

## Further Dibromotyrosine-Derived Metabolites from the Marine Sponge *Aplysina caissara*

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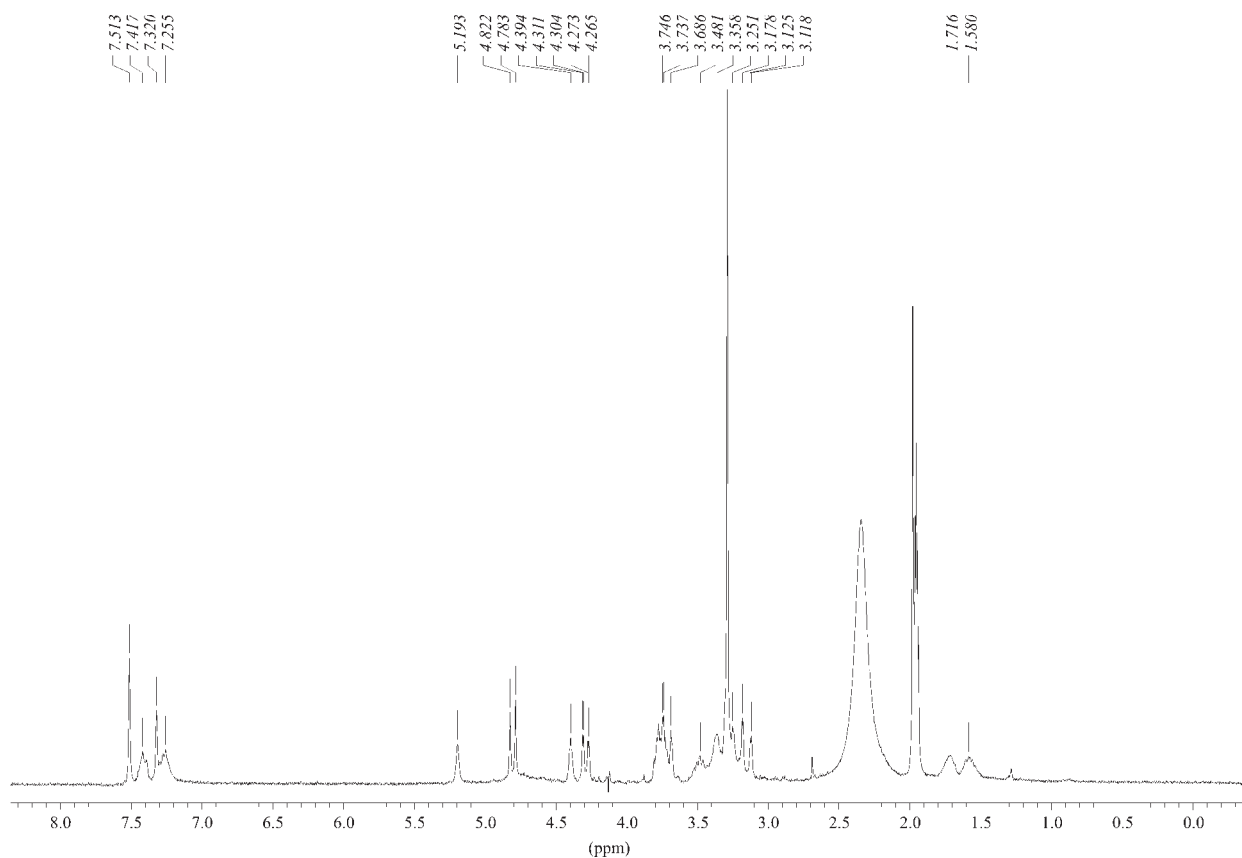


Figure S1. <sup>1</sup>H NMR spectrum (300 MHz, MeCN-*d*<sub>3</sub>) of agelocaisсарines A1 (**5**) and A2 (**6**).

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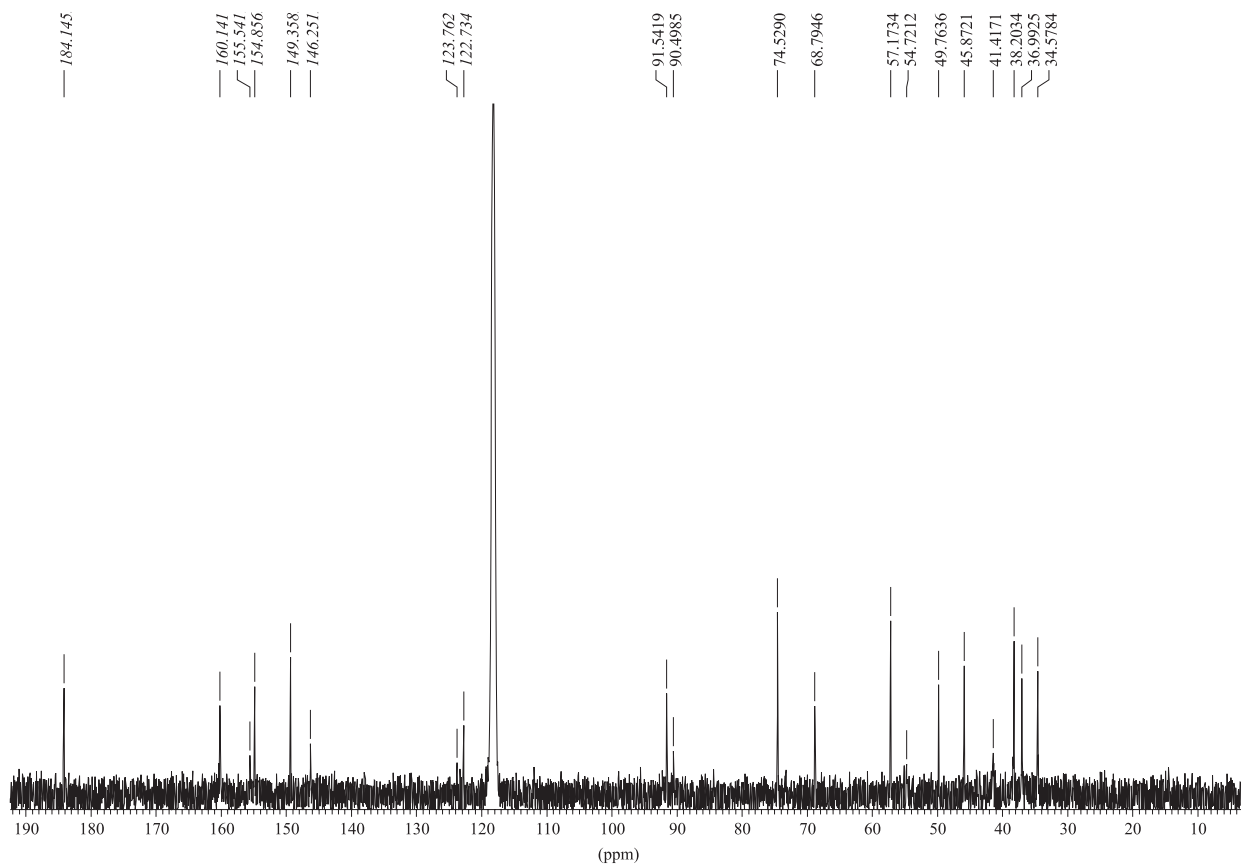


Figure S2.  $^{13}\text{C}$  NMR spectrum (75 MHz,  $\text{MeCN-}d_3$ ) of agelocaisarines A1 (5) and A2 (6).

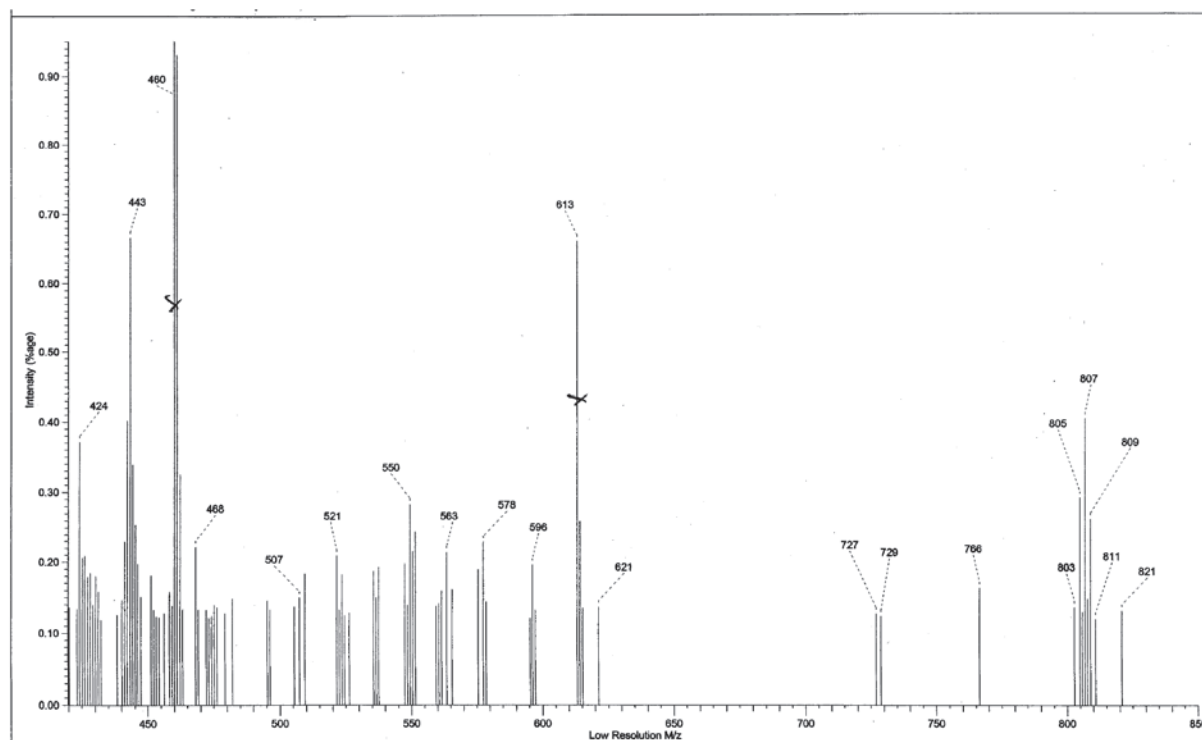


Figure S3. Scanned FAB $^+$  mass spectrum of agelocaisarines A1 (5) and A2 (6).

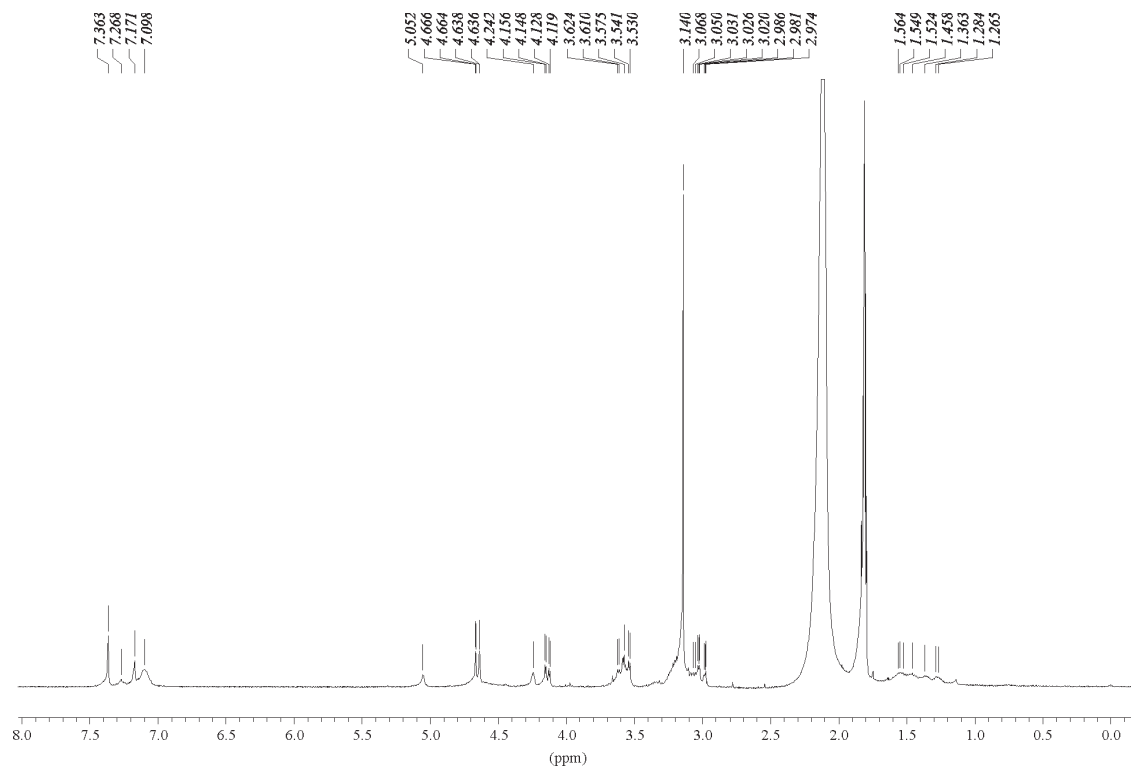


Figure S4.  $^1\text{H}$  NMR spectrum ( $\text{MeCN-}d_3$ , 400 MHz) of agelocaisarines B1 (**7**) and B2 (**8**).

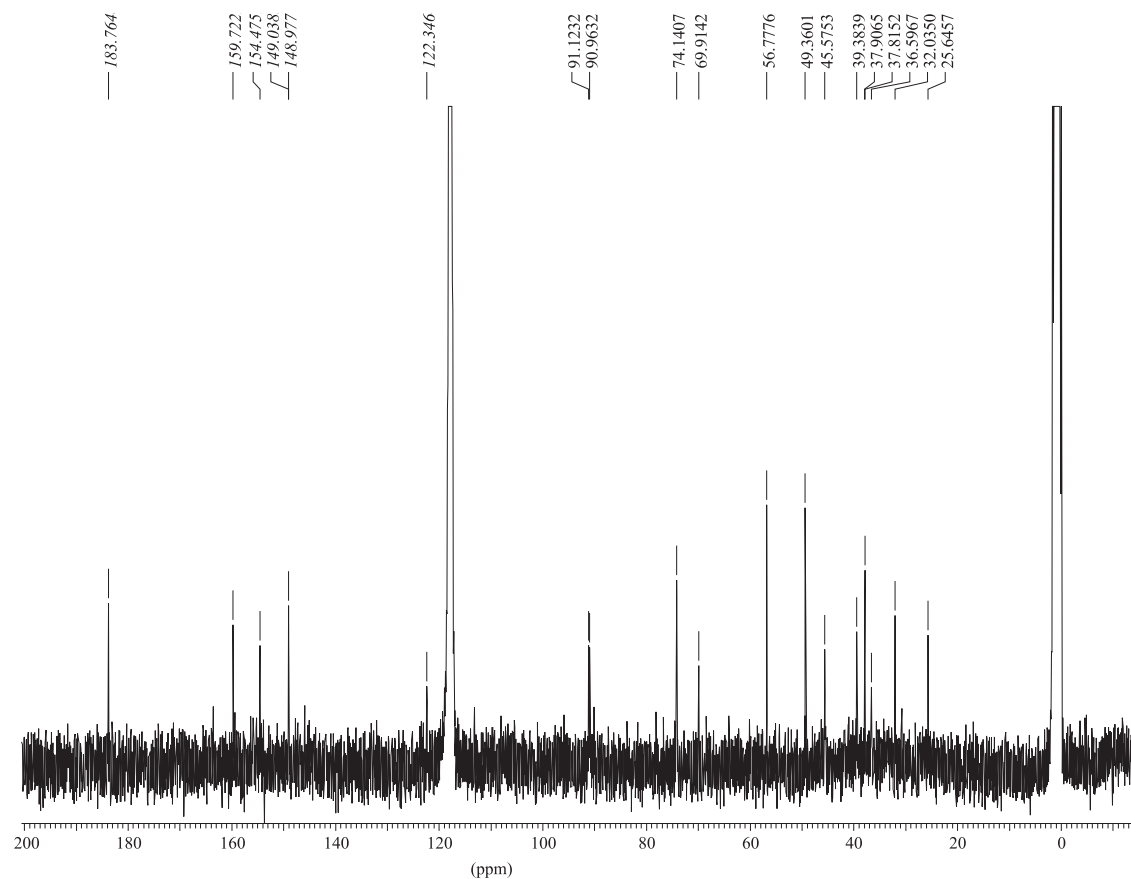


Figure S5.  $^{13}\text{C}$  NMR spectrum (75 MHz,  $\text{MeCN-}d_3$ ) of agelocaisarines B1 (**7**) and B2 (**8**).

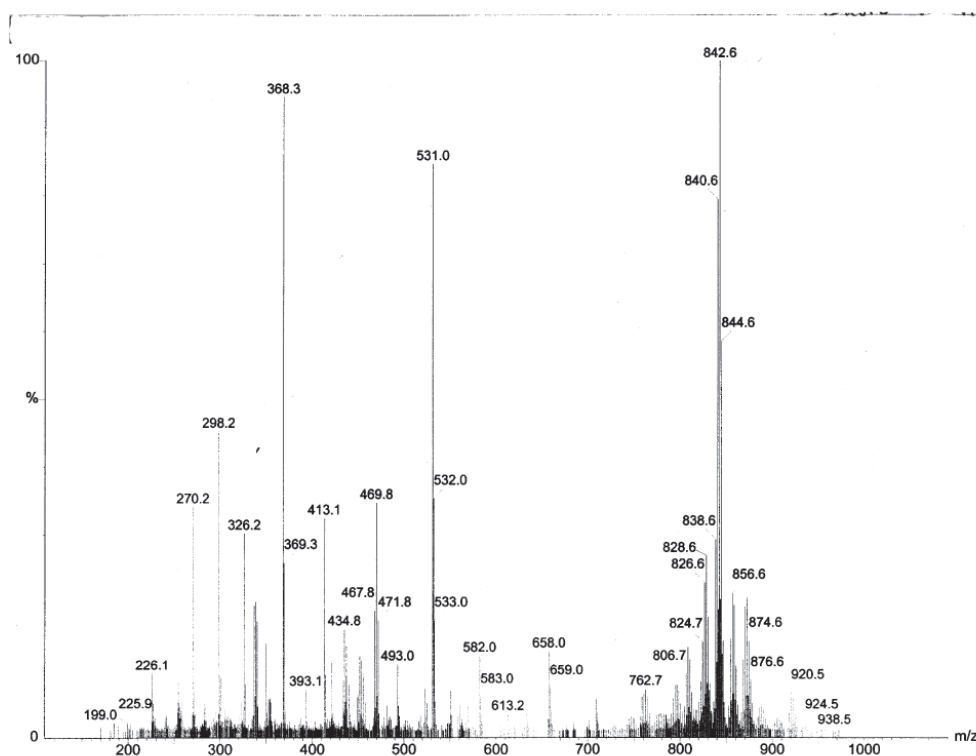


Figure S6. ESI+ mass spectrum of agelocaisarines B1 (7) and B2 (8).

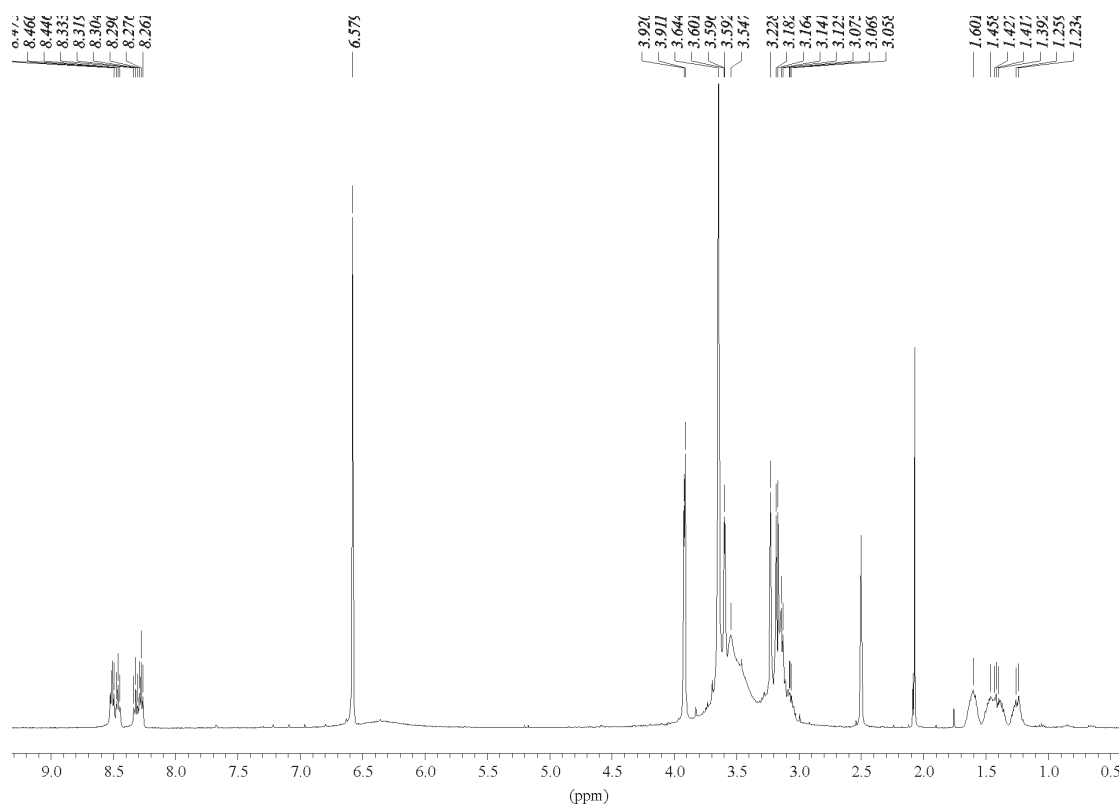


Figure S7. <sup>1</sup>H NMR spectrum (DMSO-*d*<sub>6</sub>, 400 MHz) of caissarine C (9).

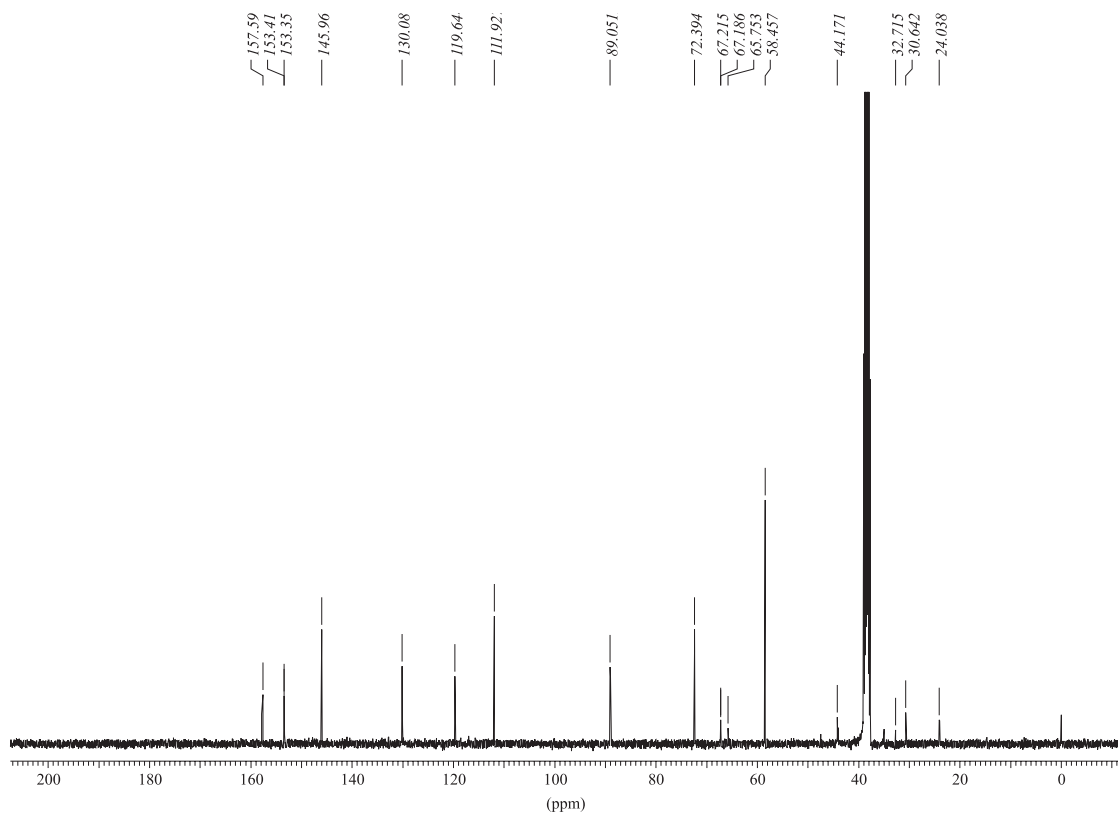


Figure S8.  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{DMSO-}d_6$ ) of caissarine C (**9**).

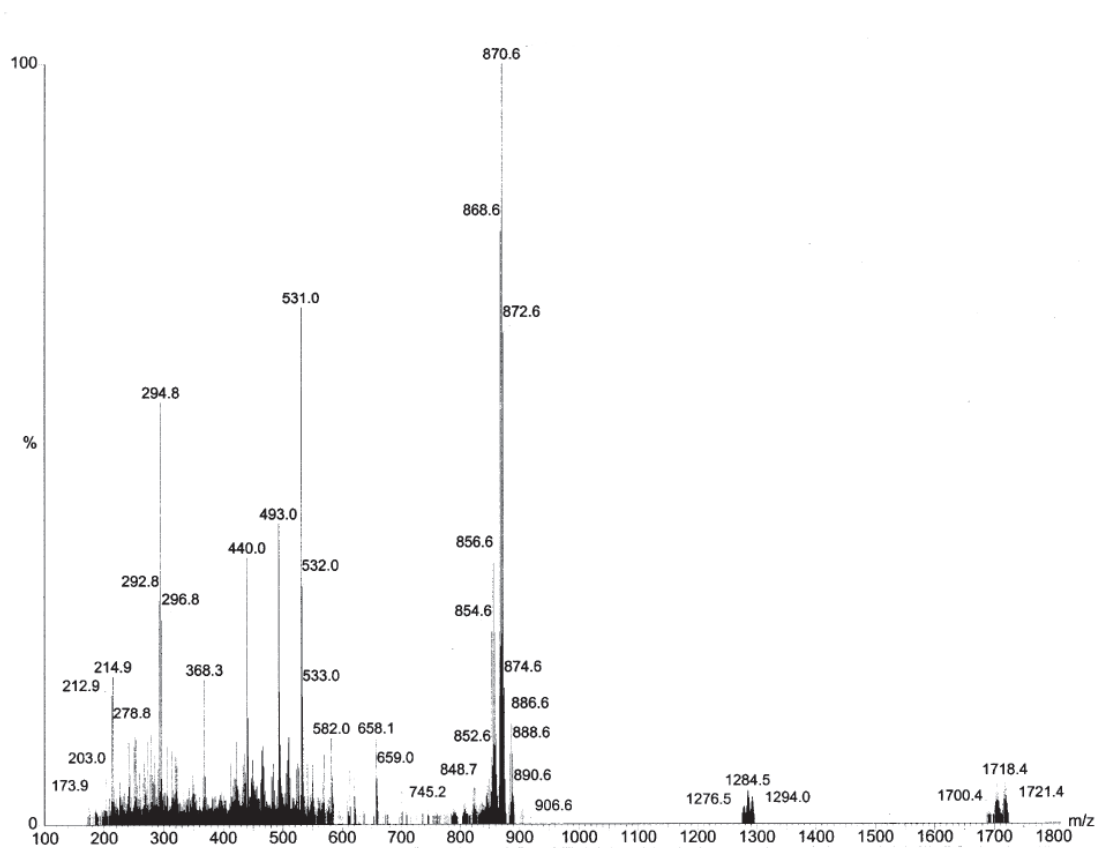


Figure S9. ESI<sup>+</sup> mass spectrum of caissarine C (**9**).