

# Supplementary Information

## Caavuranamide, a Novel Steroidal Alkaloid from the Ripe Fruits of *Solanum caavurana* Vell. (Solanaceae)

*Nelissa Pacheco Vaz,<sup>a</sup> Emmanoel V. Costa,<sup>a,b</sup> Érica L. Santos,<sup>a</sup> Sandra Bos Mikich,<sup>c</sup>  
Francisco A. Marques,<sup>a</sup> Raquel M. Braga,<sup>d</sup> Camila Delarmelina,<sup>e</sup> Marta C. T. Duarte,<sup>e</sup>  
Ana Lúcia T. G. Ruiz,<sup>f</sup> Vanessa H. S. Souza,<sup>f</sup> João E. de Carvalho<sup>f</sup> and  
Beatriz H. L. N. Sales Maia<sup>\*a</sup>*

<sup>a</sup>Departamento de Química, Universidade Federal do Paraná, Centro Politécnico,  
CP 19081, 81531-990 Curitiba-PR, Brazil

<sup>b</sup>Departamento de Química, Universidade Federal de Sergipe, Av. Marechal Rondon s/n,  
49100-000 São Cristovão-SE, Brazil

<sup>c</sup>Laboratório de Ecologia, Embrapa Florestas, CP 319, 83411-000 Colombo-PR, Brazil

<sup>d</sup>Instituto de Química, Universidade Estadual de Campinas,  
CP 6154, 13083-970 Campinas-SP, Brazil

<sup>e</sup>Divisão de Microbiologia and <sup>f</sup>Divisão de Farmacologia e Toxicologia,  
Centro Pluridisciplinar de Pesquisas Químicas Biológicas e Agrícolas (CPQBA),  
Universidade Estadual de Campinas, CP 6171, 13083-970 Campinas-SP, Brazil

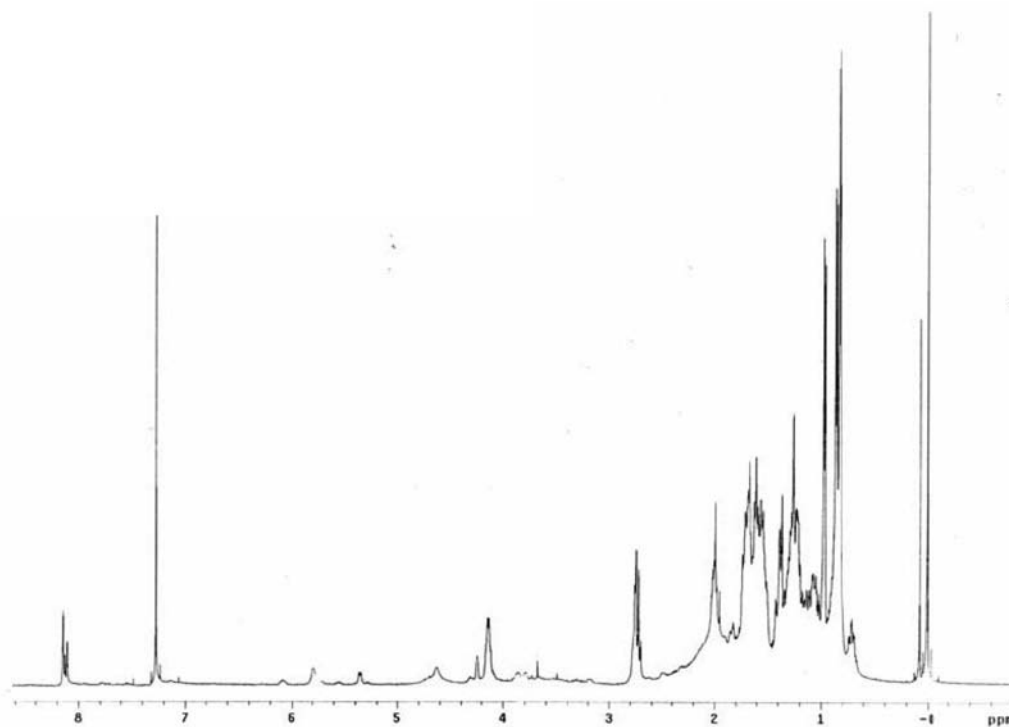


Figure S1. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of caavuranamide (1).

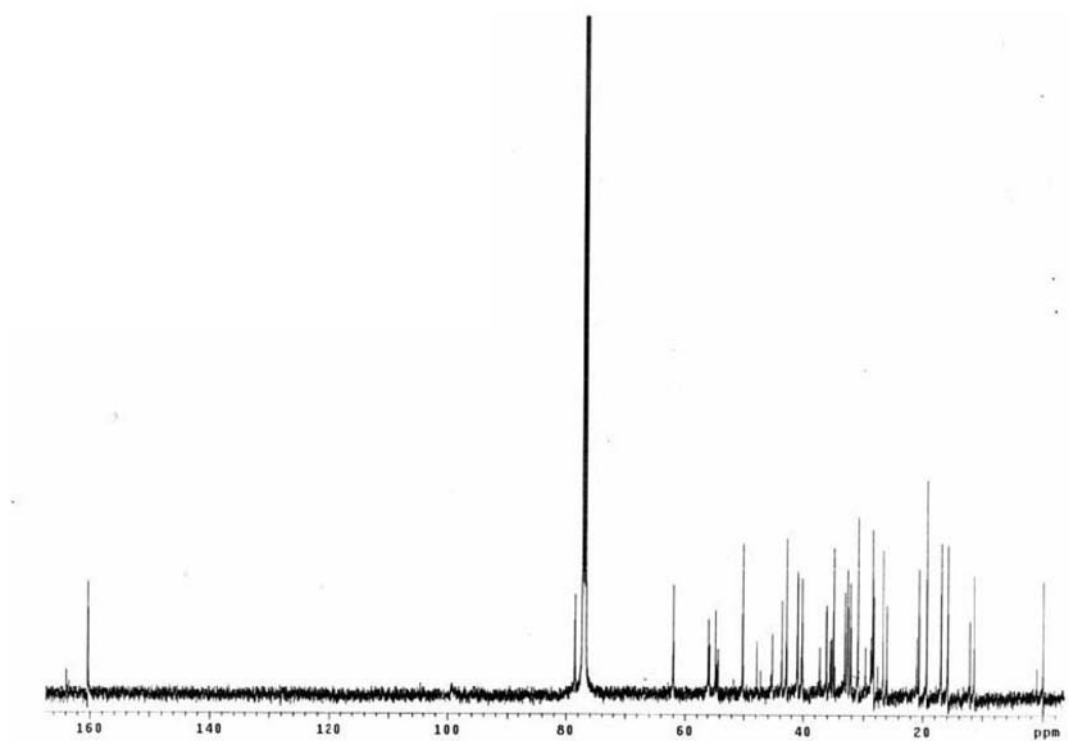


Figure S2.  $^{13}\text{C}$   $\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of caavuranamide (1).

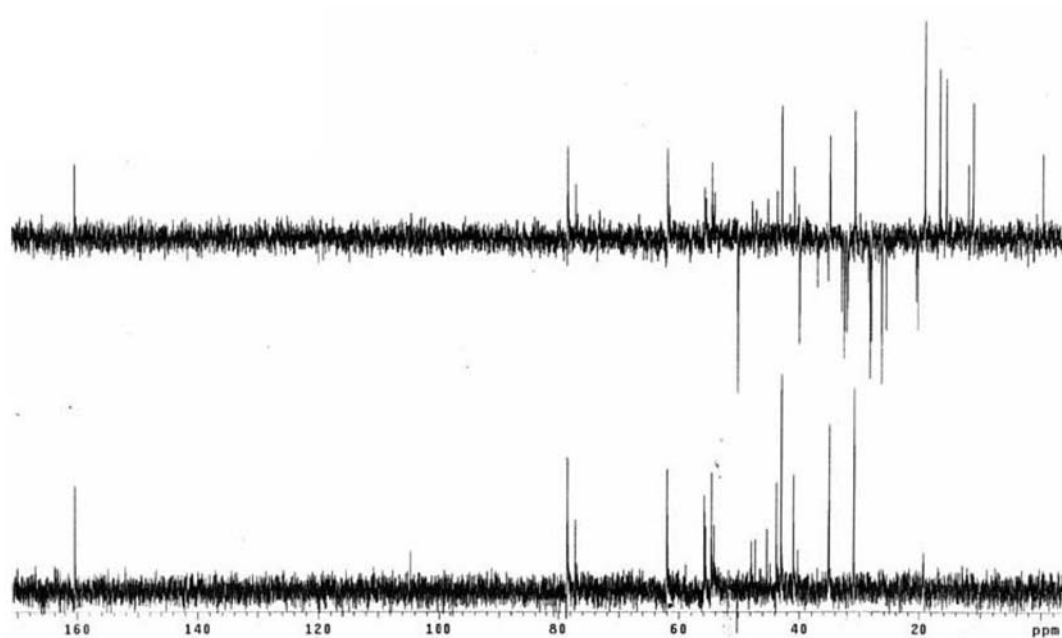


Figure S3. DEPT ( $\theta = 135^\circ$ , 125 MHz,  $\text{CDCl}_3$ ) spectrum of caavuranamide (1).

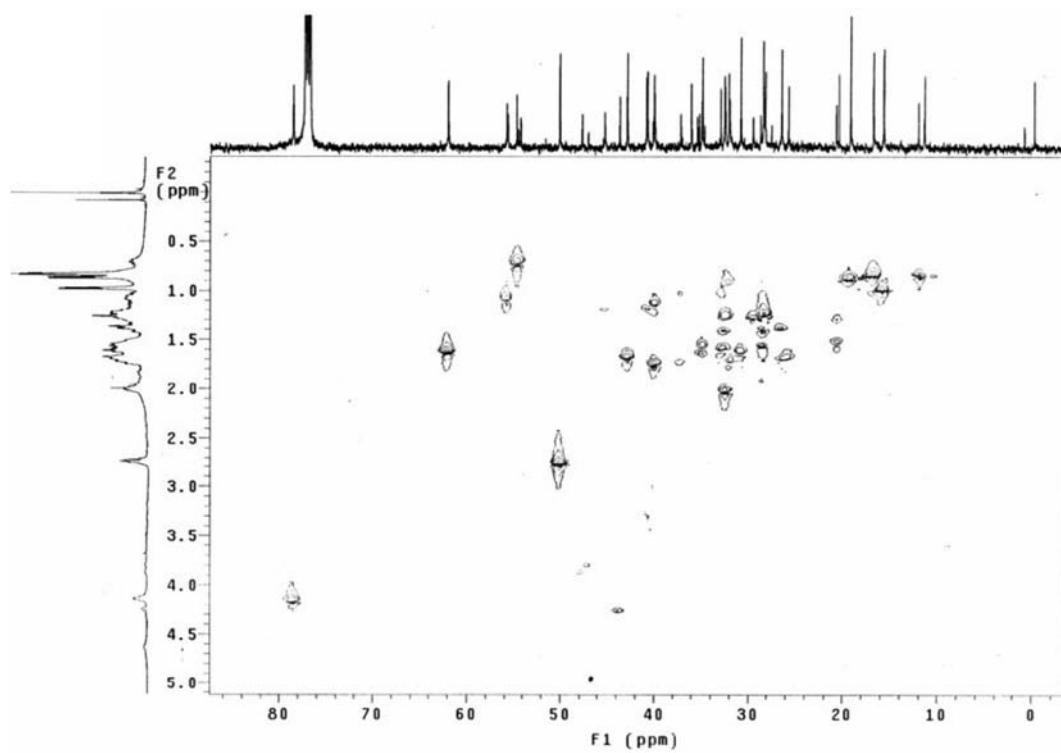


Figure S4. HSQC spectrum ( $^1\text{H}$  NMR: 500 MHz,  $^{13}\text{C}$  NMR: 125 MHz,  $\text{CDCl}_3$ ) of caavuranamide (1).

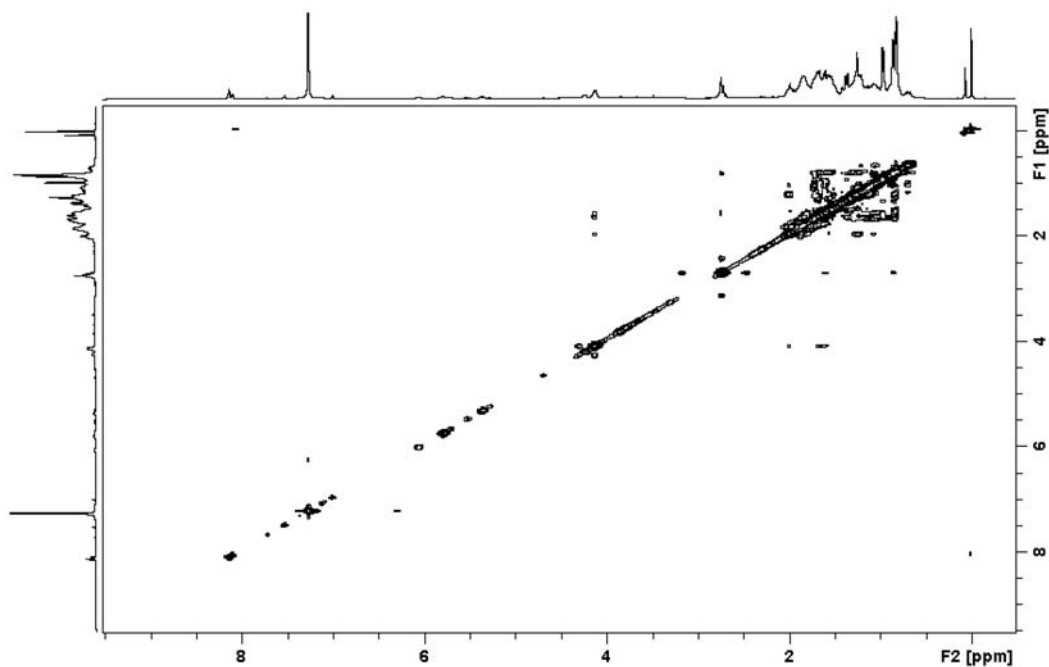


Figure S5. NOESY spectrum ( $^1\text{H}$  NMR: 400MHz,  $\text{CDCl}_3$ ) of caavuranamide (1).

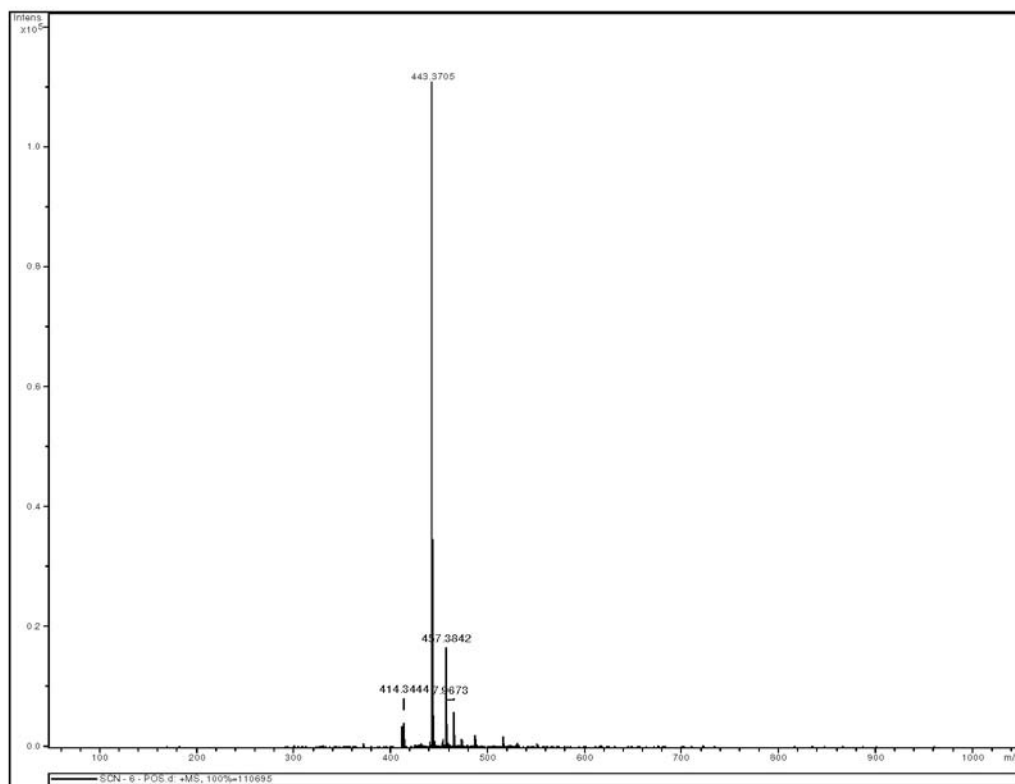


Figure S6. HRESIMS spectrum of caavuranamide (1).

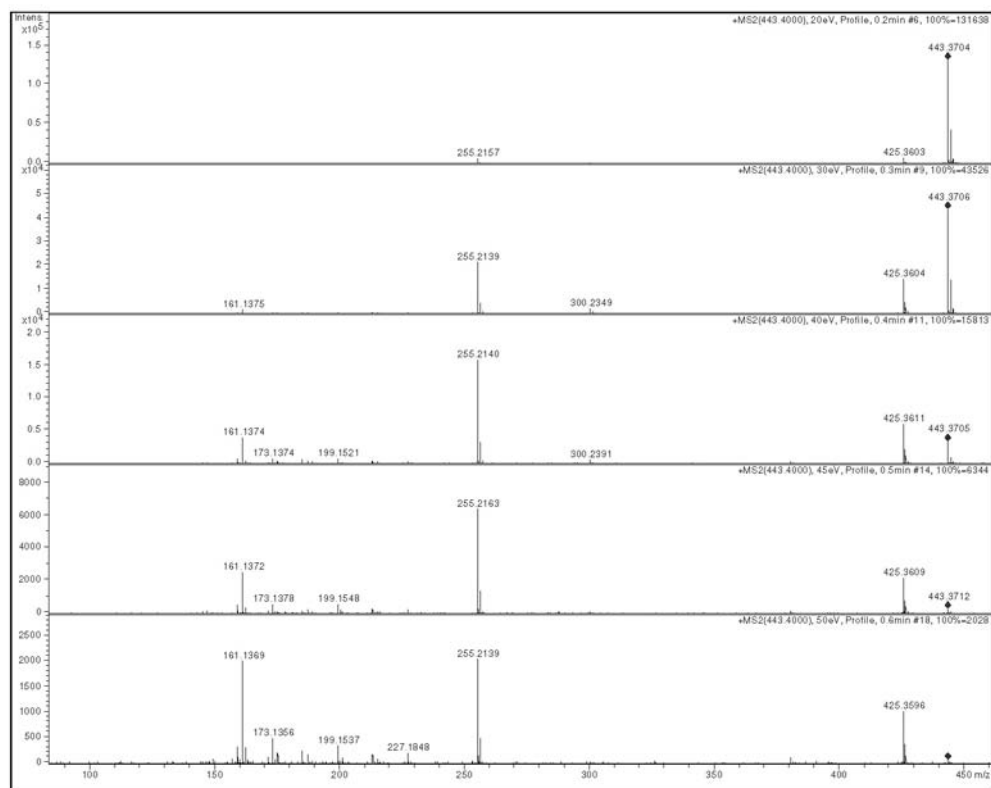
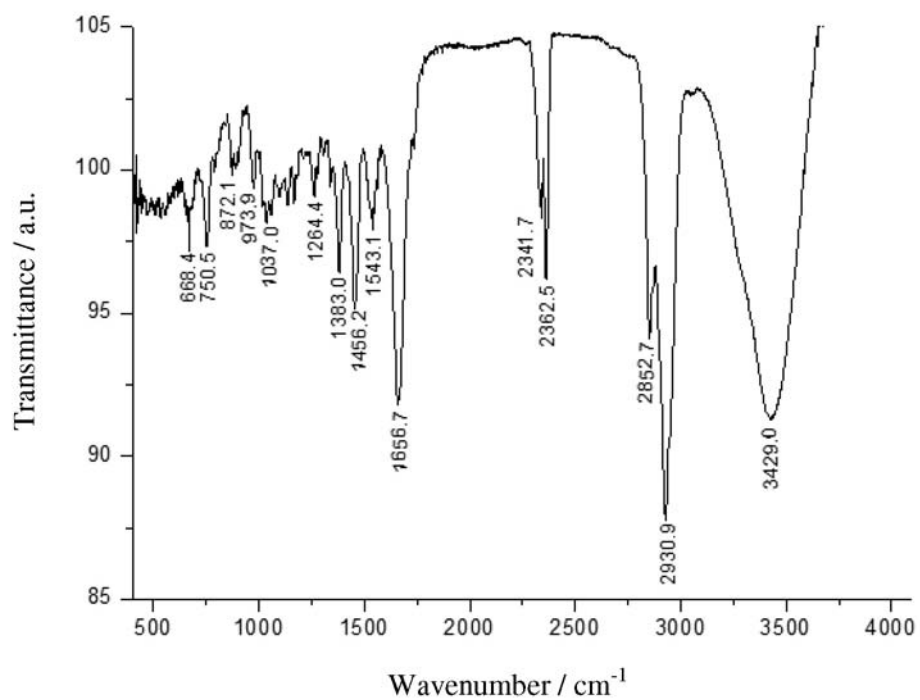
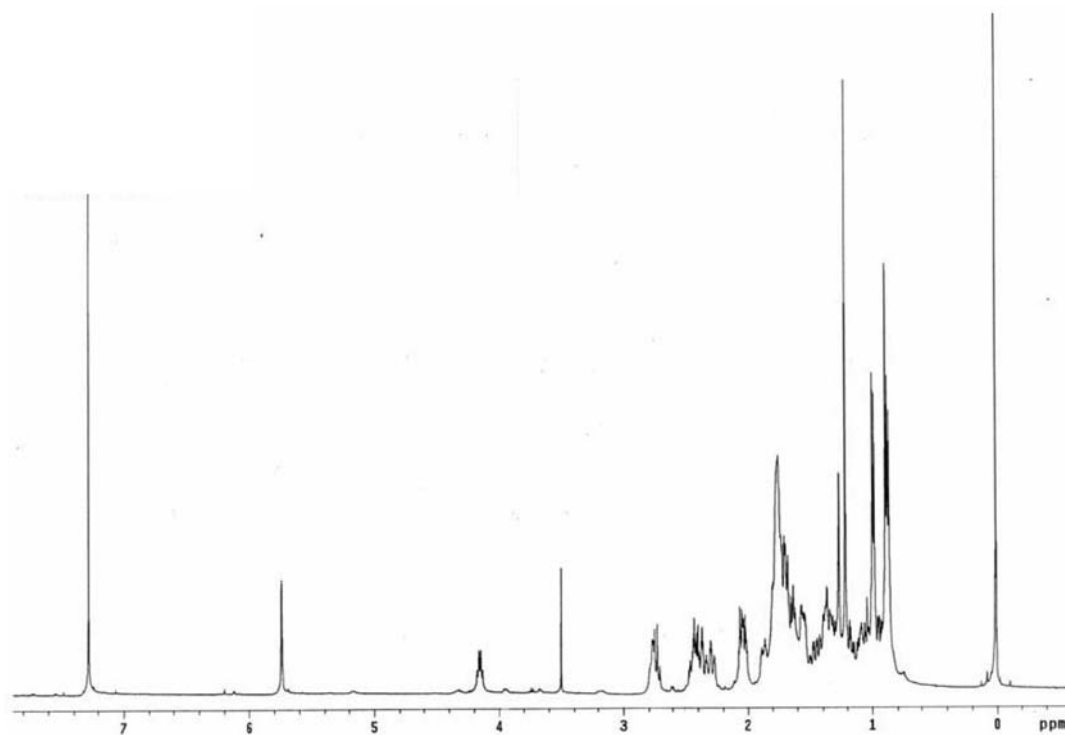


Figure S7. HRESIMS/MS spectra of caavuranamide (1).



**Figure S8.** IR (KBr) spectrum of caavuranamide (1).



**Figure S9.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of 4-tomatiden-3-one (2).

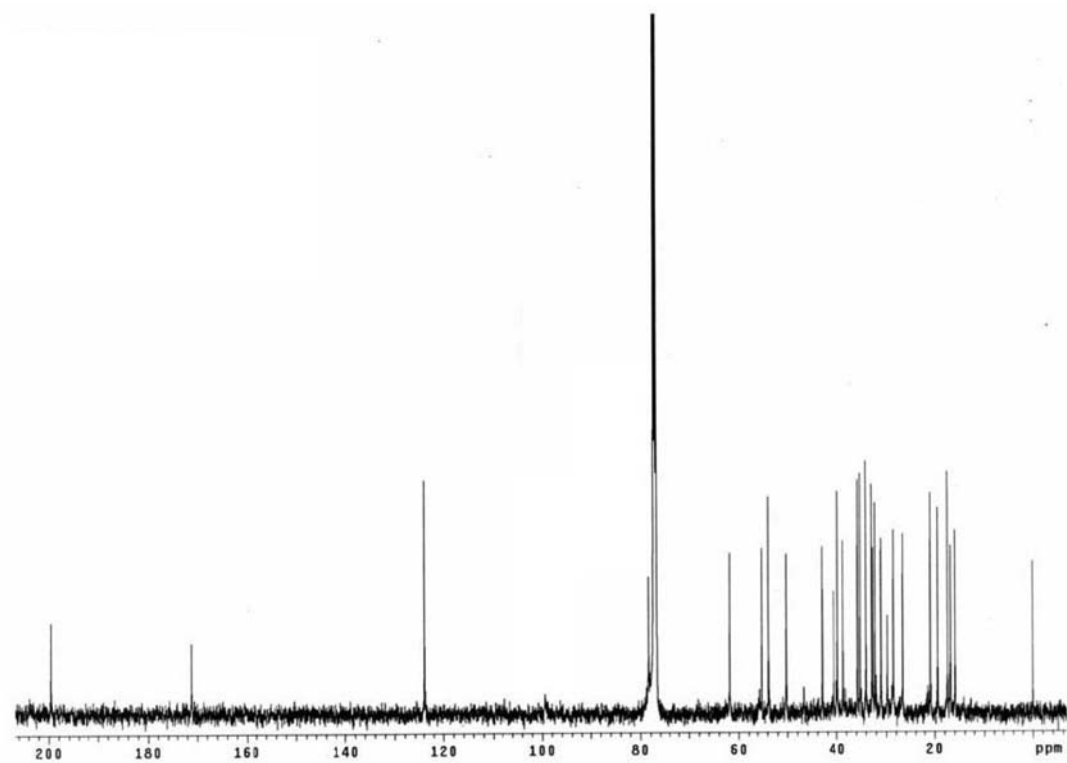


Figure S10.  $^{13}\text{C}$  { $^1\text{H}$ } NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of 4-tomatiden-3-one (2).

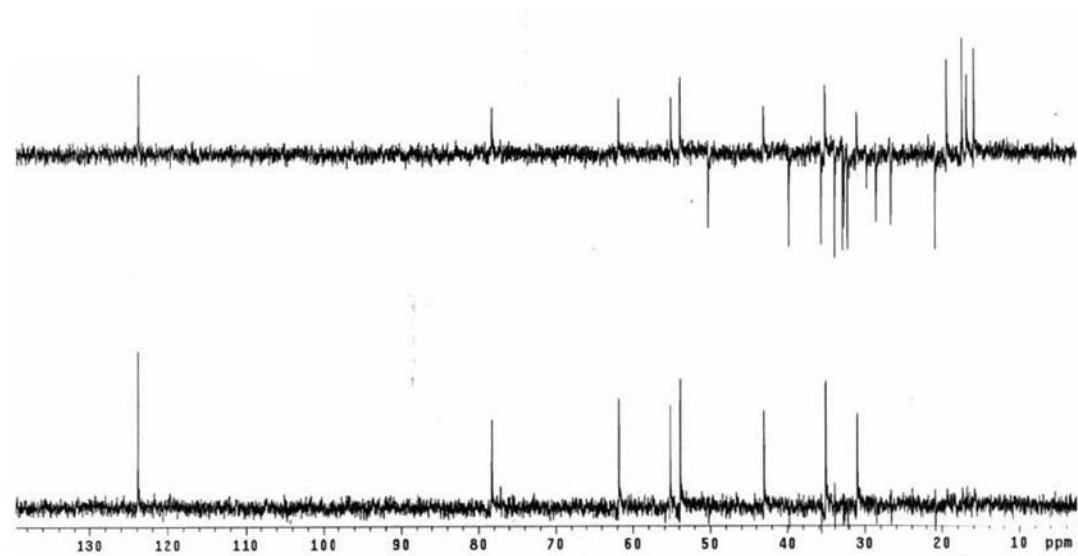


Figure S11. DEPT ( $\theta = 135^\circ$ , 125 MHz,  $\text{CDCl}_3$ ) spectrum of 4-tomatiden-3-one (2).

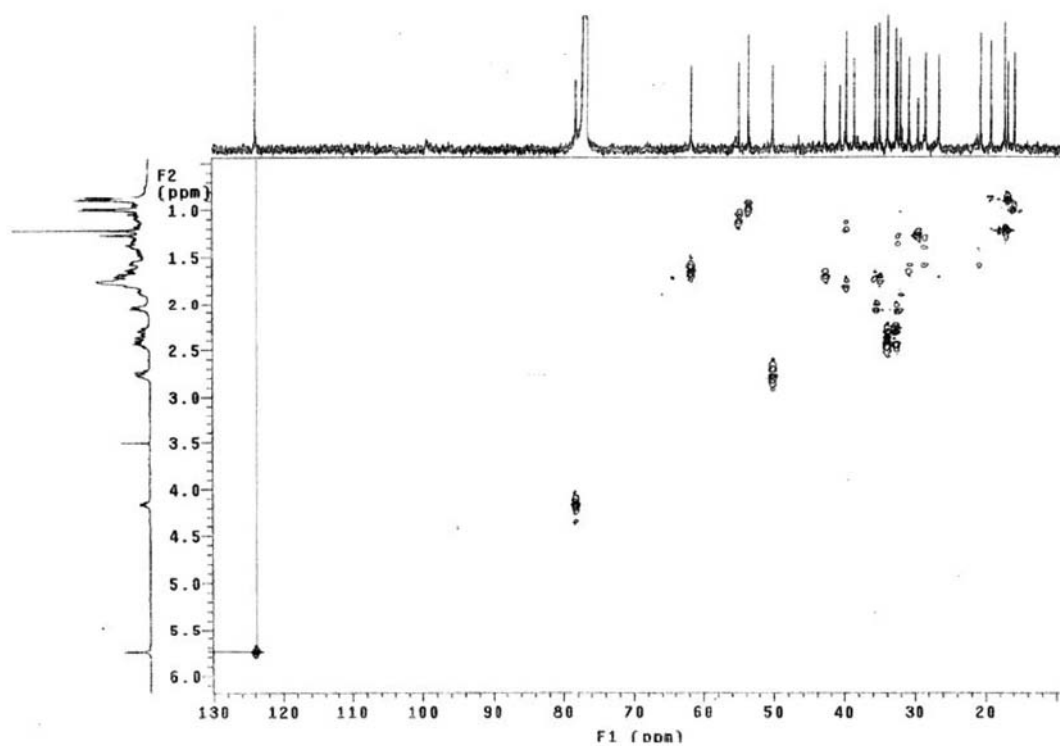


Figure S12. HSQC spectrum ( $^1\text{H}$  NMR: 500 MHz,  $^{13}\text{C}$  NMR: 125 MHz,  $\text{CDCl}_3$ ) of 4-tomatiden-3-one (2).

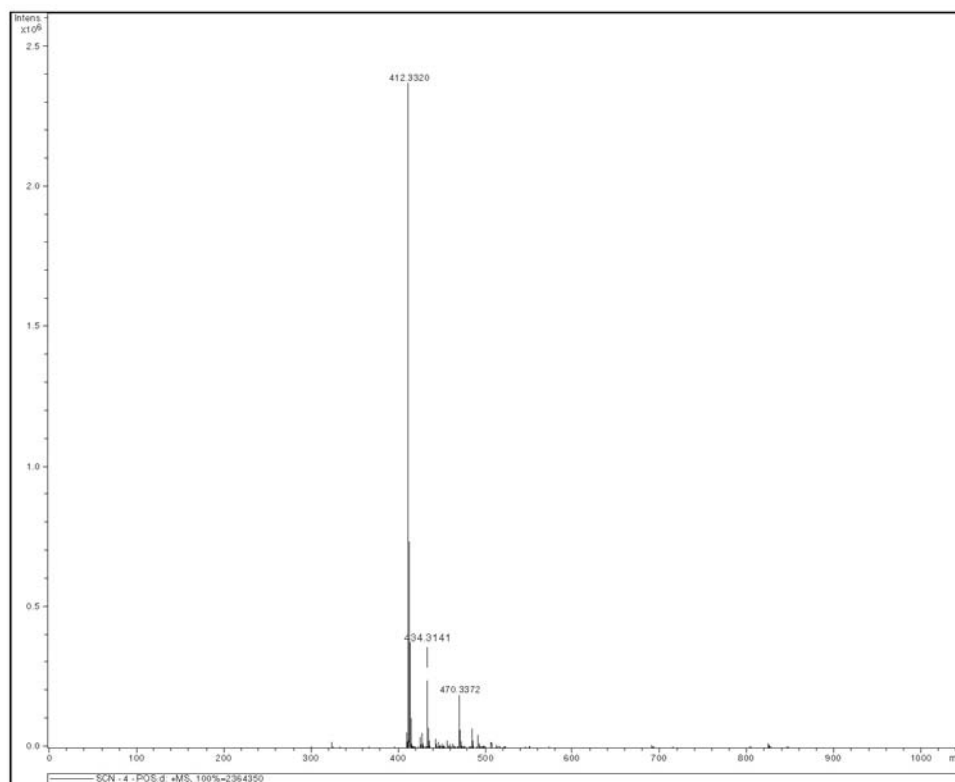


Figure S13. HRESIMS spectrum of 4-tomatiden-3-one (2).

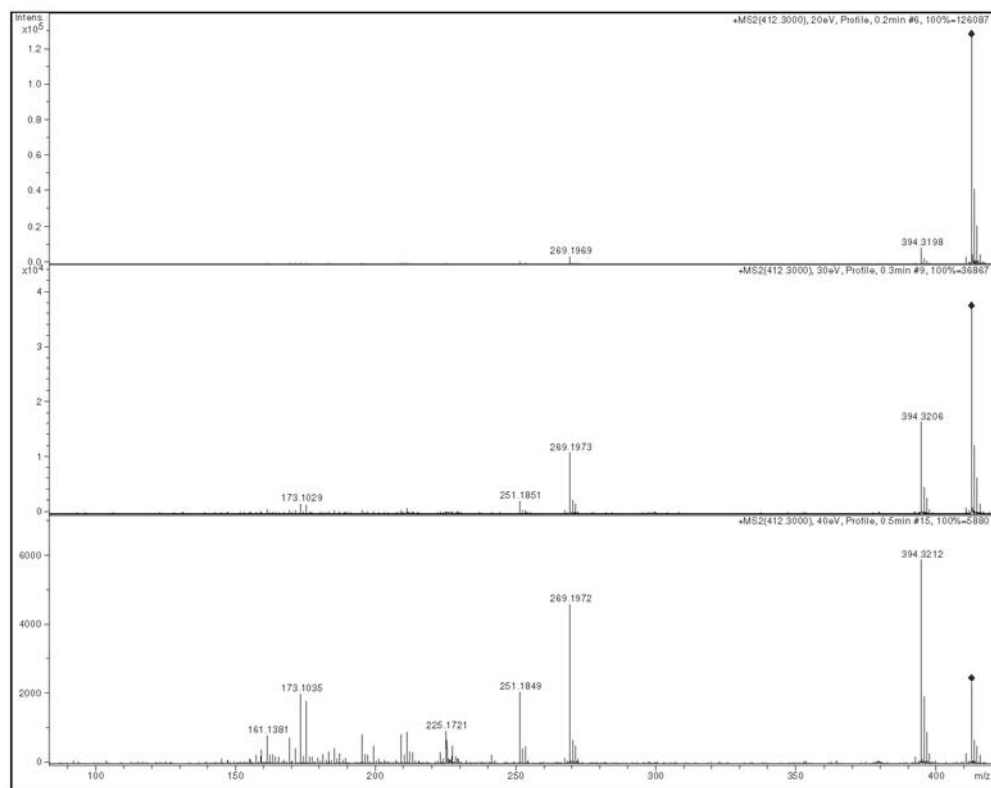


Figure S14. HRESIMS/MS spectrum of 4-tomatiden-3-one (2).

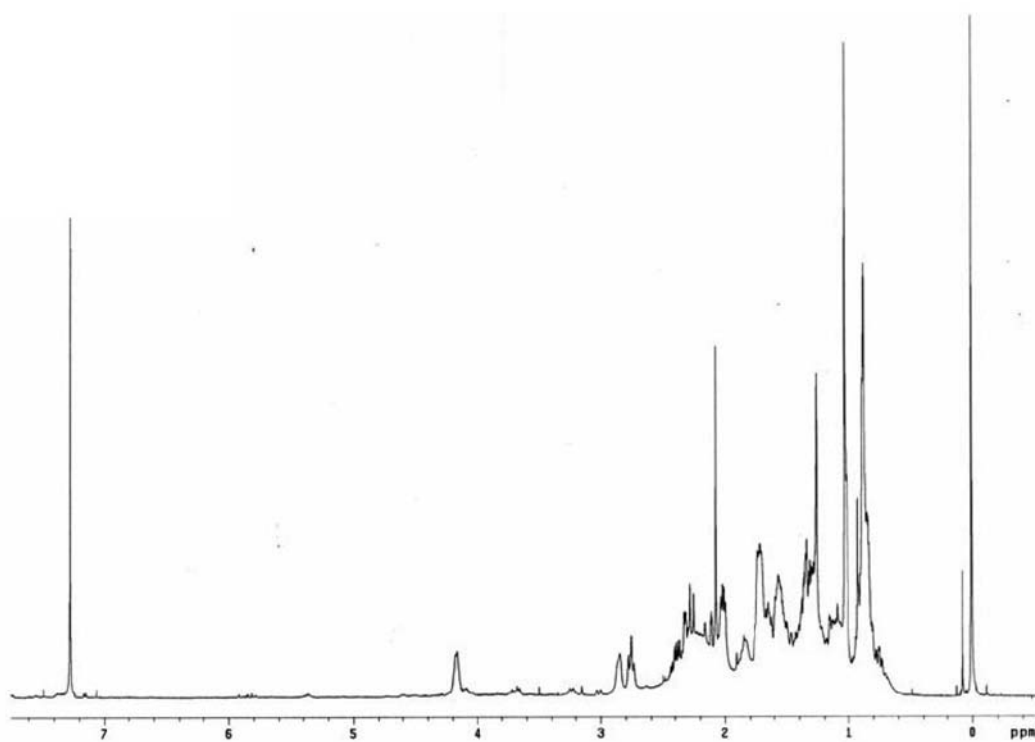


Figure S15. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of 5 $\alpha$ -tomatidan-3-one (3).



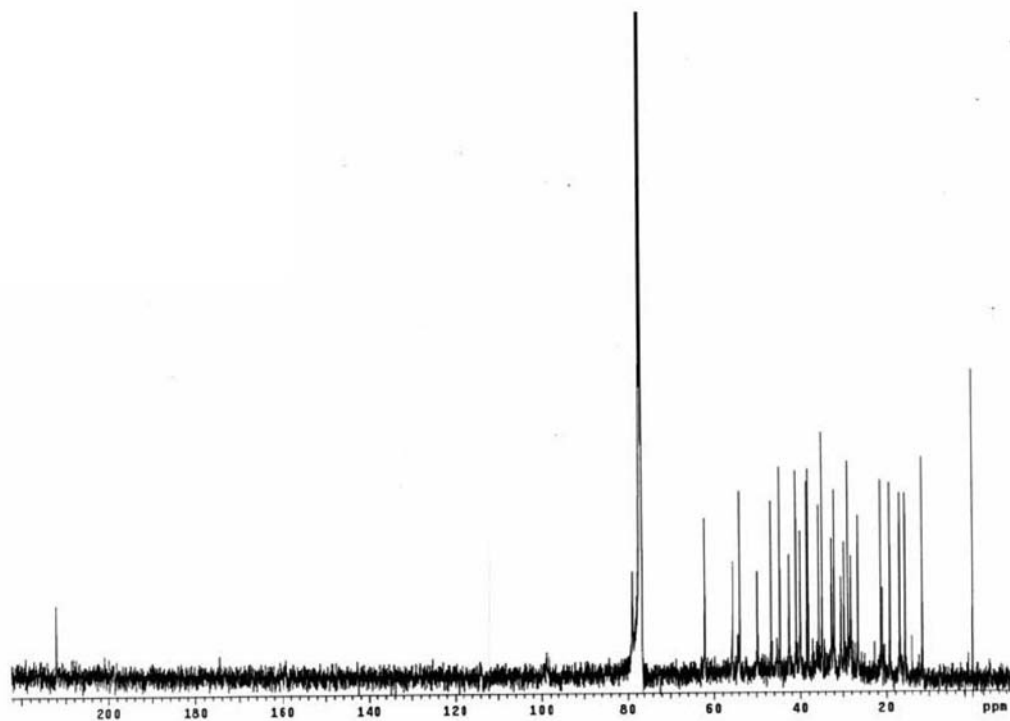


Figure S16.  $^{13}\text{C}$   $\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of 5 $\alpha$ -tomatidan-3-one (3).

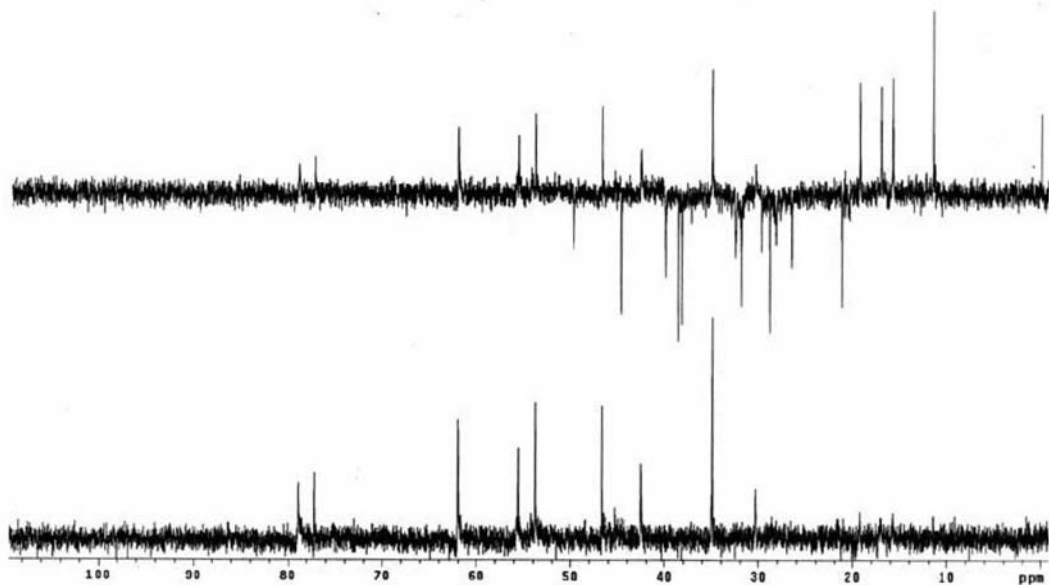


Figure S17. DEPT ( $\theta = 135^\circ$ , 125 MHz,  $\text{CDCl}_3$ ) spectrum of 5 $\alpha$ -tomatidan-3-one (3).

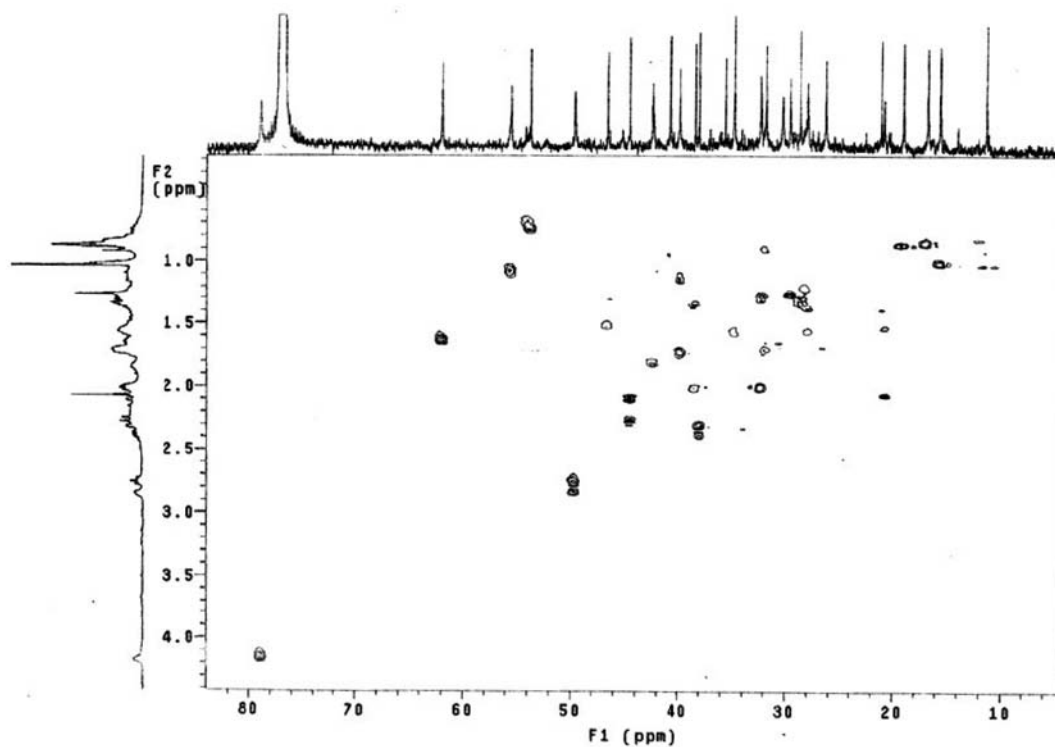


Figure S18. HSQC spectrum ( $^1\text{H}$  NMR: 500 MHz,  $^{13}\text{C}$  NMR: 125 MHz,  $\text{CDCl}_3$ ) of  $5\alpha$ -tomatidan-3-one (**3**).

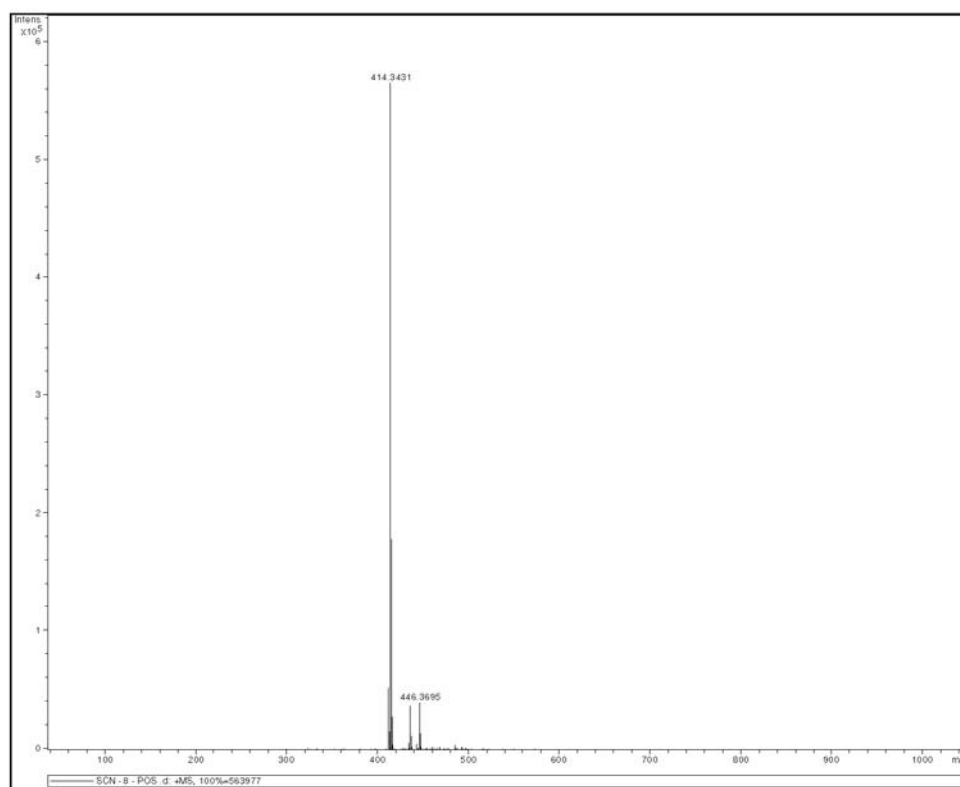


Figure S19. HRESIMS spectrum of  $5\alpha$ -tomatidan-3-one (**3**).

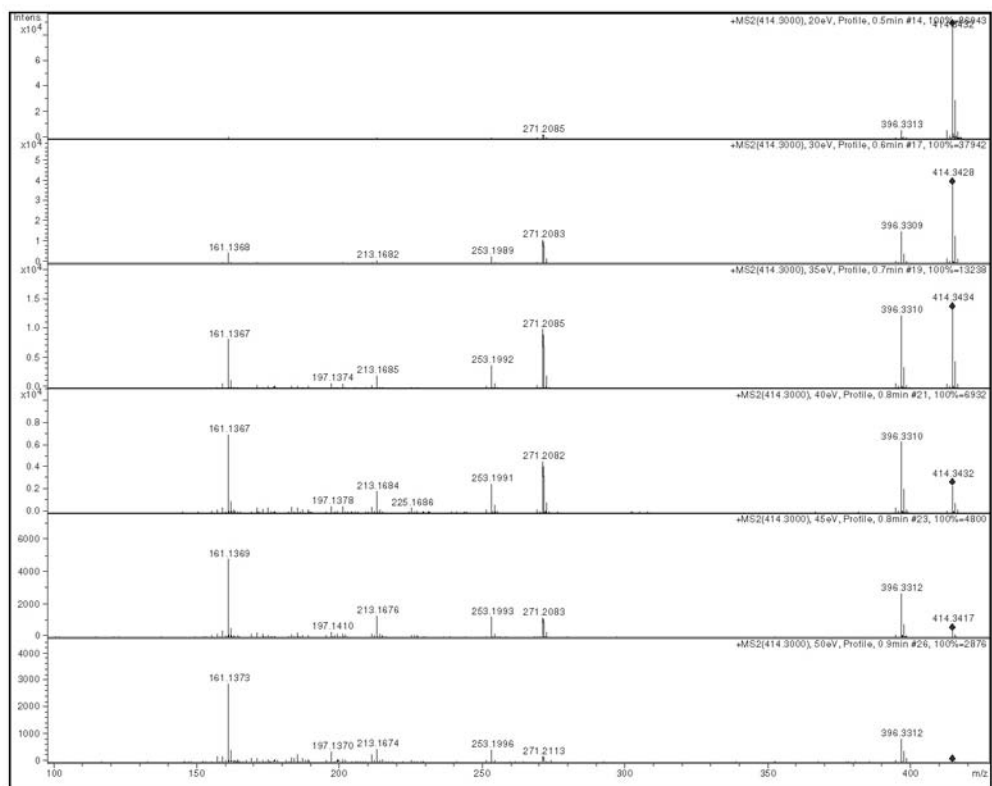


Figure S20. HRESIMS/MS spectra of 5 $\alpha$ -tomatidan-3-one (3).