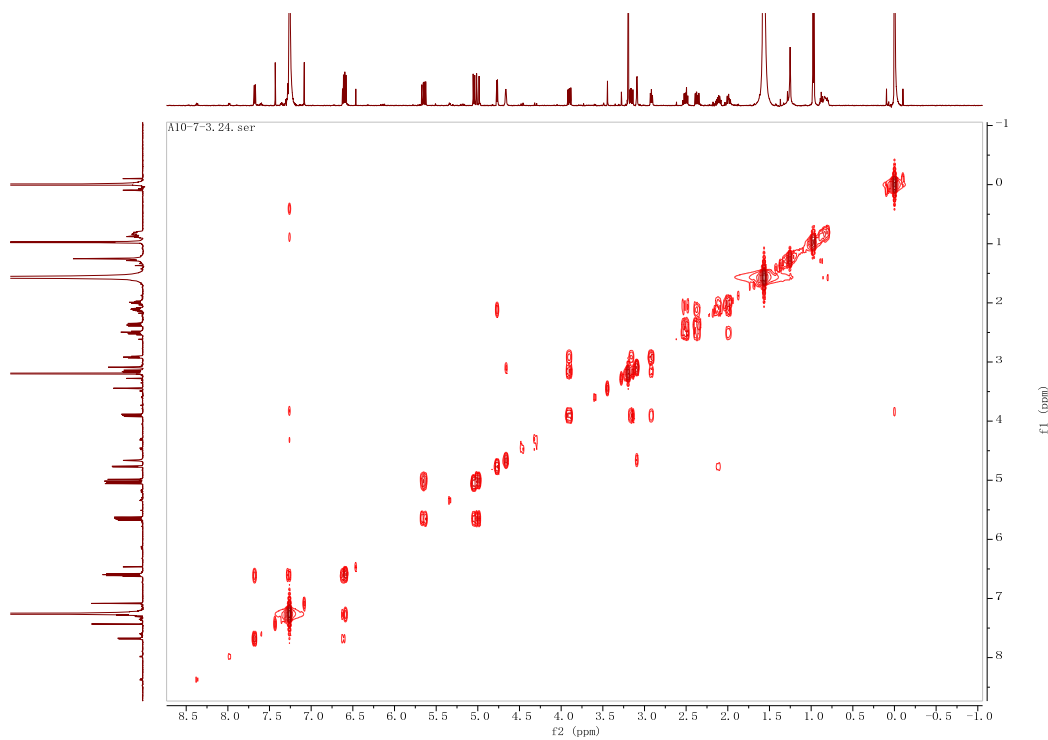


Figure S4. ¹H-¹H COSY spectrum (600 MHz, Chloroform-d) of **1**

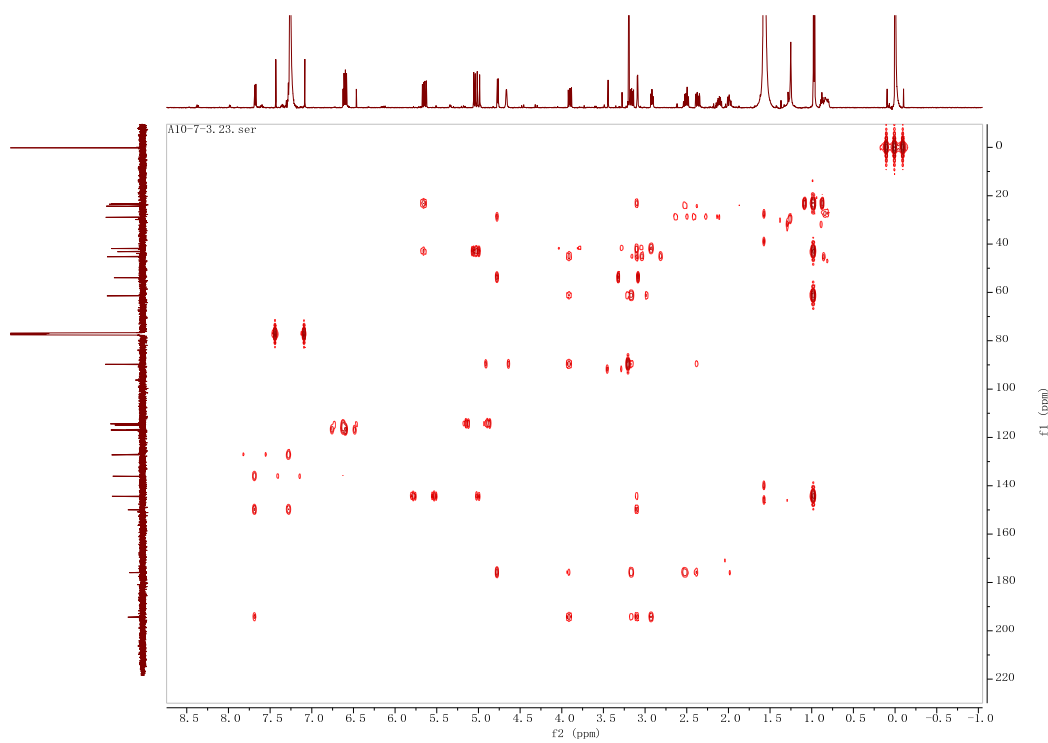


Figure S5. HMBC spectrum (600 MHz, Chloroform-d) of **1**

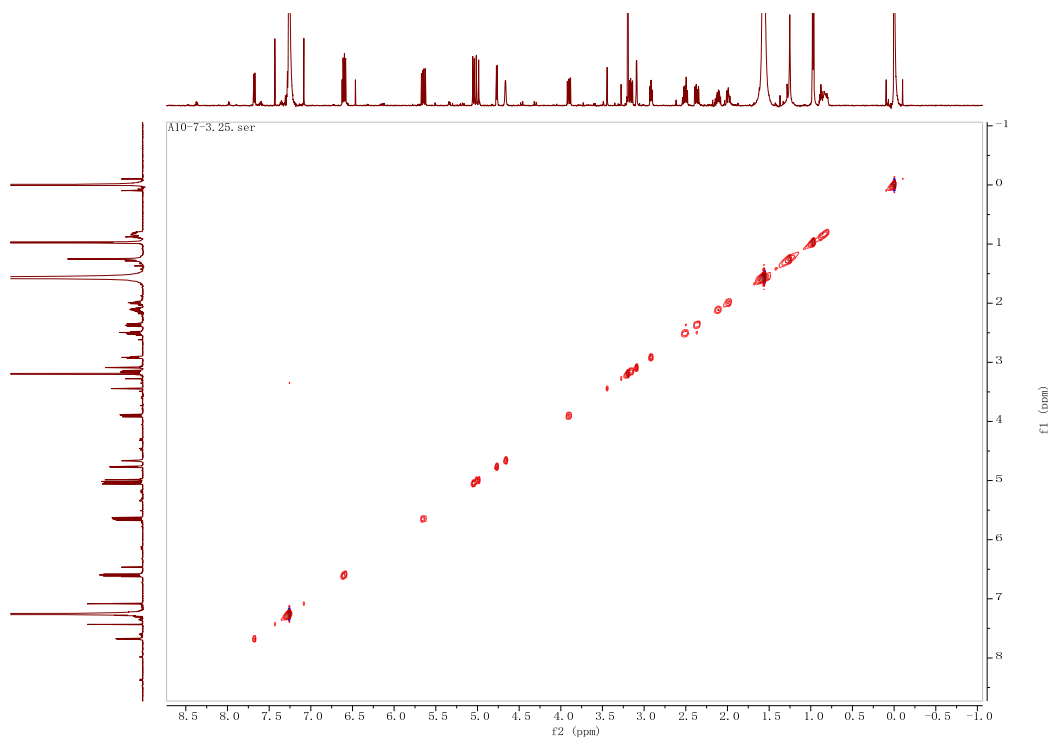


Figure S6. NOESY spectrum (600 MHz, Chloroform-d) of **1**

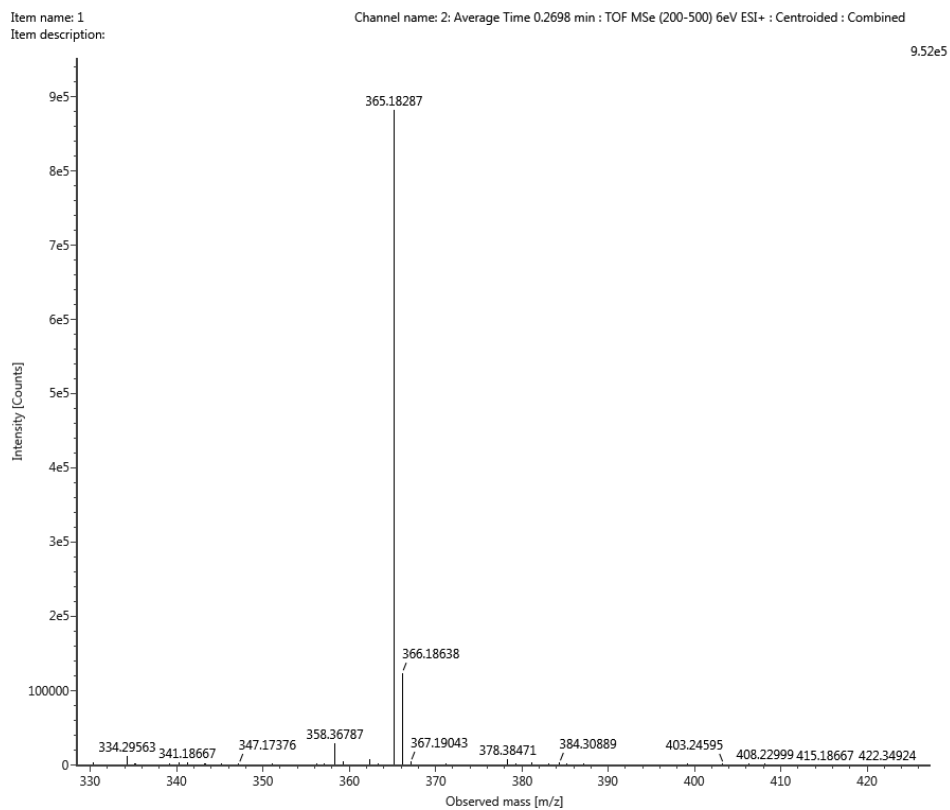


Figure S7. HRESIMS spectrum of **1**

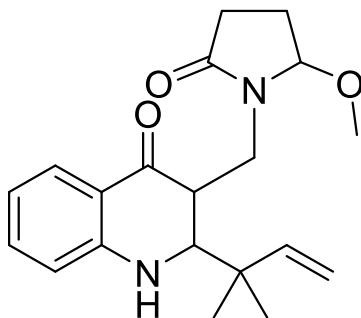


Figure S8. Chemical structure of compound **1**

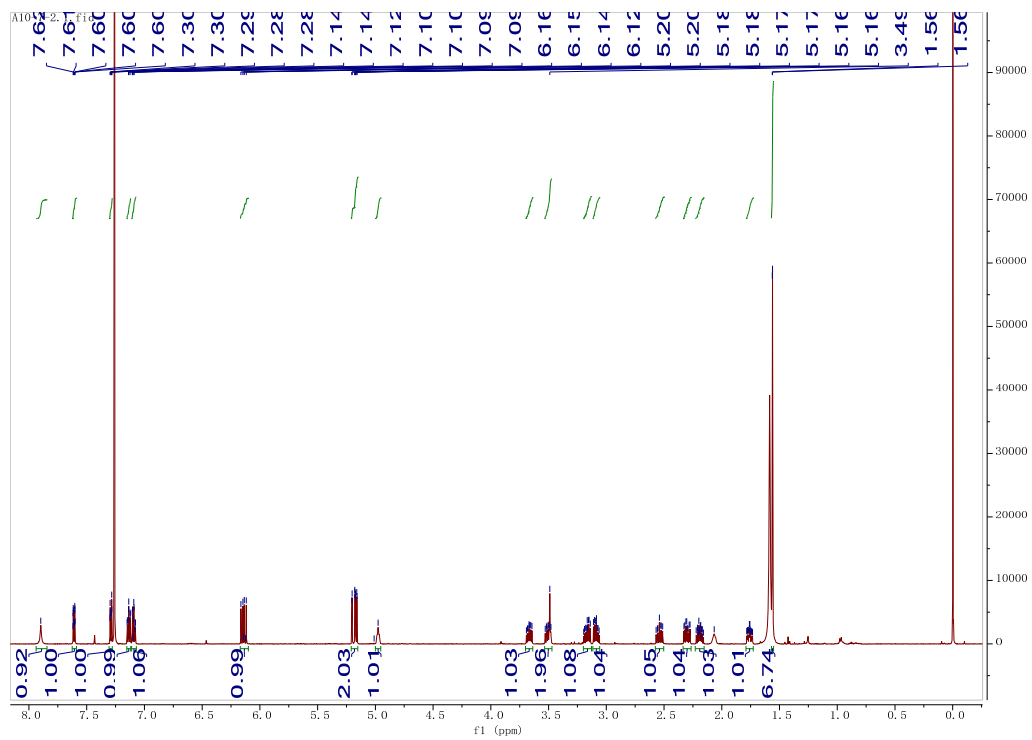


Figure S9. ^1H NMR spectrum (600 MHz, Chloroform-d) of **2**

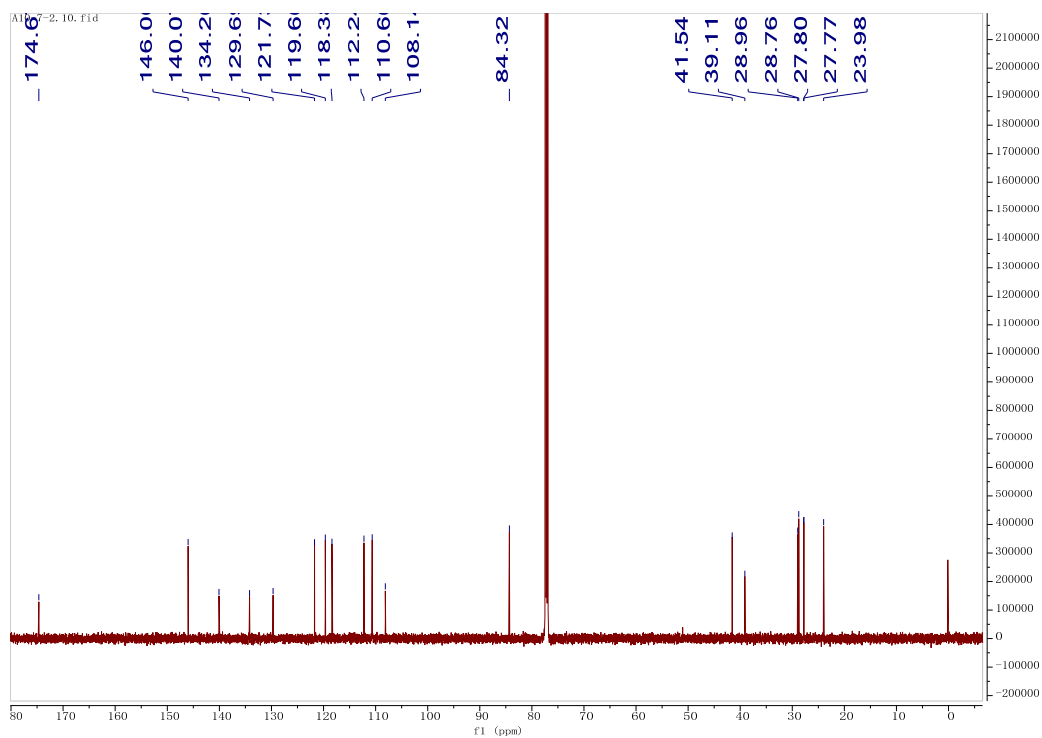


Figure S10. ^{13}C NMR spectrum (600 MHz, Chloroform-d) of **2**

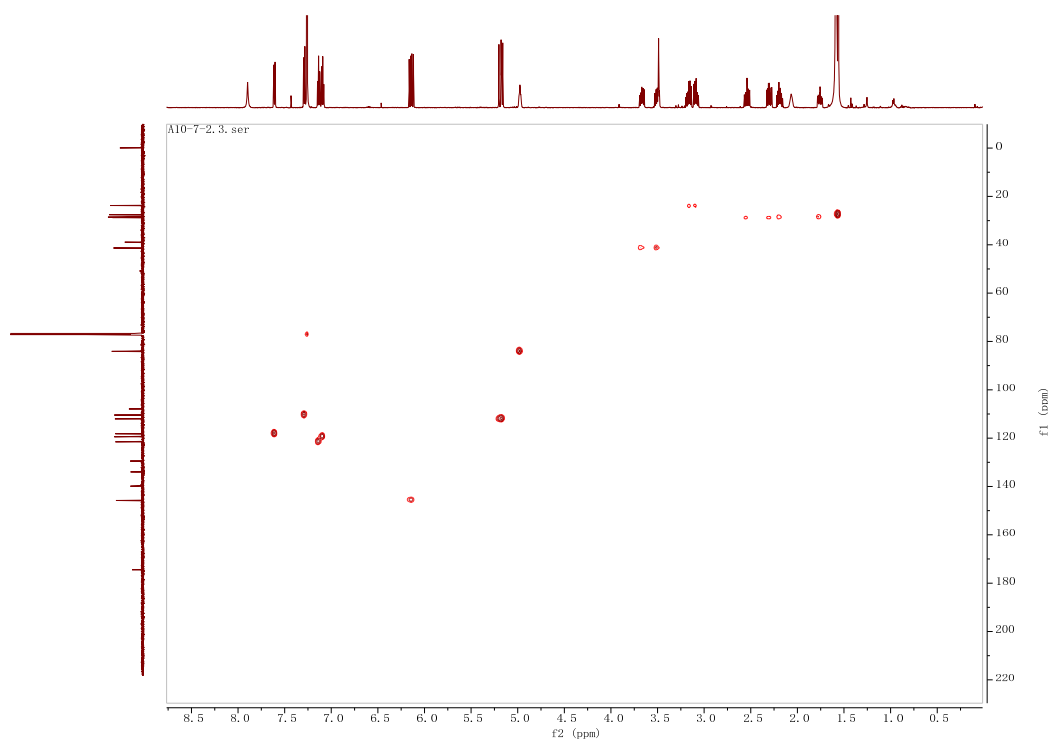


Figure S11. HSQC spectrum (600 MHz, Chloroform-d) of **2**

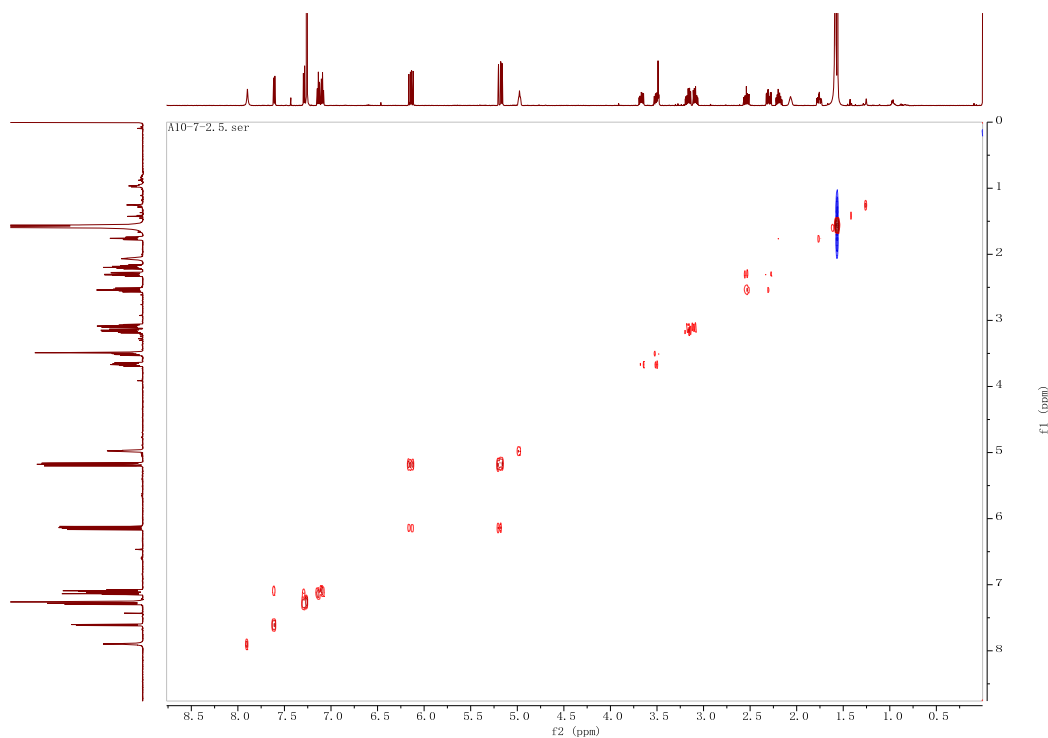


Figure S12. ^1H - ^1H COSY spectrum (600 MHz, Chloroform-d) of **2**

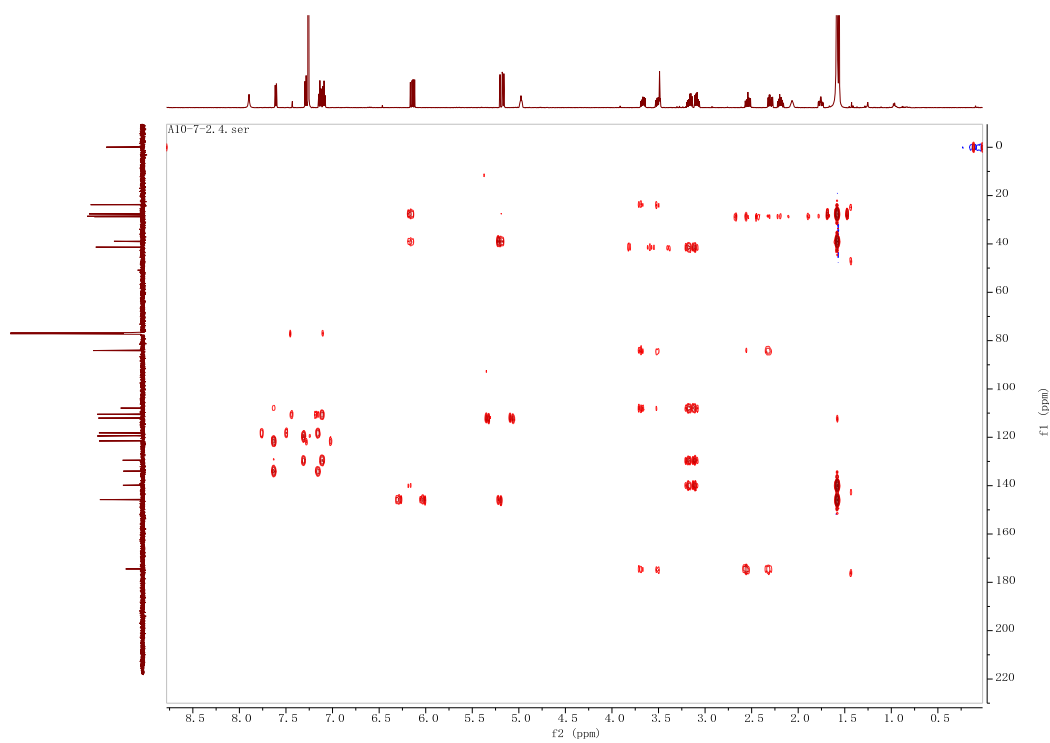


Figure S13. HMBC spectrum (600 MHz, Chloroform-d) of **2**

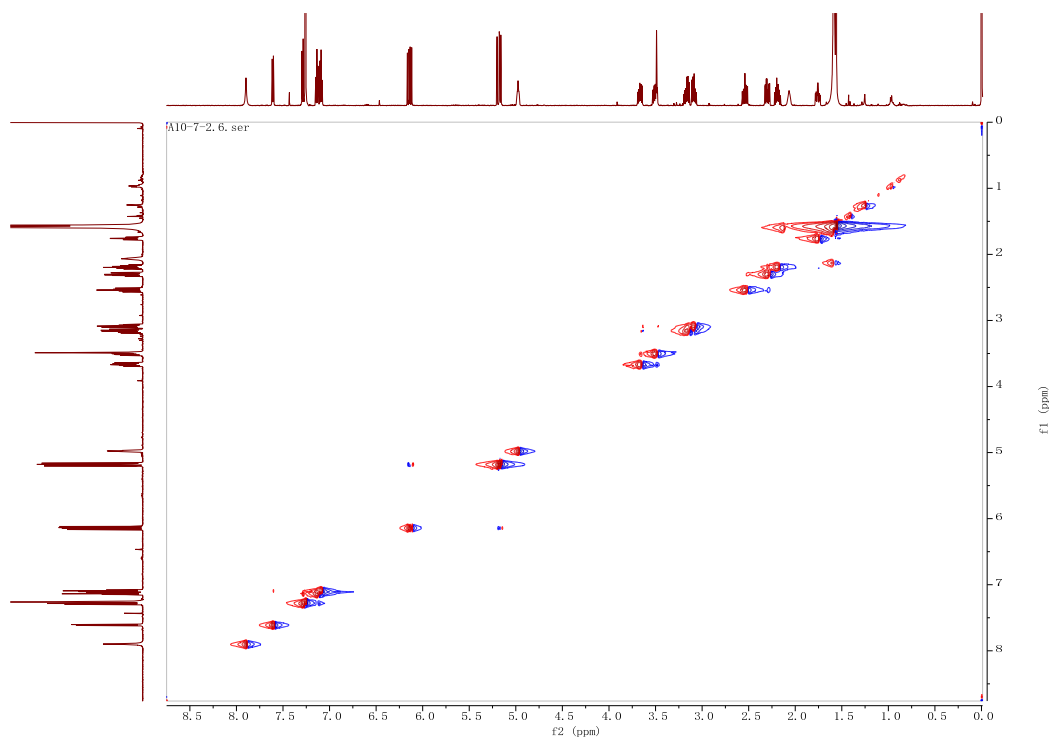


Figure S14. NOESY spectrum (600 MHz, Chloroform-d) of **2**

Item name: 2
Item description:

Channel name: 2: Average Time 0.2492 min : TOF MSe (200-500) 6eV ESI+ : Centroided : Combined

2.05e6

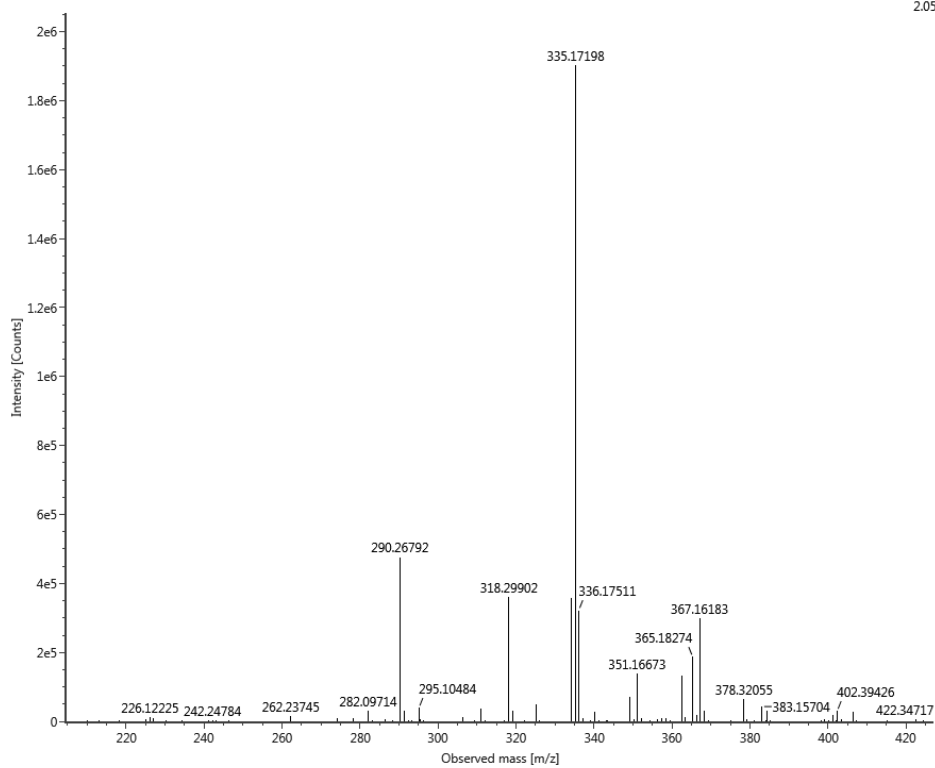


Figure S15. HRESIMS spectrum of **2**

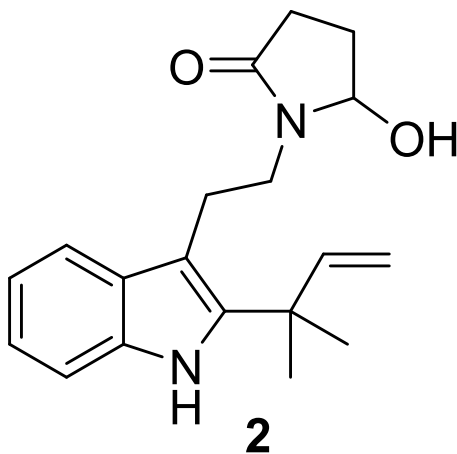


Figure S16. Chemical structure of compound **2**

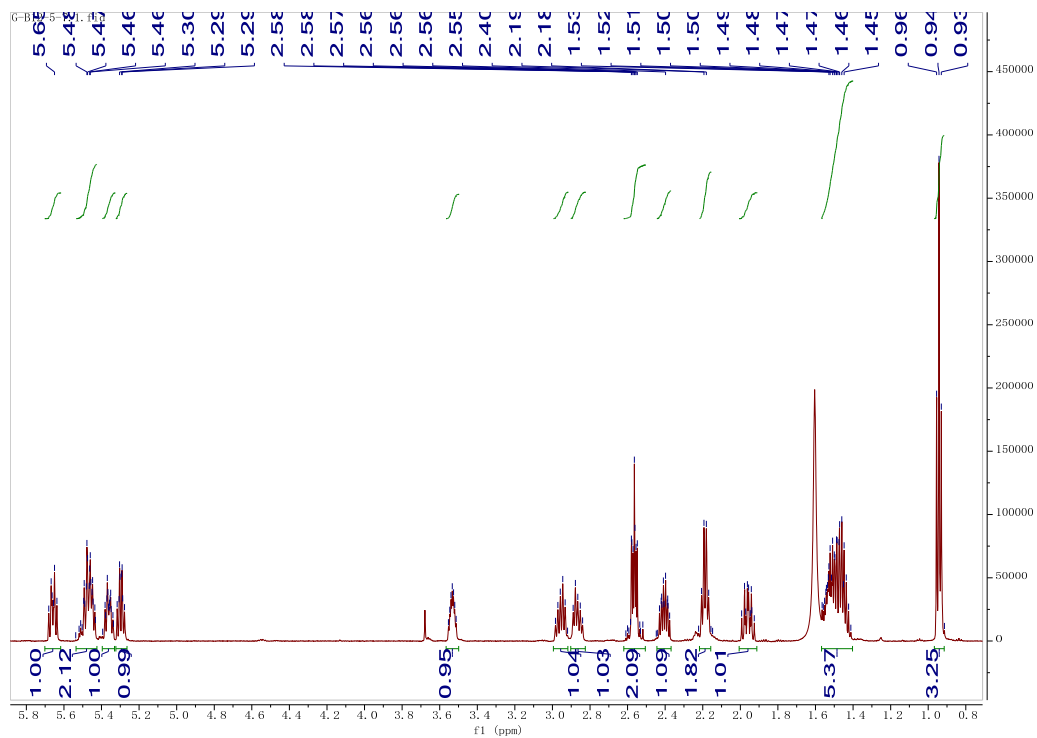


Figure S17. ^1H NMR spectrum (600 MHz, Chloroform-d) of **3**

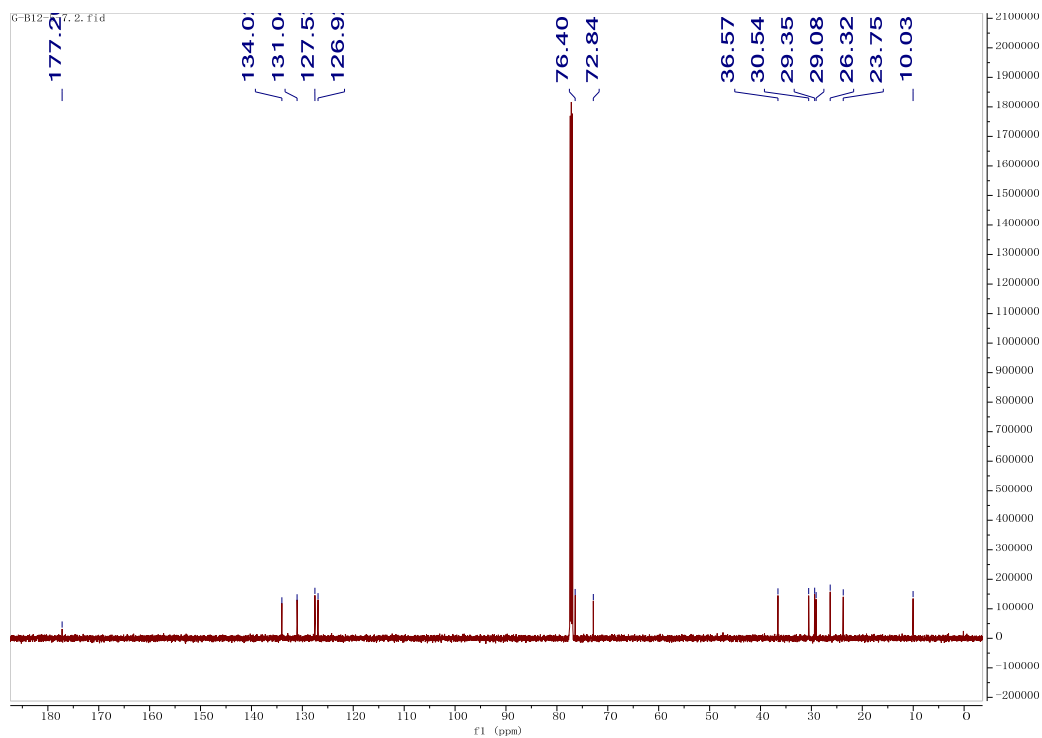


Figure S18. ^{13}C NMR spectrum (600 MHz, Chloroform-d) of **3**

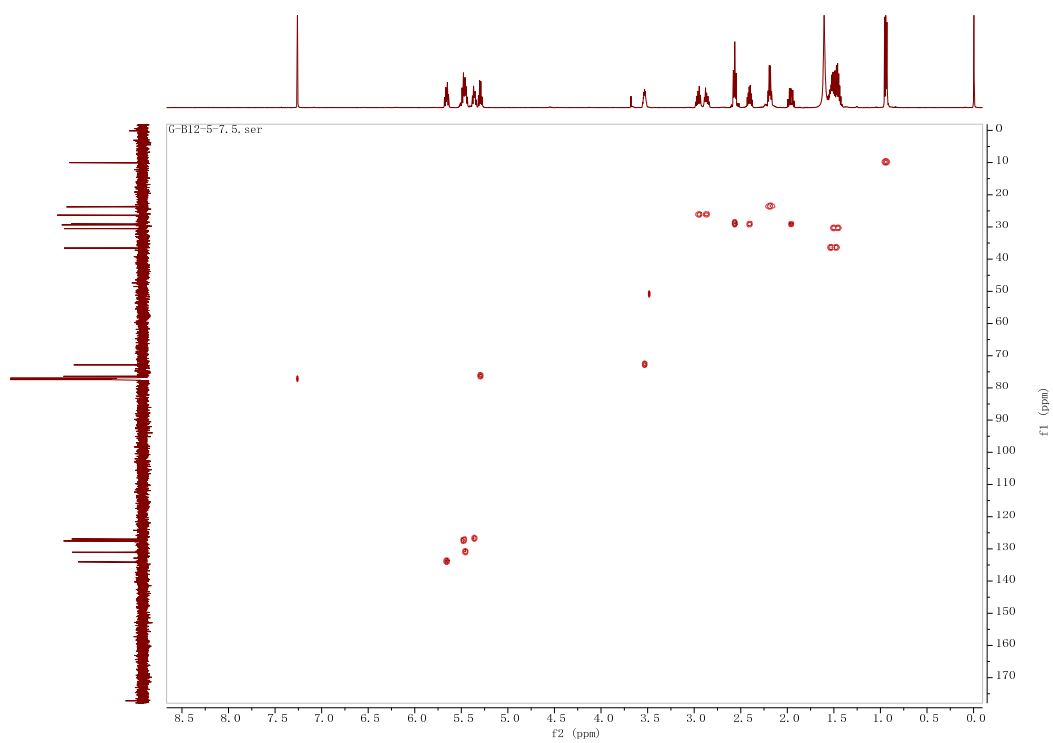


Figure S19. HSQC spectrum (600 MHz, Chloroform-d) of **3**

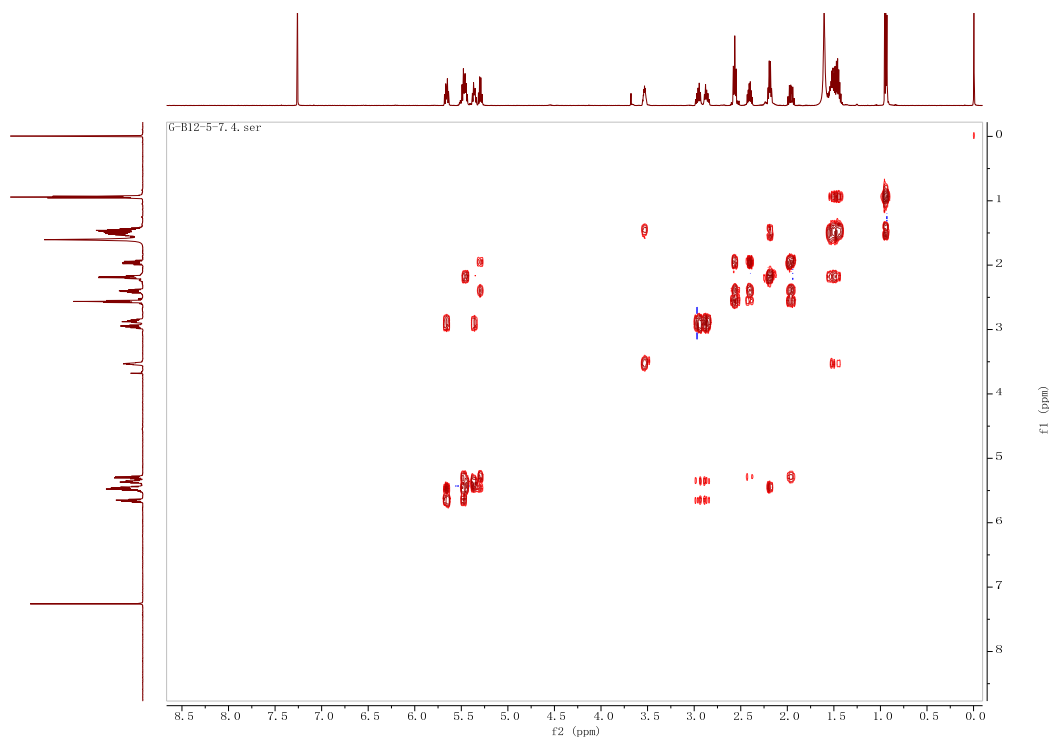


Figure S20. ^1H - ^1H COSY spectrum (600 MHz, Chloroform-d) of **3**

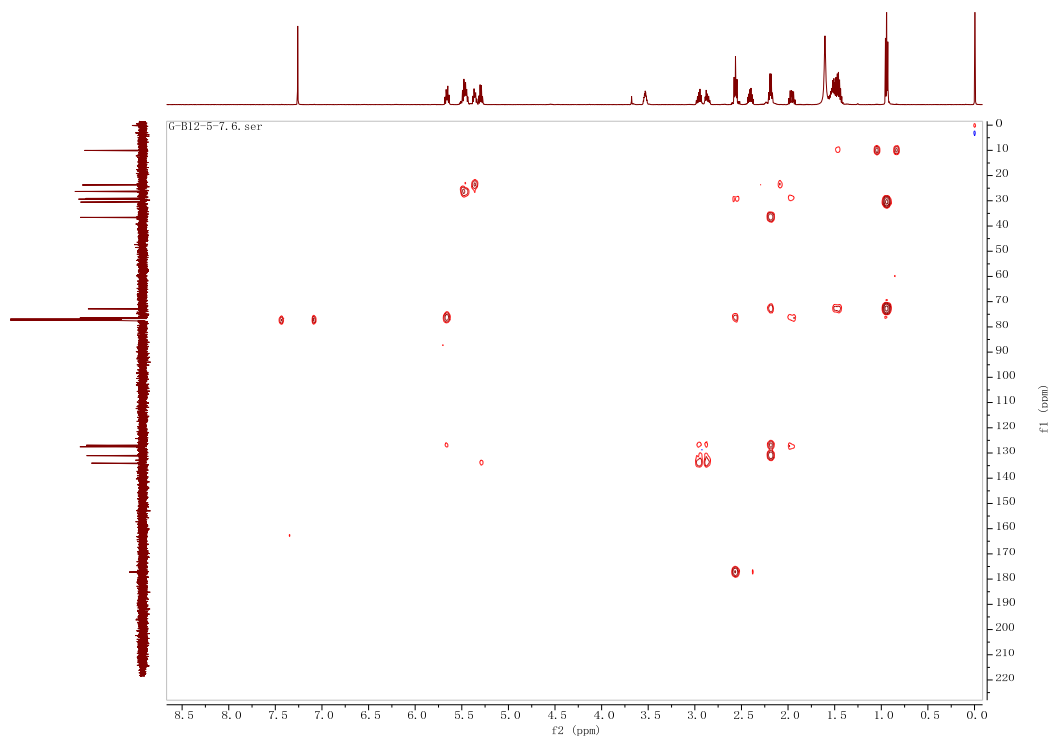


Figure S121. HMBC spectrum (600 MHz, Chloroform-d) of **3**

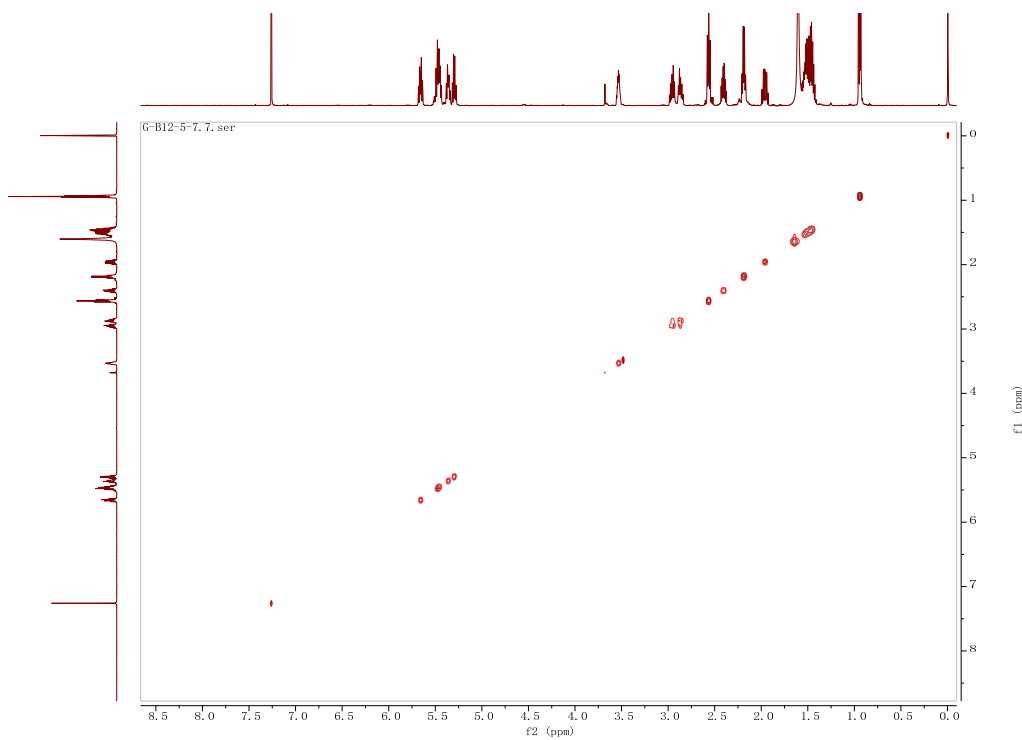


Figure S22. NOESY spectrum (600 MHz, Chloroform-d) of **3**

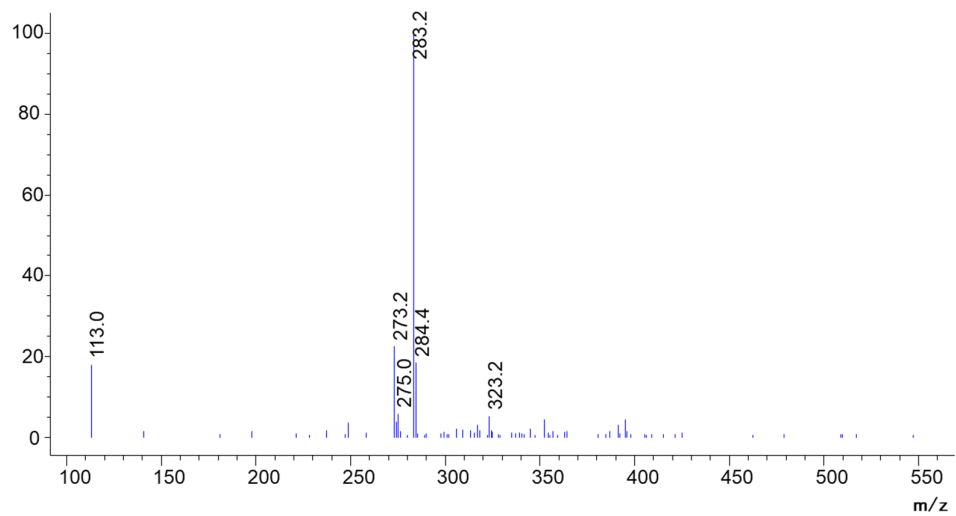


Figure S23. LC-MS spectrum of **3**

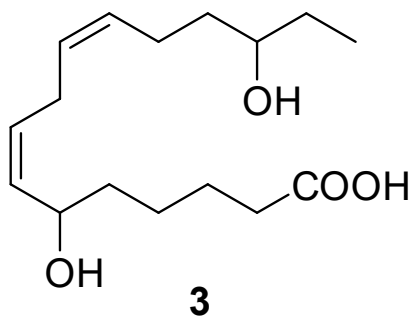


Figure S24. Chemical structure of compounds **3**

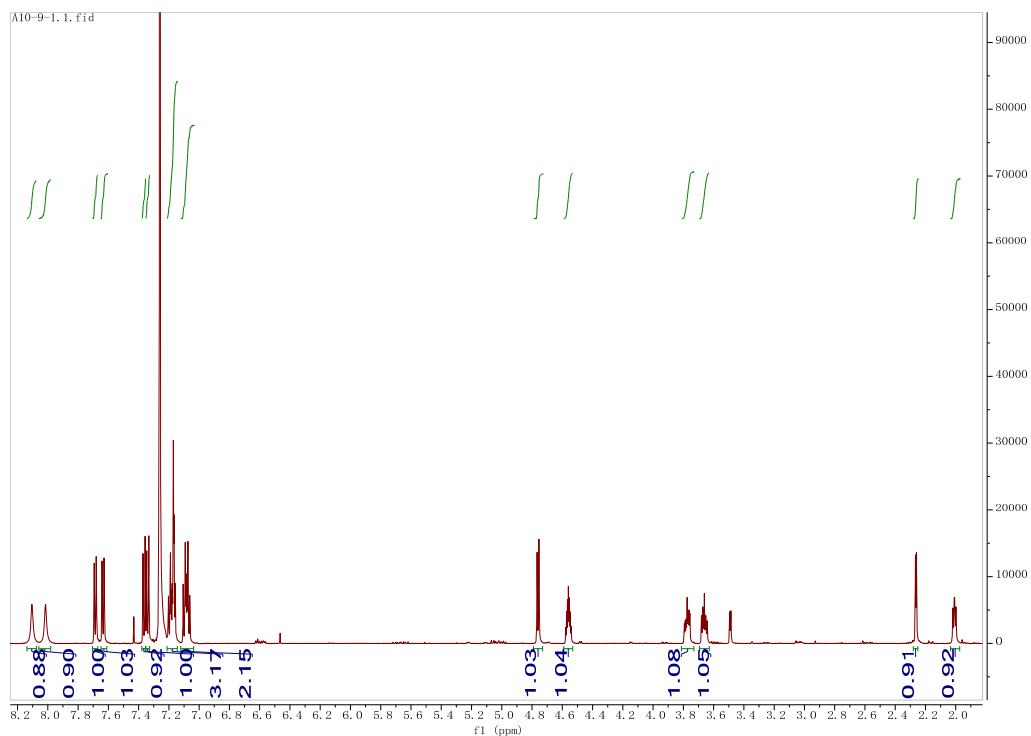


Figure S25. ¹H NMR spectrum (600 MHz, Chloroform-d) of **4**

¹H NMR (600 MHz, Chloroform-d) δ 8.11 (s, 1H), 8.02 (s, 1H), 7.69 (dd, J = 8.0, 1.0 Hz, 1H), 7.63 (dd, J = 8.0, 1.0 Hz, 1H), 7.36 (d, J = 8.2 Hz, 1H), 7.34 (d, J = 8.1 Hz, 1H), 7.22 – 7.15 (m, 3H), 7.12 – 7.05 (m, 2H), 4.76 (d, J = 7.2 Hz, 1H), 4.56 (tt, J = 7.1, 3.6 Hz, 1H), 3.78 (ddd, J = 10.9, 7.2, 3.5 Hz, 1H), 3.66 (ddd, J = 11.4, 6.7, 4.9 Hz, 1H), 2.26 (d, J = 3.9 Hz, 1H), 2.01 (dd, J = 7.3, 5.1 Hz, 1H). Compound **4** was determined by comparison of its spectroscopic data with fusarindole B in the literature [1].

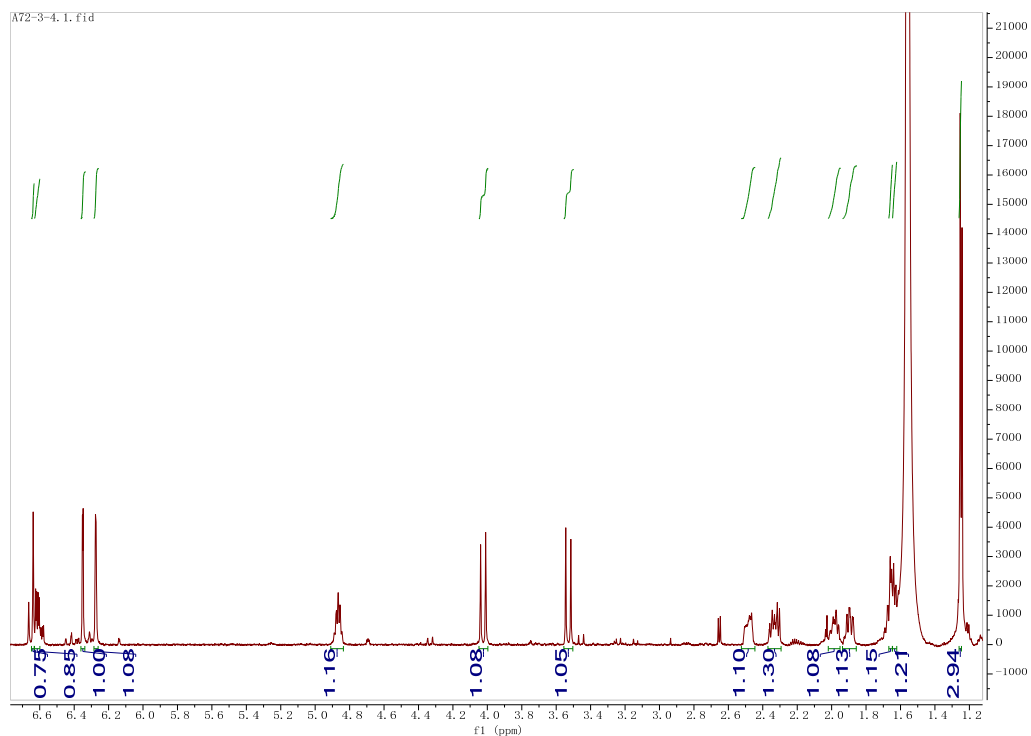


Figure S26. ^1H NMR spectrum (600 MHz, Chloroform-d) of **5**

^1H NMR (600 MHz, Chloroform-d) δ 6.64 (d, $J = 1.5$ Hz, 1H), 6.61 (dd, $J = 8.6, 3.8$ Hz, 1H), 6.35 (d, $J = 2.5$ Hz, 1H), 6.27 (d, $J = 2.6$ Hz, 1H), 4.92 – 4.84 (m, 1H), 4.02 (d, $J = 17.7$ Hz, 1H), 3.53 (d, $J = 17.7$ Hz, 1H), 2.47 (d, $J = 8.5$ Hz, 1H), 2.38 – 2.29 (m, 1H), 1.98 (q, $J = 9.3, 7.6$ Hz, 1H), 1.93 – 1.86 (m, 1H), 1.66 (d, $J = 4.9$ Hz, 1H), 1.65 – 1.63 (m, 1H), 1.25 (s, 3H). Compound **5** was determined by comparison of its spectroscopic data with dehydrocurvularin in the literature [2].

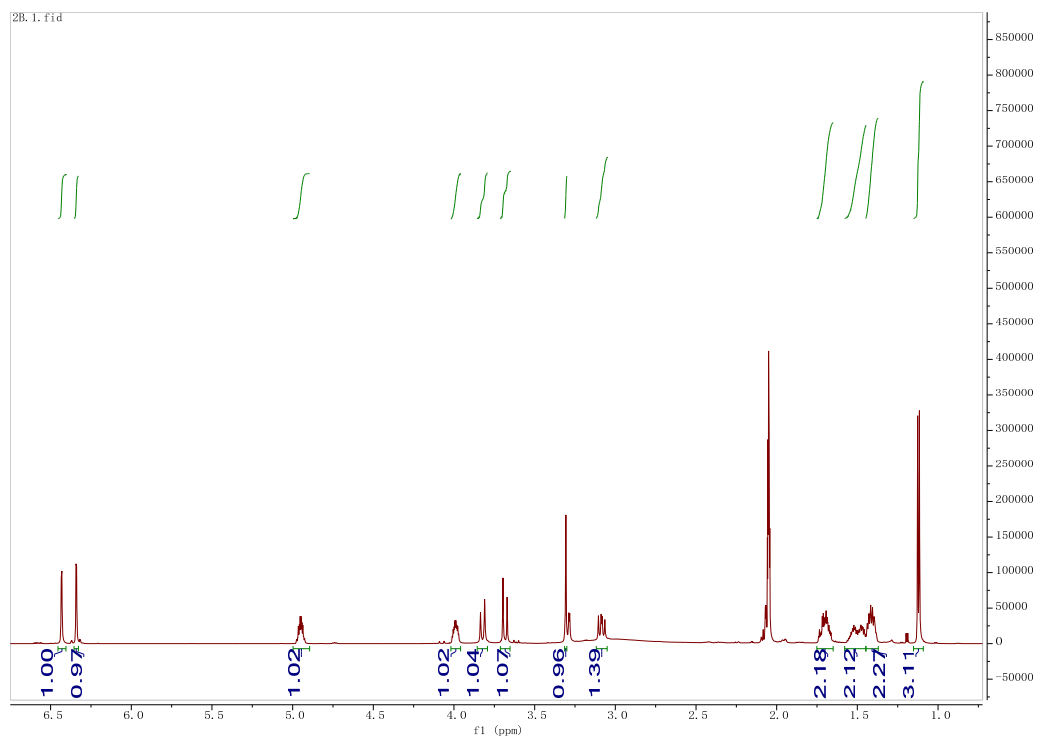


Figure S27. ^1H NMR spectrum (600 MHz, Acetone- d_6) of **6**

^1H NMR (600 MHz, Acetone- d_6) δ 6.43 (d, J = 2.3 Hz, 1H), 6.34 (d, J = 2.3 Hz, 1H), 4.95 (td, J = 6.6, 3.5 Hz, 1H), 3.99 (ddt, J = 10.4, 7.0, 3.6 Hz, 1H), 3.82 (d, J = 15.4 Hz, 1H), 3.68 (d, J = 15.4 Hz, 1H), 3.31 (d, J = 3.2 Hz, 1H), 3.08 (dd, J = 13.9, 10.0 Hz, 1H), 1.81 – 1.33 (m, 6H), 1.12 (d, J = 6.4 Hz, 3H). Compound **6** was determined by comparison of its spectroscopic data with hydroxycurvularin in the literature [3].

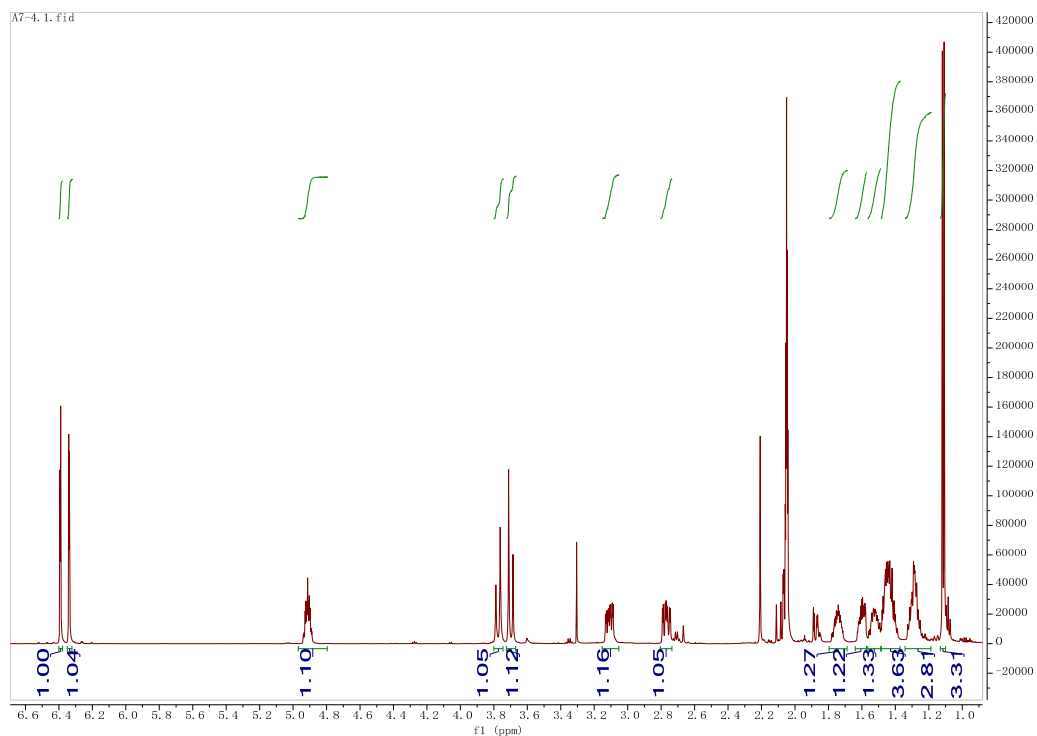


Figure S28. ^1H NMR spectrum (600 MHz, Acetone- d_6) of **7**

^1H NMR (600 MHz, Acetone- d_6) δ 6.39 (d, J = 2.3 Hz, 1H), 6.34 (d, J = 2.3 Hz, 1H), 4.91 (dq, J = 9.0, 6.3, 2.8 Hz, 1H), 3.77 (d, J = 15.7 Hz, 1H), 3.70 (d, J = 15.6 Hz, 1H), 3.11 (ddd, J = 15.5, 8.6, 3.0 Hz, 1H), 2.77 (ddd, J = 15.5, 9.8, 3.0 Hz, 1H), 1.80 – 1.68 (m, 1H), 1.60 (ddt, J = 14.3, 7.9, 3.2 Hz, 1H), 1.56 – 1.49 (m, 1H), 1.49 – 1.37 (m, 3H), 1.35 – 1.21 (m, 2H), 1.11 (d, J = 6.3 Hz, 3H). Compound **7** was determined by comparison of its spectroscopic data with curvularin in the literature [4].

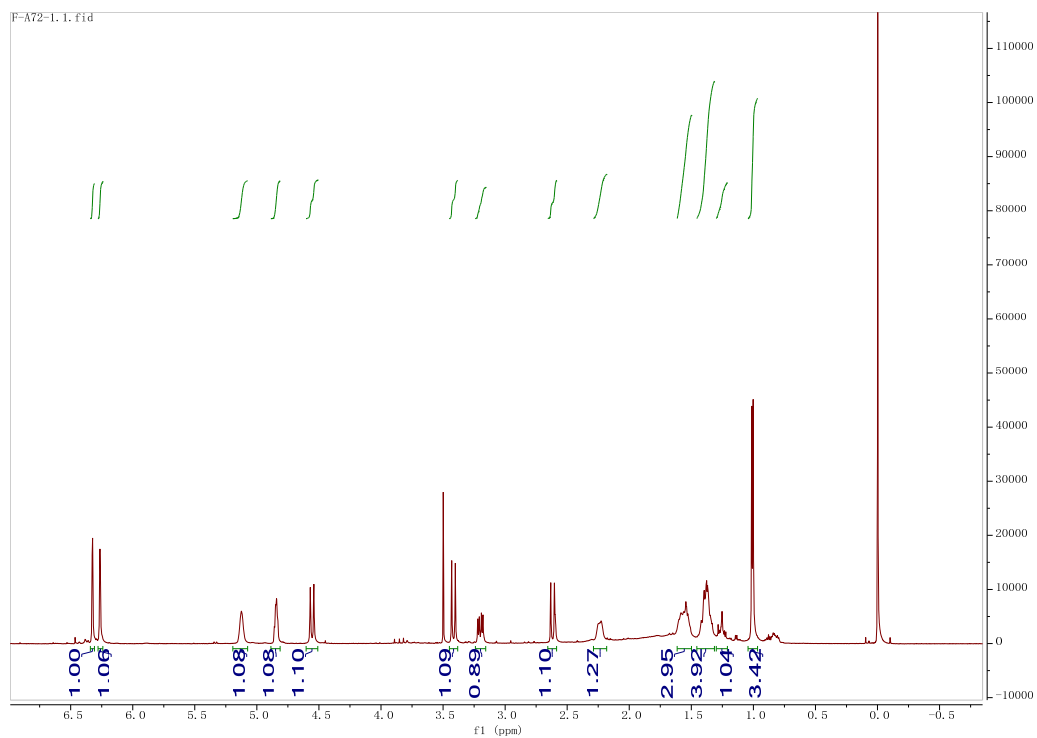


Figure S29. ¹H NMR spectrum (600 MHz, Chloroform-d) of **8**

¹H NMR (600 MHz, Chloroform-d) δ 6.32 (d, J = 2.3 Hz, 1H), 6.28 – 6.24 (m, 1H), 5.12 (s, 1H), 4.85 (q, J = 6.1, 5.6 Hz, 1H), 4.56 (d, J = 17.4 Hz, 1H), 3.42 (d, J = 17.4 Hz, 1H), 3.20 (dd, J = 17.7, 7.6 Hz, 1H), 2.62 (d, J = 17.7 Hz, 1H), 2.23 (s, 1H), 1.66 – 1.49 (m, 2H), 1.44 – 1.31 (m, 3H), 1.30 – 1.22 (m, 1H), 1.01 (d, J = 6.6 Hz, 3H). Compound **8** was determined by comparison of its spectroscopic data with curvulopyran in the literature [5].

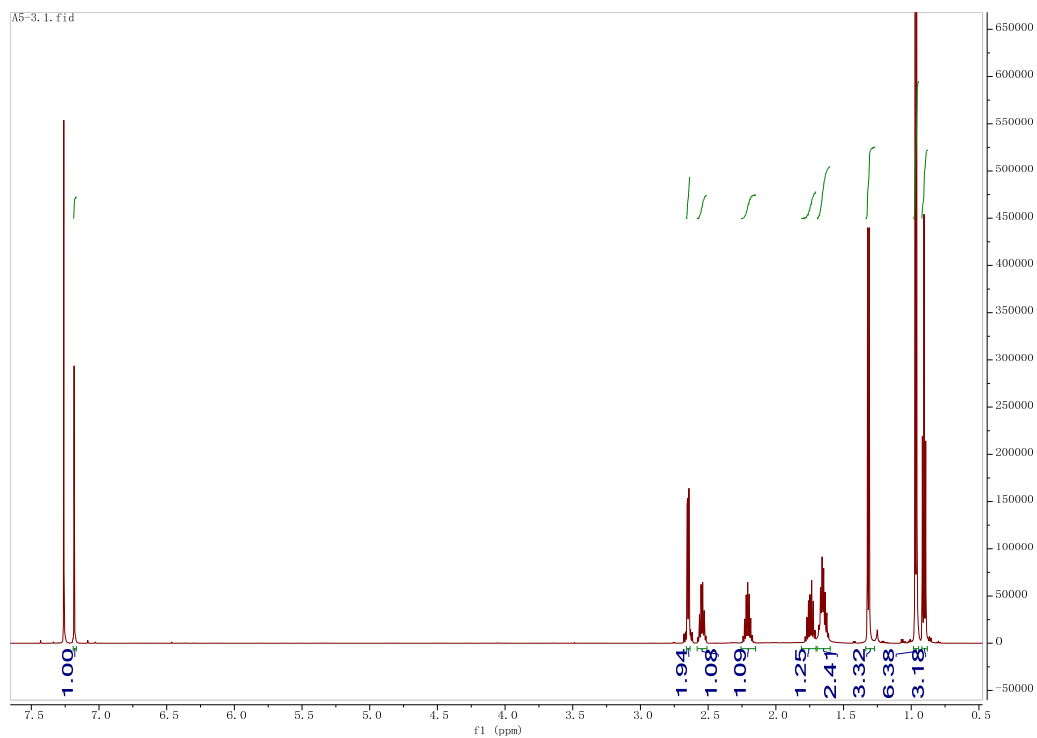


Figure S30. ^1H NMR spectrum (600 MHz, Chloroform-d) of **9**

^1H NMR (600 MHz, Chloroform-d) δ 7.18 (s, 1H), 2.65 (dd, $J = 7.1, 1.9$ Hz, 2H), 2.55 (h, $J = 7.1$ Hz, 1H), 2.21 (dh, $J = 13.5, 6.7$ Hz, 1H), 1.75 (dt, $J = 13.7, 7.5$ Hz, 1H), 1.65 (dp, $J = 14.4, 7.3$ Hz, 2H), 1.32 (d, $J = 7.0$ Hz, 3H), 0.97 (d, $J = 6.7$ Hz, 6H), 0.91 (t, $J = 7.4$ Hz, 3H). Compound **9** was determined by comparison of its spectroscopic data with (S)-6-(sec-butyl)-3-isobutylpyrazin-2(1H)-one in the literature [6].

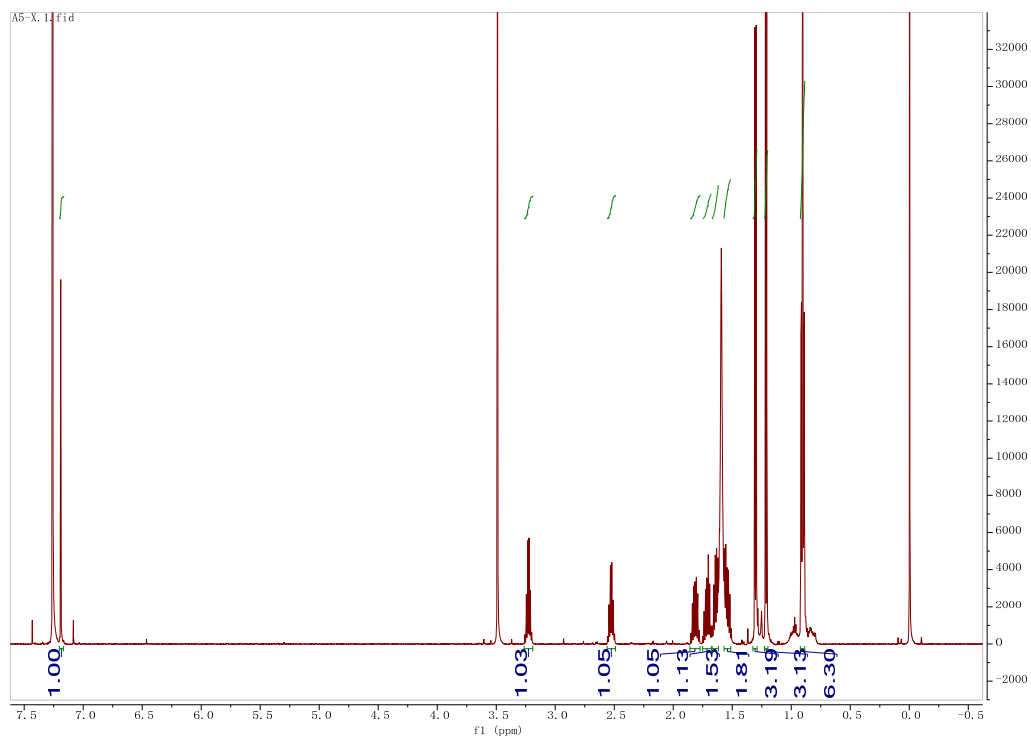


Figure S31. ^1H NMR spectrum (600 MHz, Chloroform-d) of **10**

^1H NMR (600 MHz, Chloroform-d) δ 7.19 (s, 1H), 3.23 (h, $J = 6.9$ Hz, 1H), 2.53 (h, $J = 7.1$ Hz, 1H), 1.87 – 1.77 (m, 1H), 1.71 (dt, $J = 13.8, 7.5$ Hz, 1H), 1.64 (dt, $J = 14.1, 7.2$ Hz, 1H), 1.54 (dt, $J = 13.4, 7.3$ Hz, 1H), 1.30 (d, $J = 7.0$ Hz, 3H), 1.21 (d, $J = 6.9$ Hz, 3H), 0.90 (td, $J = 7.4, 2.9$ Hz, 6H). Compound **10** was determined by comparison of its spectroscopic data with 3,6-di-sec-butyl-2(1H)-pyrazinone in the literature [6].

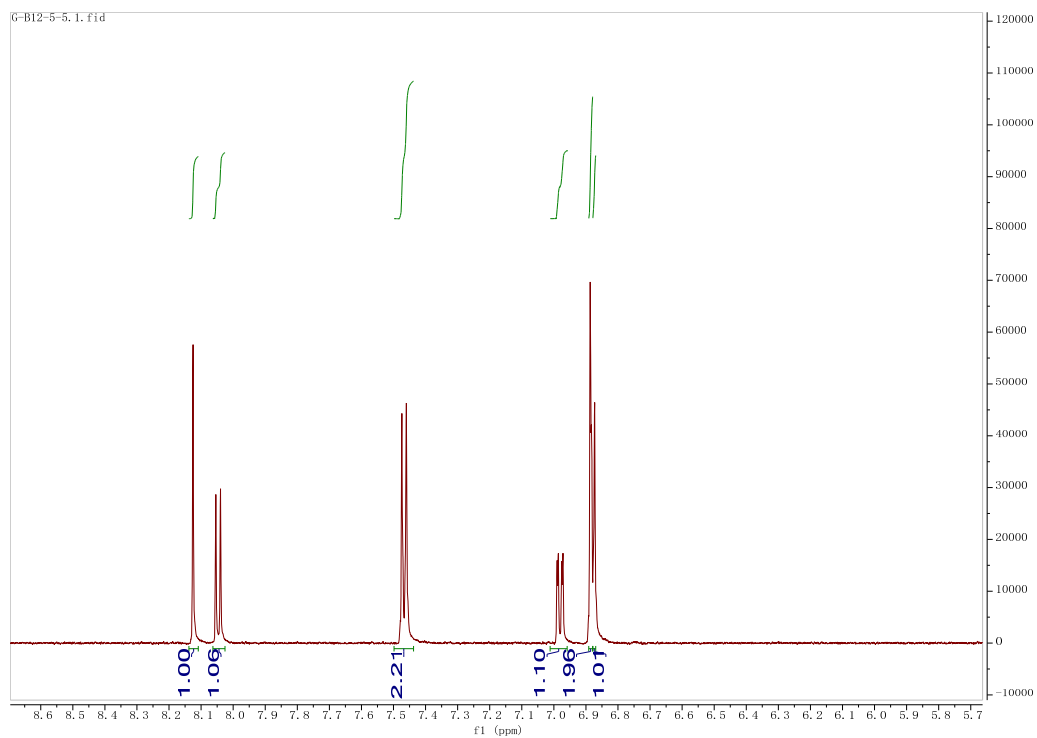


Figure S32. ^1H NMR spectrum (600 MHz, Acetone-d) of **11**

^1H NMR (600 MHz, Acetone- d_6) δ 8.13 (s, 1H), 8.05 (d, $J = 8.7$ Hz, 1H), 7.47 (d, $J = 8.5$ Hz, 2H), 6.98 (dd, $J = 8.8, 2.3$ Hz, 1H), 6.88 (d, $J = 2.6$ Hz, 2H), 6.87 (d, $J = 2.3$ Hz, 1H). Compound **11** was determined by comparison of its spectroscopic data with daidzein in the literature [7].

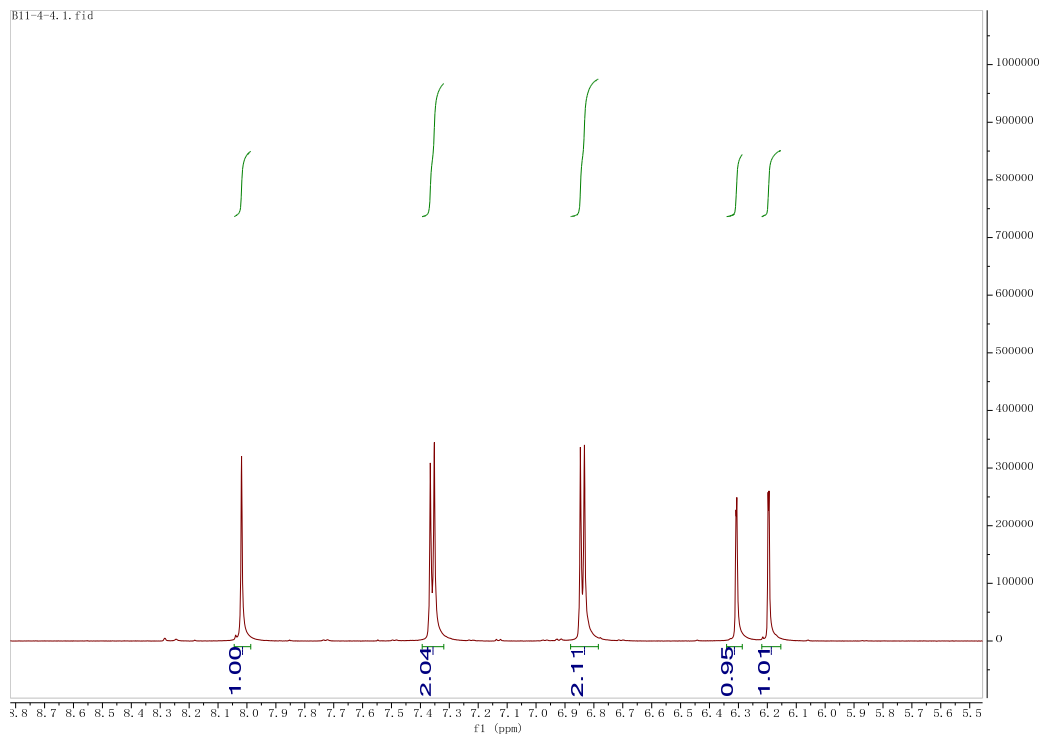


Figure S33.1H NMR spectrum (600 MHz, Methanol-d4) of **12**

^1H NMR (600 MHz, Methanol-d4) δ 8.02 (s, 1H), 7.36 (d, J = 8.3 Hz, 2H), 6.84 (d, J = 8.3 Hz, 2H), 6.31 (d, J = 2.1 Hz, 1H), 6.20 (d, J = 2.1 Hz, 1H). Compound **12** was determined by comparison of its spectroscopic data with genistein in the literature [8].

Supplementary References

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8. M. A. Selepe; S. Drewes; F. V. van Heerden. van Heerden, et al. *J. Nat. Prod.* **2010**, *73*, 1680–1685. doi: 10.1021/np100407n.