

## SUPPLEMENTARY MATERIAL

### Two new flavans from the roots of *Dianella ensifolia* (L.) DC

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Abstract: Two new flavans, named (2*S*)-2',4'-dihydroxy-7-methoxy-8-methylflavan (**1**) and (2*S*)-2'-hydroxy-4',7-dimethoxy-8-methylflavan (**2**) were isolated from the roots of *Dianella ensifolia*. Their structures were elucidated by extensive spectroscopic measurements and comparison with data reported in literatures. Compounds **1** and **2** displayed cytotoxic effects against cancer cell lines MDA-MB-231, B16-F10, HCT116 and A549.

Keywords: *Dianella ensifolia*; flavans; cytotoxicity

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## Supplementary data for the paper

- Figure S1  $^1\text{H}$  NMR spectrum of compound **1** in DMSO- $d_6$  (400 MHz).
- Figure S2  $^{13}\text{C}$  NMR spectrum of compound **1** in DMSO- $d_6$  (100 MHz).
- Figure S3 DEPT-135 spectrum of compound **1** in DMSO- $d_6$  (100 MHz).
- Figure S4  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1** in DMSO- $d_6$ .
- Figure S5 HSQC spectrum of compound **1** in DMSO- $d_6$ .
- Figure S6 HMBC spectrum of compound **1** in DMSO- $d_6$ .
- Figure S7 NOESY spectrum of compound **1** in DMSO- $d_6$ .
- Figure S8 HR-ESI-MS of **1**.
- Figure S9 UV spectrum of **1** in  $\text{CH}_3\text{OH}$ .
- Figure S10 IR (KBr disc) spectrum of **1**.
- Figure S11 Key HMBC correlations (arrows) and COSY (bold lines) of compound **1**.
- Figure S12  $^1\text{H}$  NMR spectrum of compound **2** in DMSO- $d_6$  (400 MHz).
- Figure S13  $^{13}\text{C}$  NMR spectrum of compound **2** in DMSO- $d_6$  (100 MHz).
- Figure S14 DEPT-135 spectrum of compound **2** in DMSO- $d_6$  (100 MHz).
- Figure S15  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **2** in DMSO- $d_6$ .
- Figure S16 HSQC spectrum of compound **2** in DMSO- $d_6$ .
- Figure S17 HMBC spectrum of compound **2** in DMSO- $d_6$ .
- Figure S18 NOESY spectrum of compound **2** in DMSO- $d_6$ .
- Figure S19 HR-ESI-MS of **2**.
- Figure S20 UV spectrum of **2** in  $\text{CH}_3\text{OH}$ .
- Figure S21 IR (KBr disc) spectrum of **2**.
- Figure S22 Key HMBC correlations (arrows) and COSY (bold lines) of compound **2**.

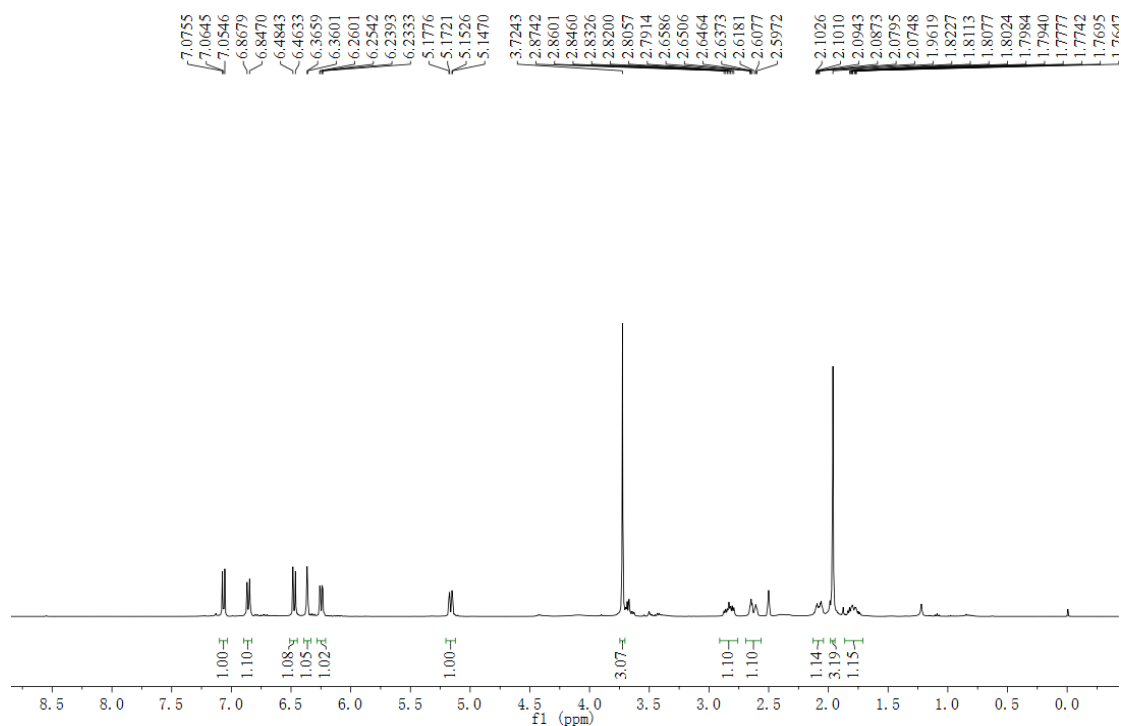


Figure S1 <sup>1</sup>H NMR spectrum of compound **1** in DMSO-*d*<sub>6</sub> (400 MHz).

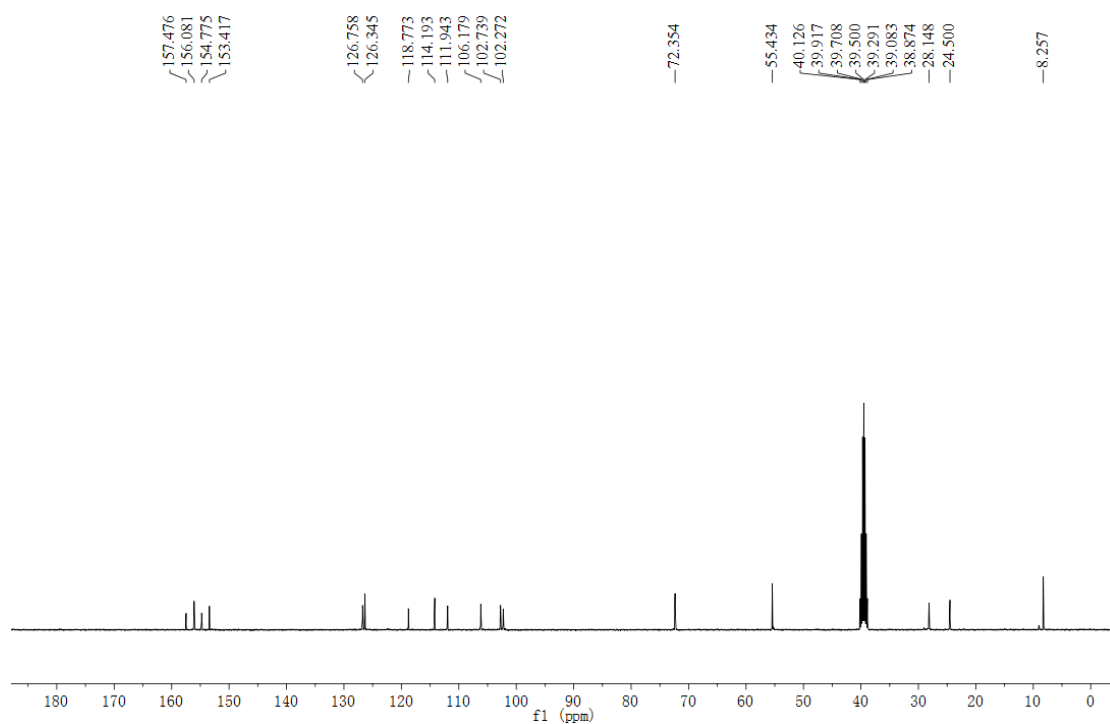


Figure S2 <sup>13</sup>C NMR spectrum of compound **1** in DMSO-*d*<sub>6</sub> (100 MHz).



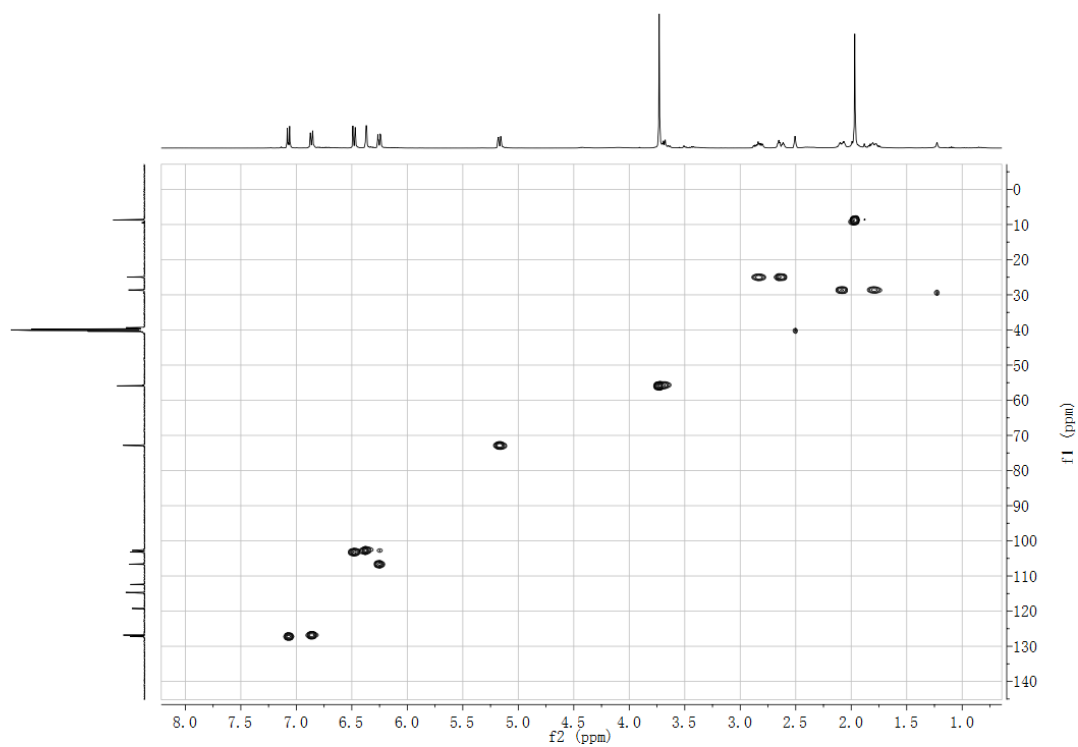


Figure S5 HSQC spectrum of compound **1** in DMSO- $d_6$ .

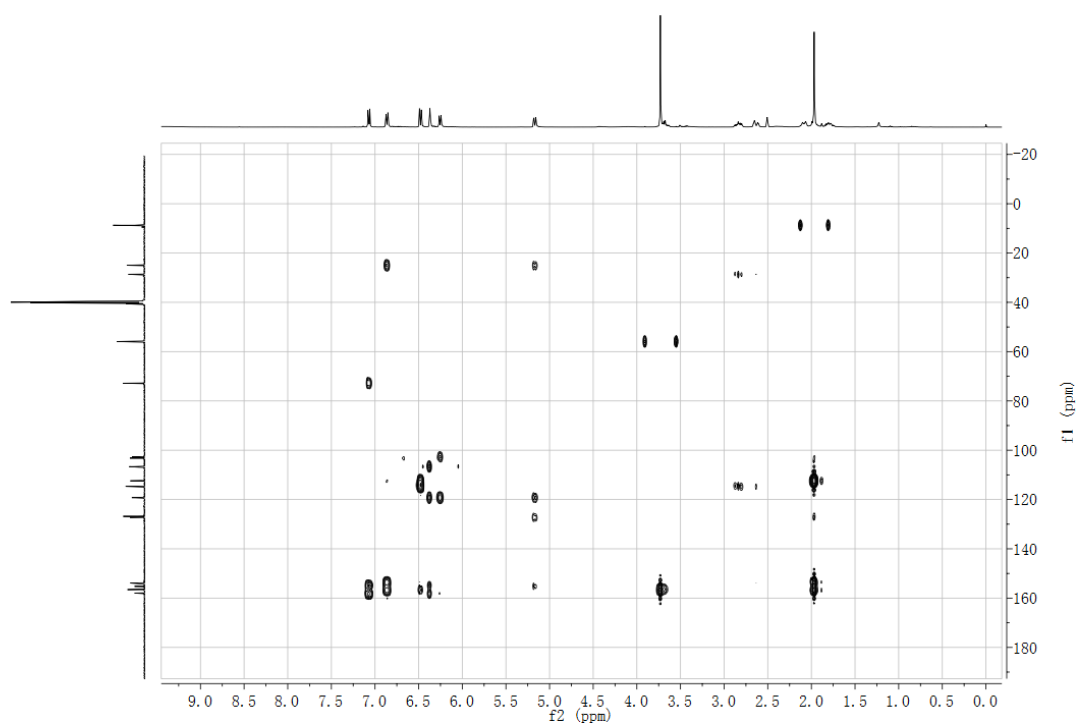


Figure S6 HMBC spectrum of compound **1** in DMSO- $d_6$ .

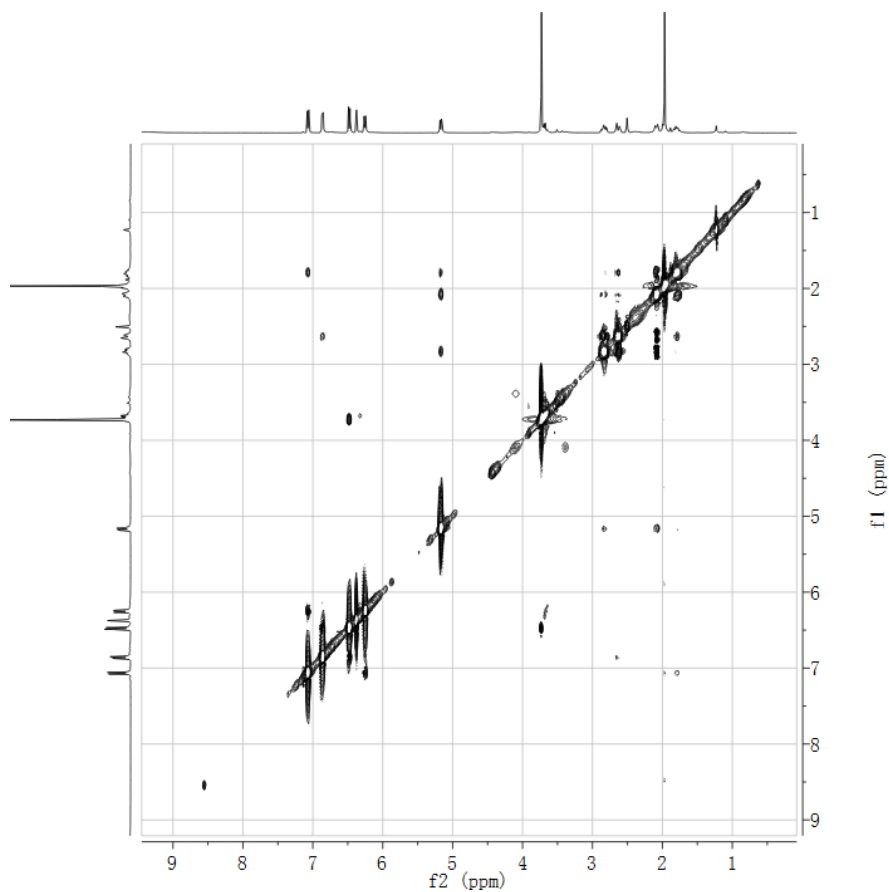


Figure S7 NOESY spectrum of compound **1** in DMSO- $d_6$ .

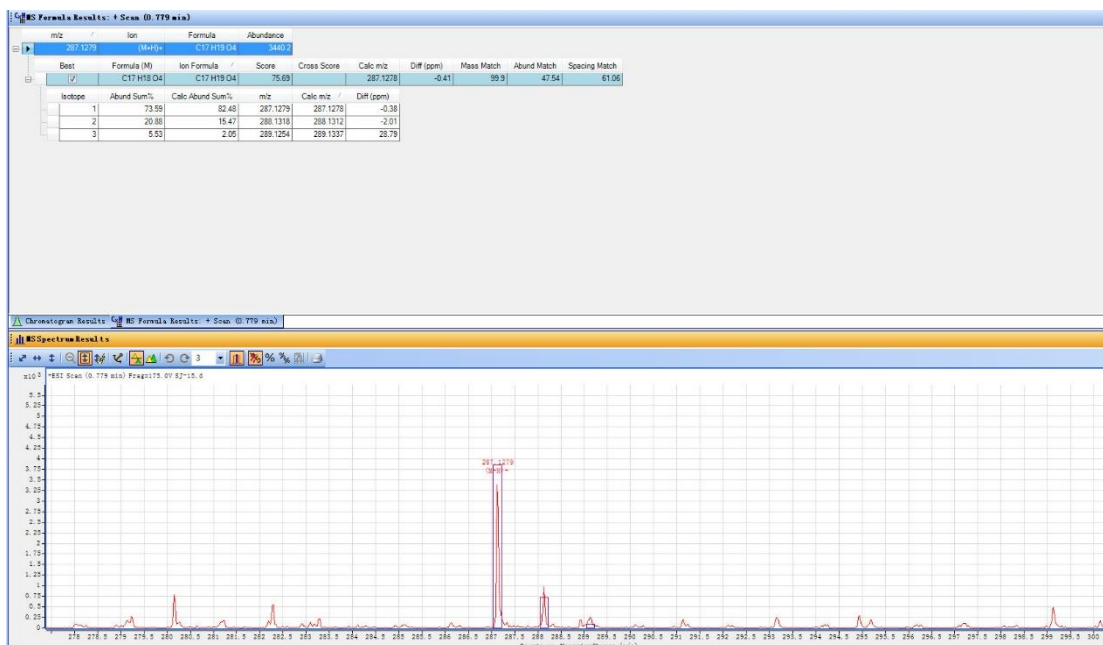


Figure S8 HR-ESI-MS of **1**.

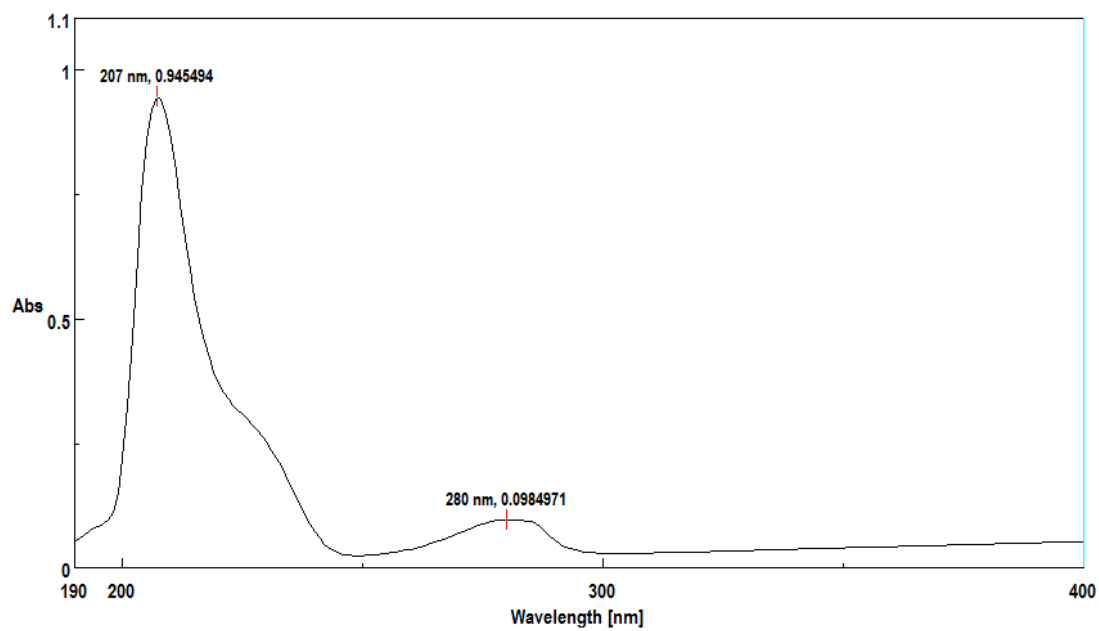


Figure S9 UV spectrum of **1** in CH<sub>3</sub>OH.

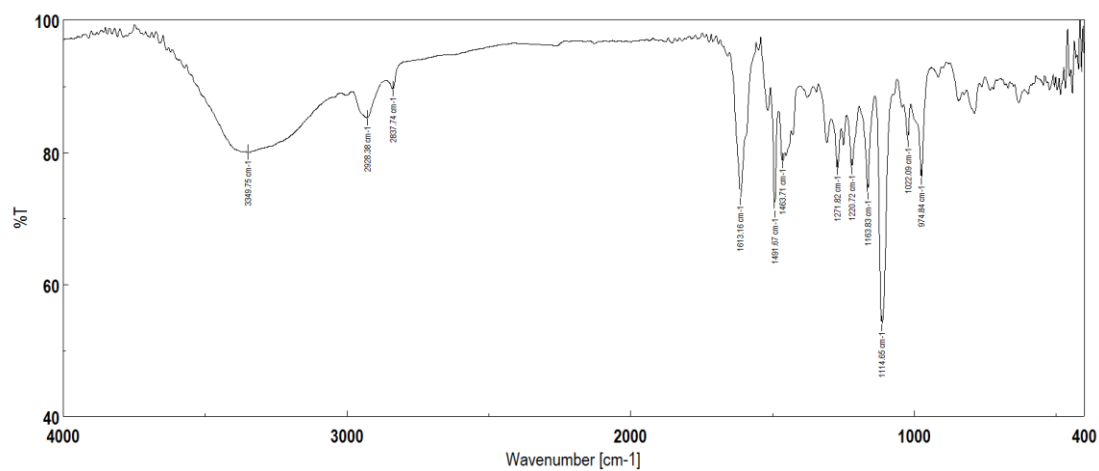


Figure S10 IR (KBr disc) spectrum of **1**.

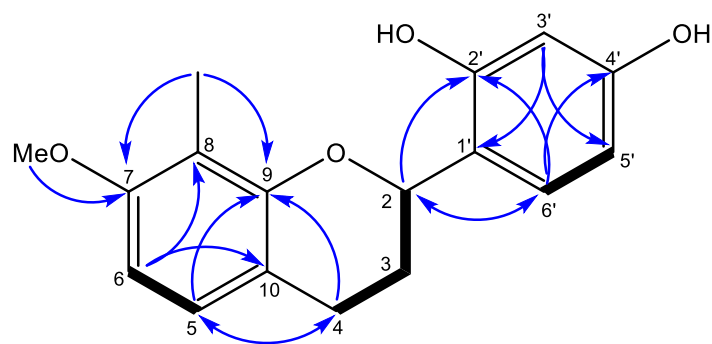
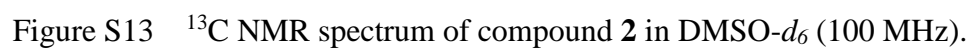
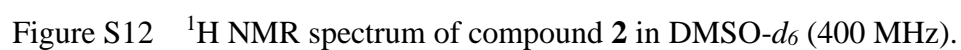


Figure S11 Key HMBC correlations (arrows) and COSY (bold lines) of compound **1**.





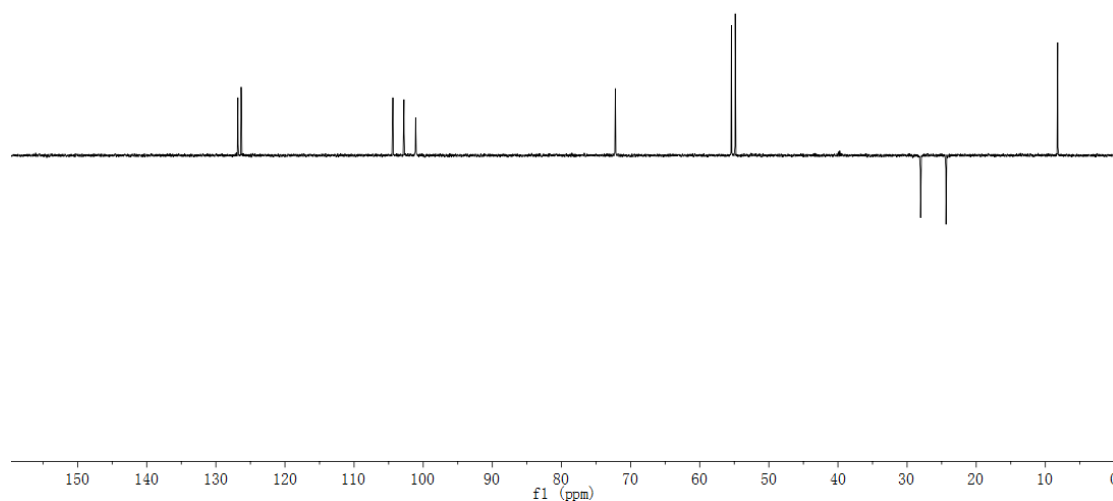


Figure S14 DEPT-135 spectrum of compound **2** in DMSO- $d_6$  (100 MHz).

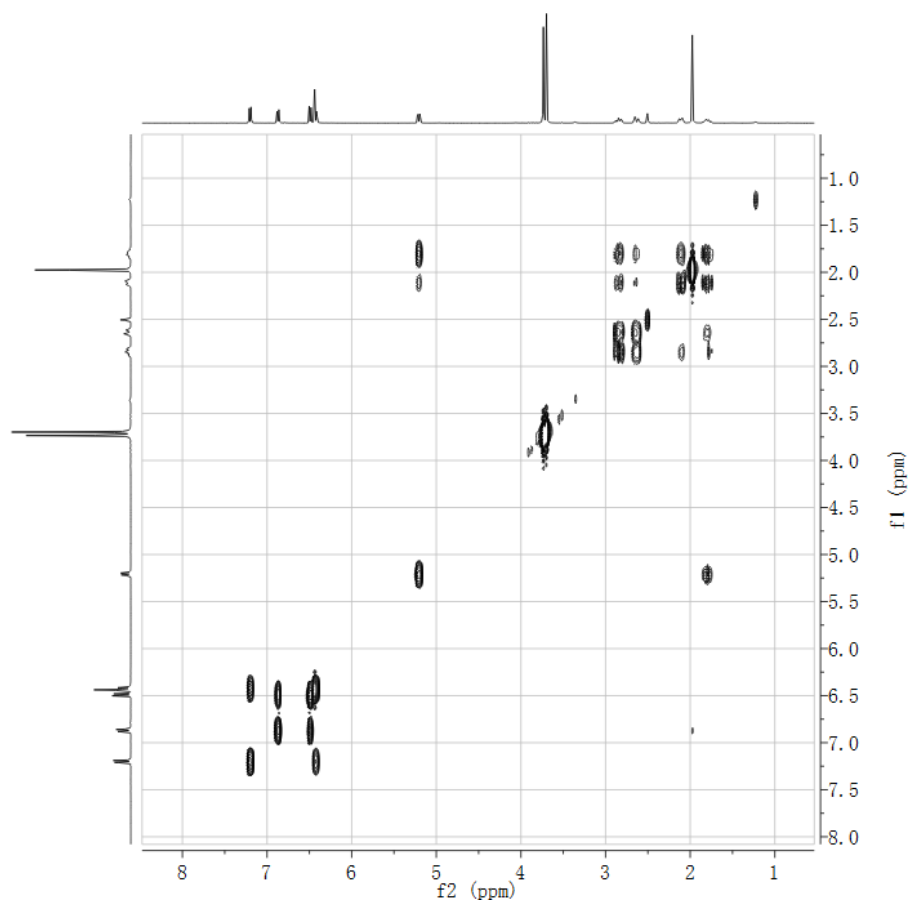


Figure S15  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **2** in DMSO- $d_6$ .

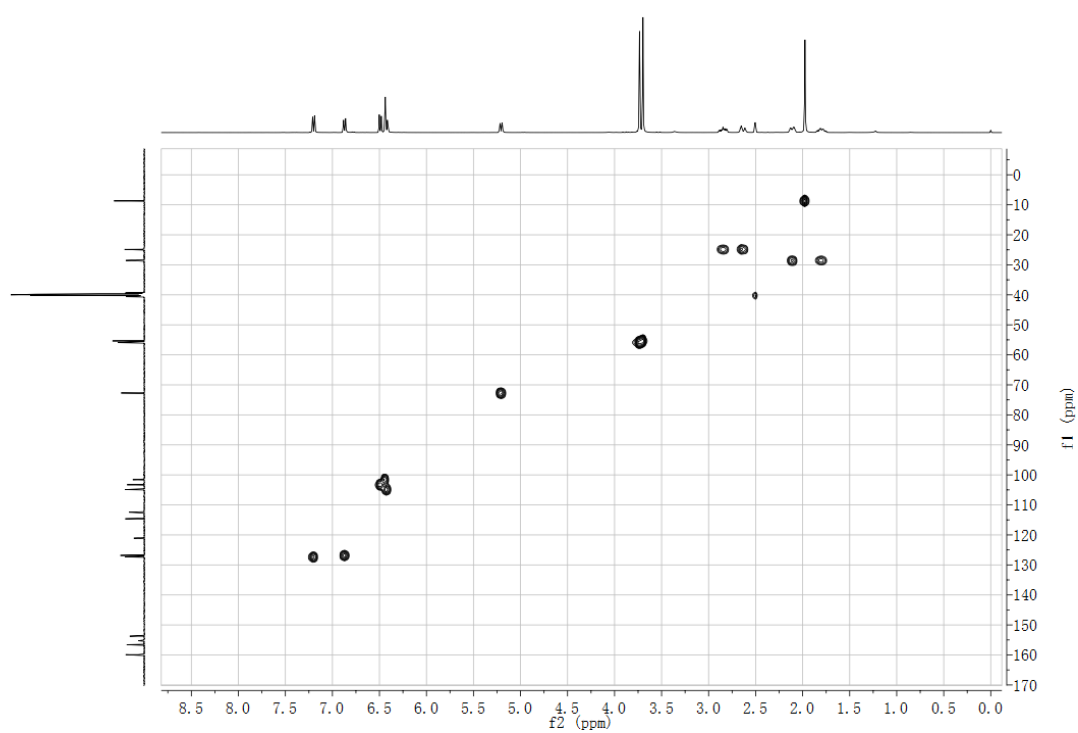


Figure S16 HSQC spectrum of compound **2** in DMSO-*d*<sub>6</sub>.

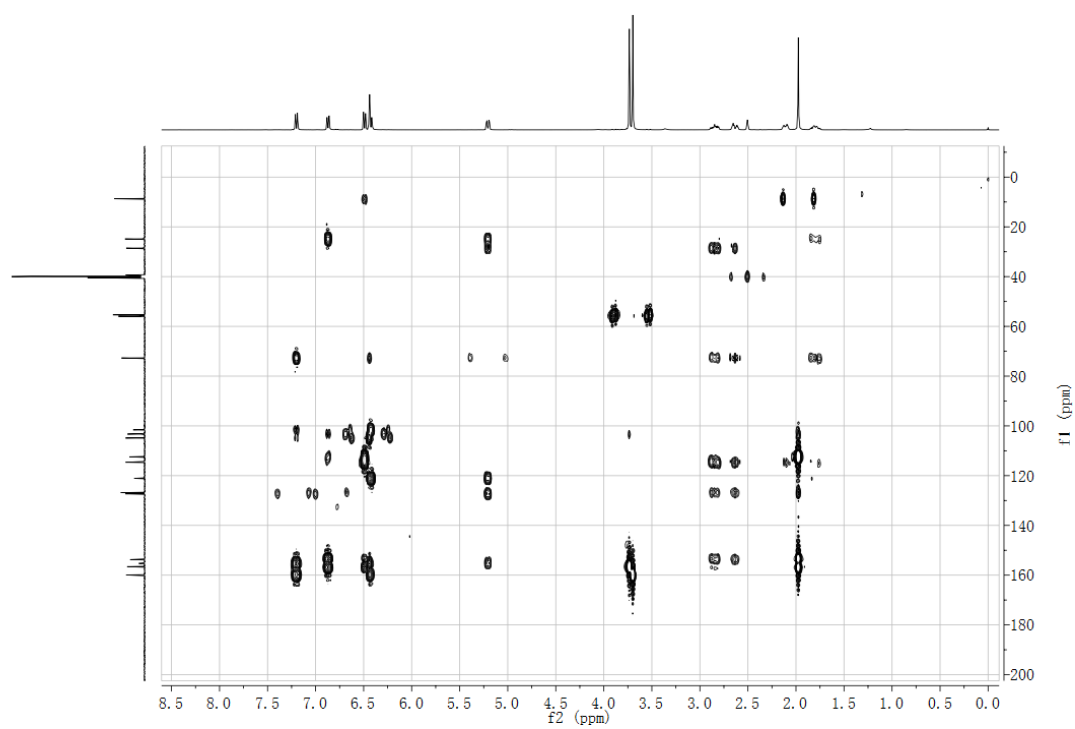


Figure S17 HMBC spectrum of compound **2** in DMSO-*d*<sub>6</sub>.

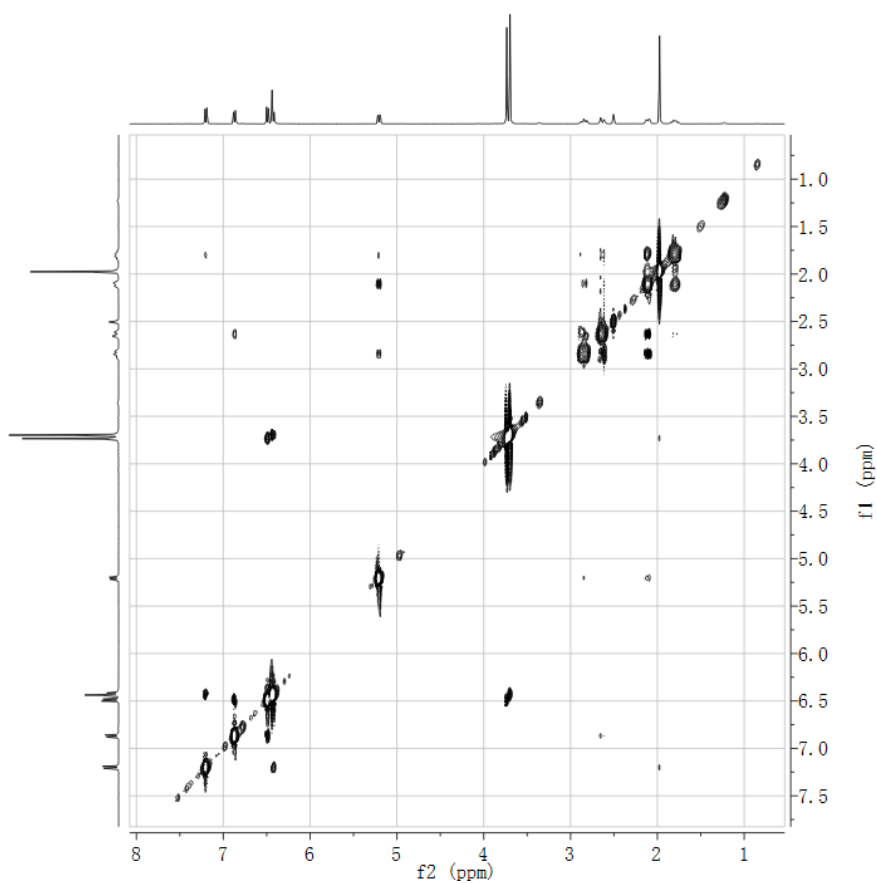


Figure S18 NOESY spectrum of compound **2** in DMSO-*d*<sub>6</sub>.

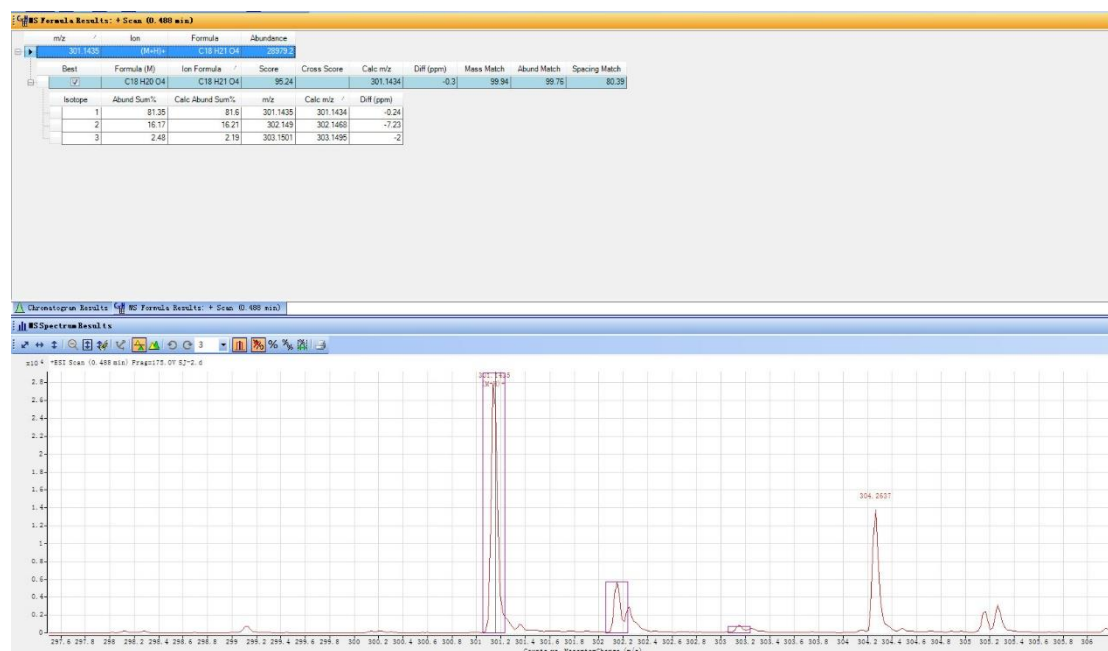


Figure S19 HR-ESI-MS of **2**.

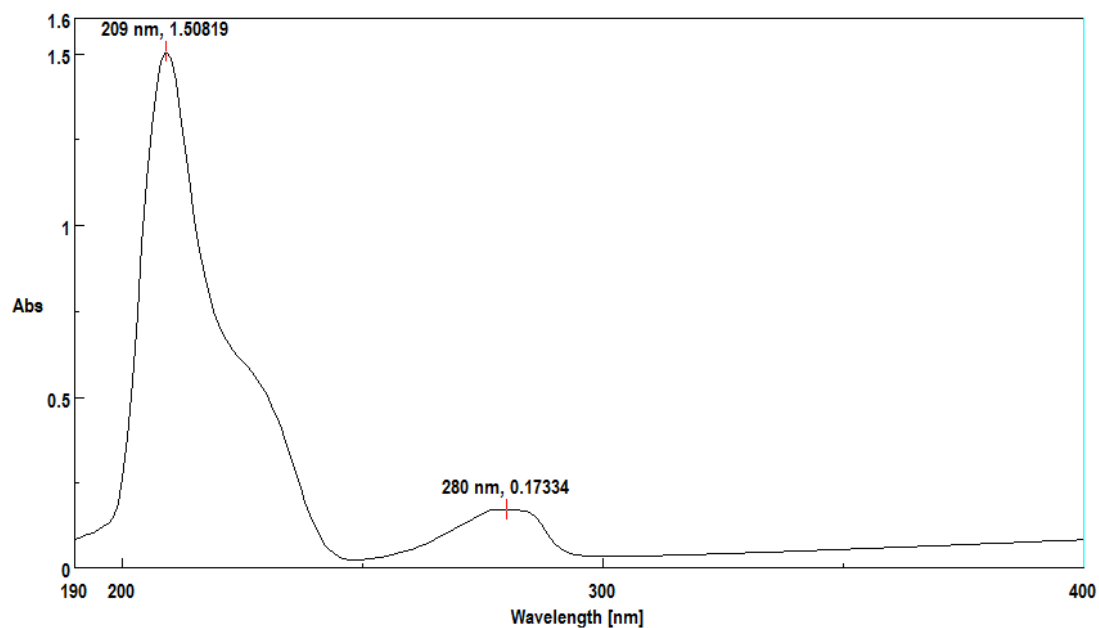


Figure S20 UV spectrum of **2** in CH<sub>3</sub>OH.

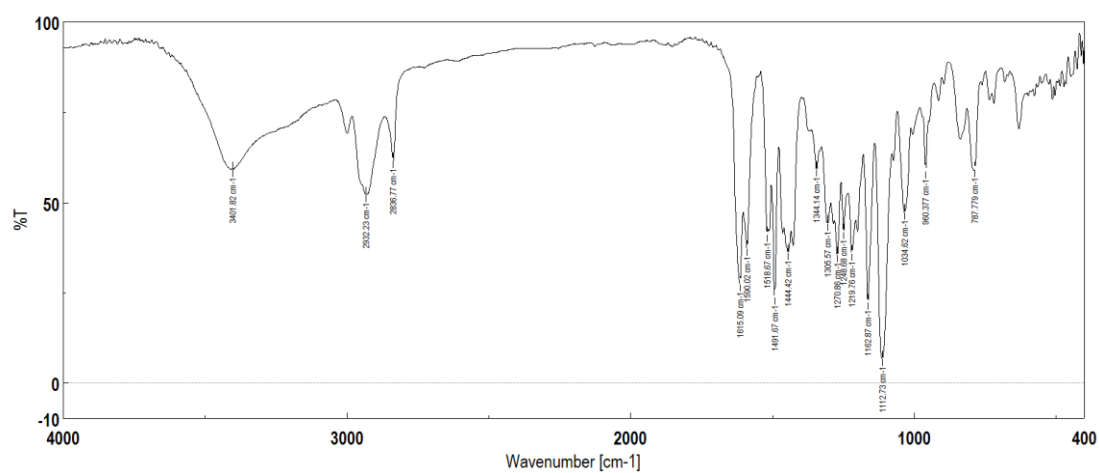


Figure S21 IR (KBr disc) spectrum of **2**.

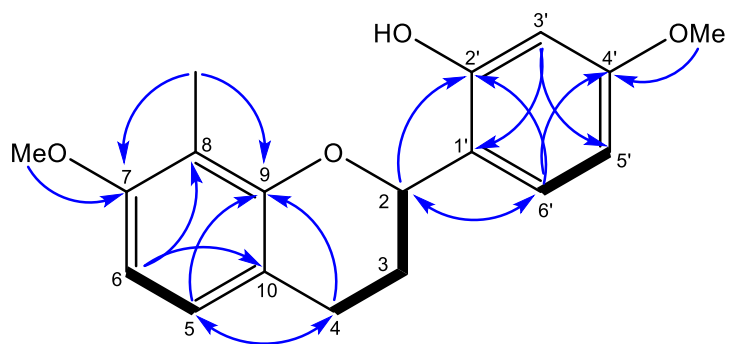


Figure S22 Key HMBC correlations (arrows) and COSY (bold lines) of compound **2**.