

# Supplementary Information

## Pentacyclic Triterpenes from Branches of *Maytenus robusta* and *in vitro* Cytotoxic Property Against 4T1 Cancer Cells

Grasiely Faria de Sousa,<sup>a</sup> Daniel Crístian Ferreira Soares,<sup>b</sup> Wagner da Nova Mussel,<sup>a</sup>  
Nana Flora Elias Pompeu,<sup>a</sup> Grácia Divina de Fátima Silva,<sup>a</sup>  
Sidney Augusto Vieira Filho<sup>c</sup> and Lucienir Pains Duarte<sup>\*a</sup>

<sup>a</sup>Departamento de Química, Universidade Federal de Minas Gerais,  
Avenida Presidente Antônio Carlos, 6627, Pampulha, 31270-901 Belo Horizonte-MG, Brazil

<sup>b</sup>Universidade Federal de Itajubá, Campus Itabira, Rua Irmã Ivone Drumond, 200,  
Distrito Industrial II, 35903-087 Itabira-MG, Brazil

<sup>c</sup>Escola de Farmácia, Universidade Federal de Ouro Preto,  
Rua Costa Sena, 171, Centro, 35400-000 Ouro Preto-MG, Brazil

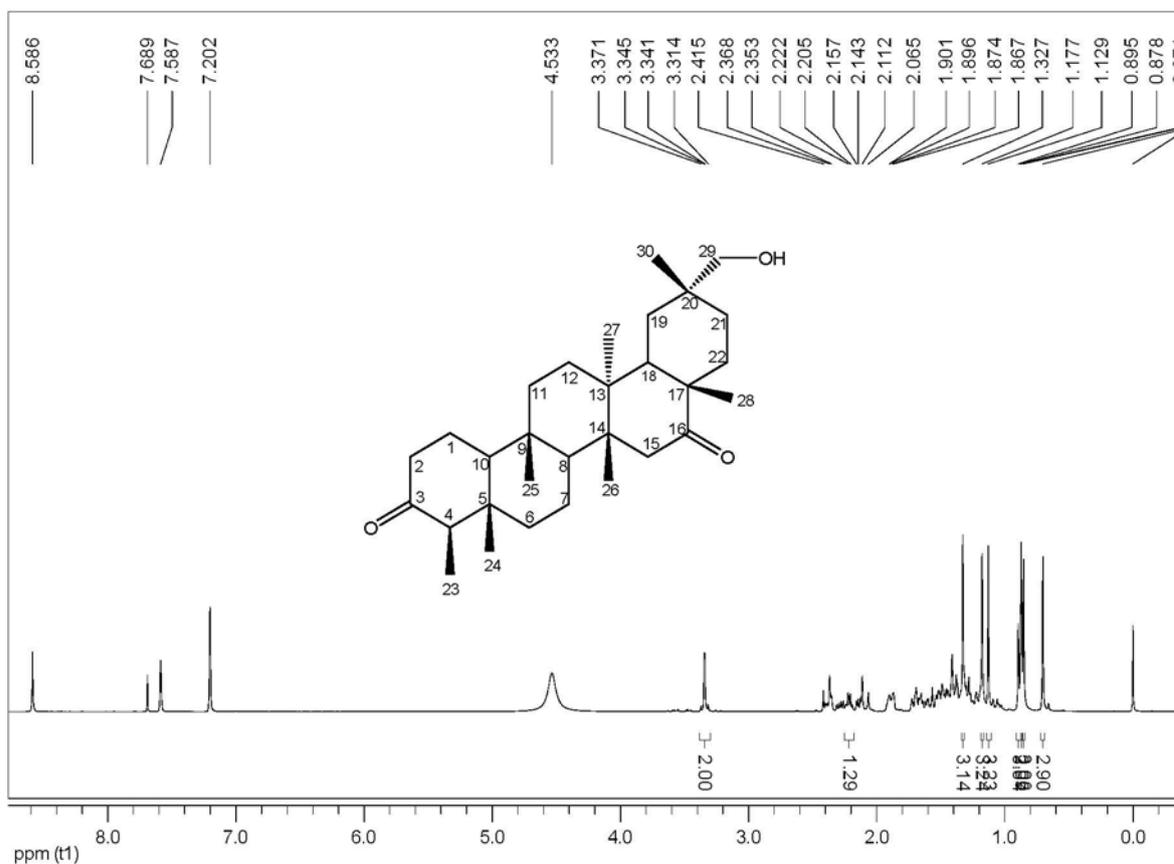
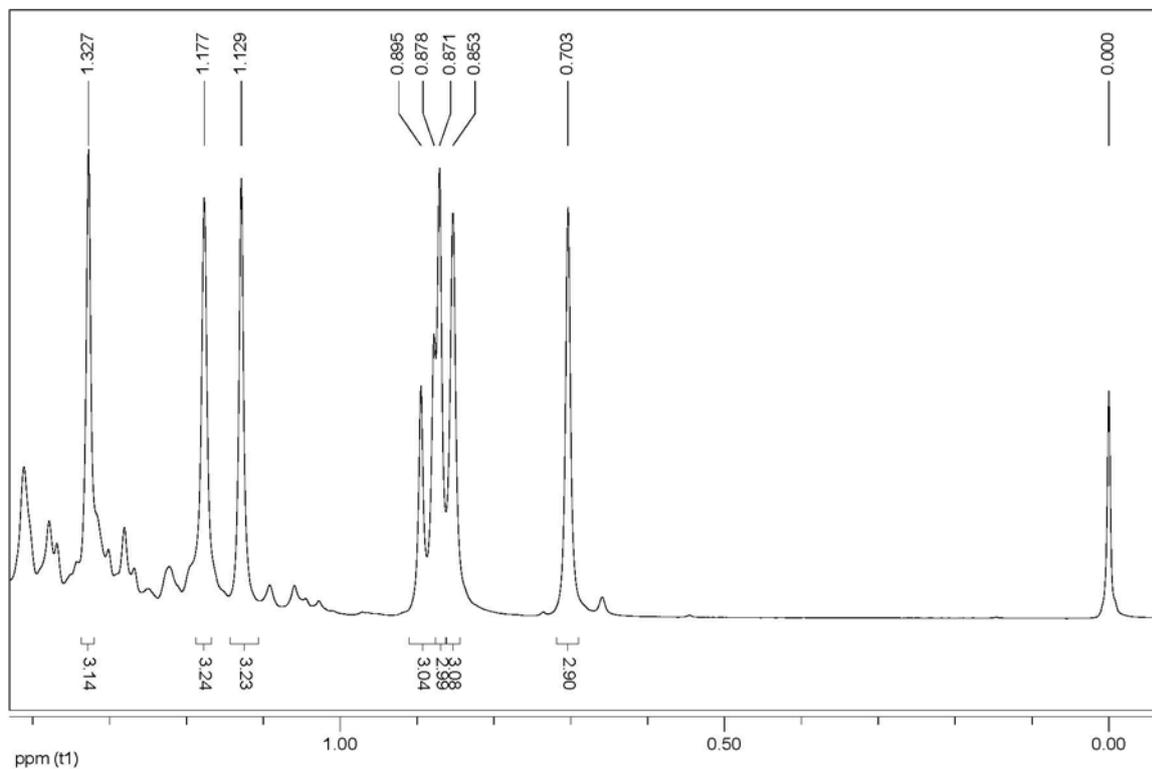
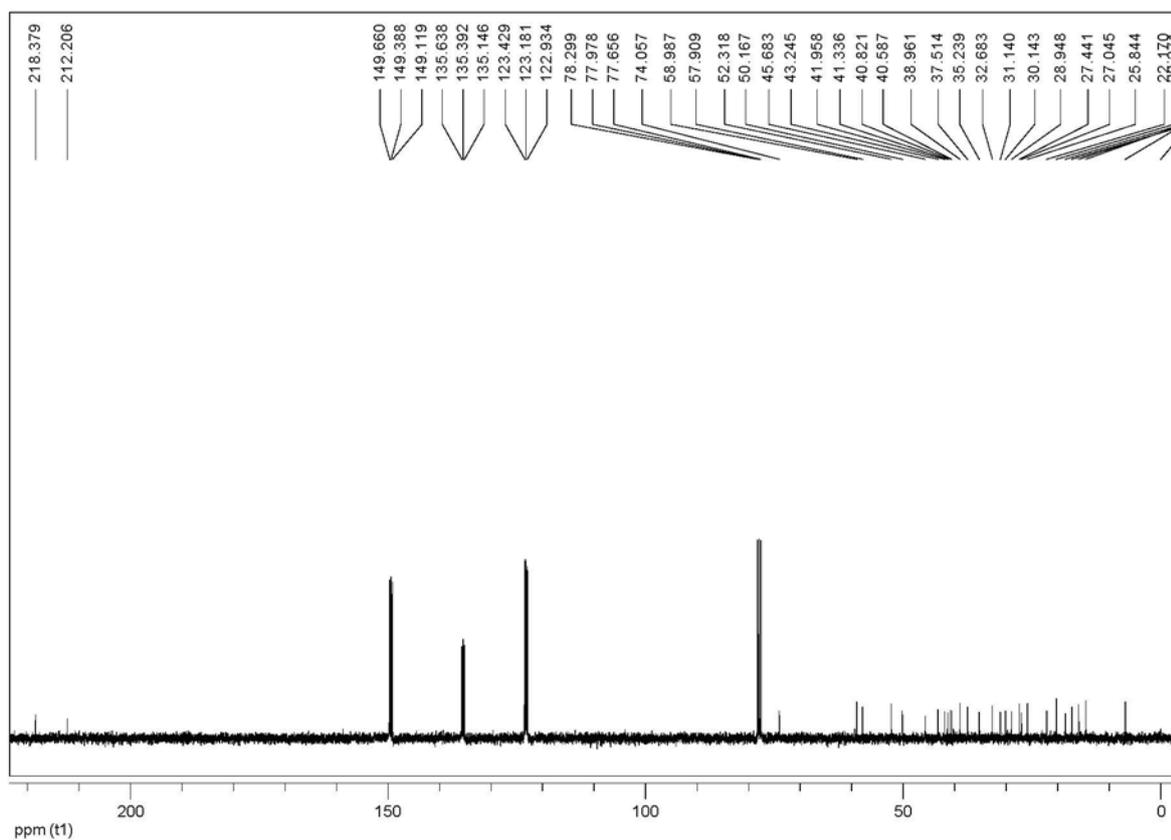


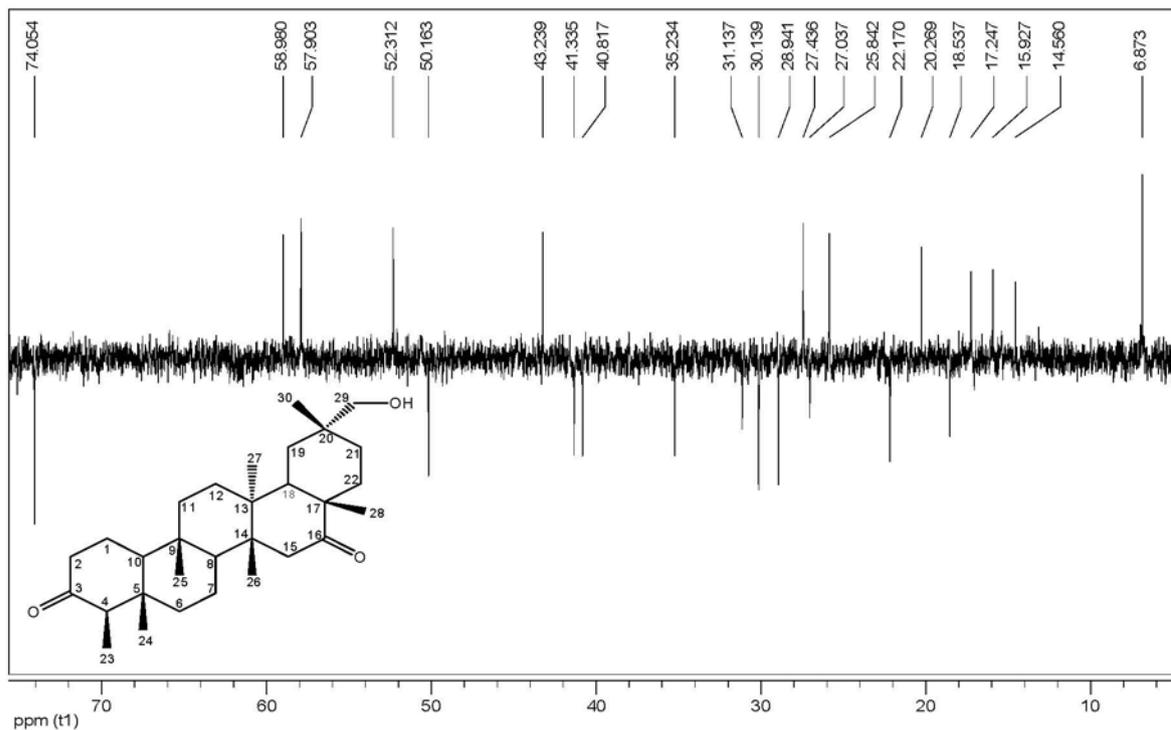
Figure S1. <sup>1</sup>H NMR spectrum of compound 1 (CDCl<sub>3</sub> + Py-*d*<sub>5</sub>, 400 MHz).



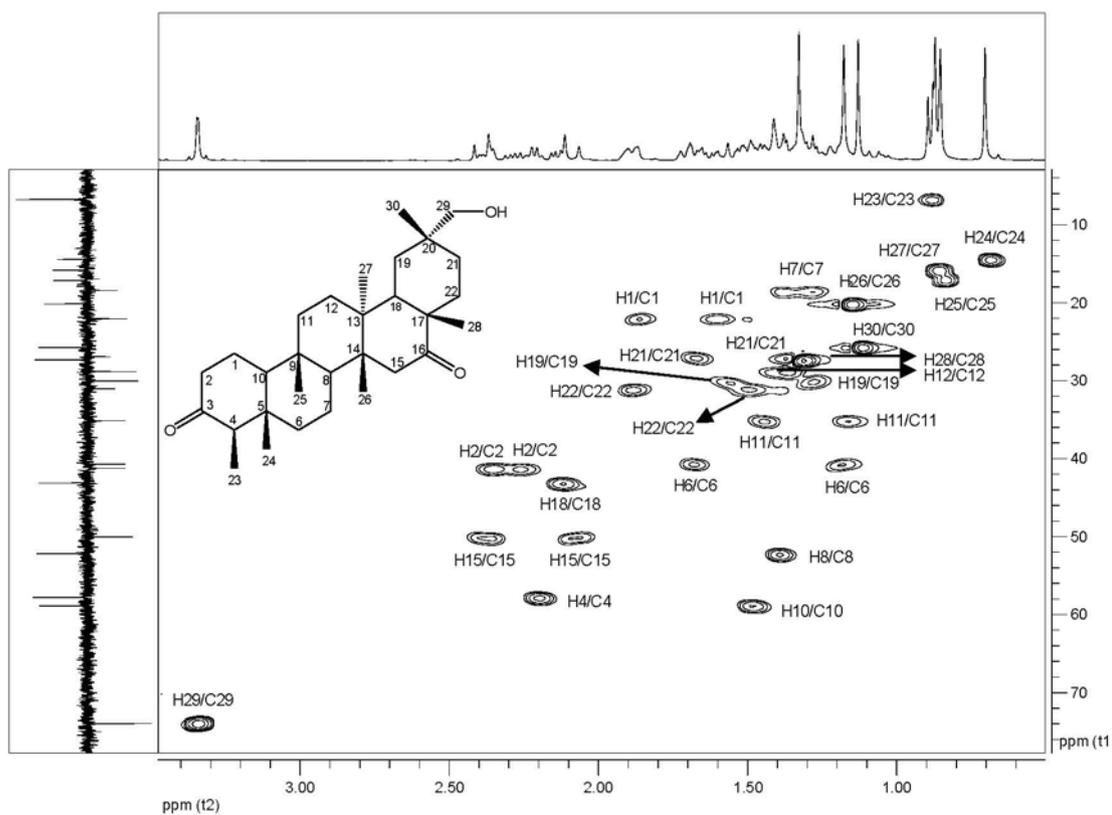
**Figure S2.**  $^1\text{H}$  NMR spectrum of compound **1** (region of 1.4 to 0 ppm and 0.91 to 0.84 ppm,  $\text{CDCl}_3 + \text{Py}-d_5$ , 400 MHz).



**Figure S3.**  $^{13}\text{C}$  NMR spectrum of compound **1** ( $\text{CDCl}_3 + \text{Py}-d_5$ , 100 MHz).



**Figure S4.** Subspectrum DEPT135 of compound **1** ( $\text{CDCl}_3$  +  $\text{Py}-d_5$ , 100 MHz).



**Figure S5.** HSQC correlation of compound **1** ( $\text{CDCl}_3$  +  $\text{Py}-d_5$ , 400 MHz).

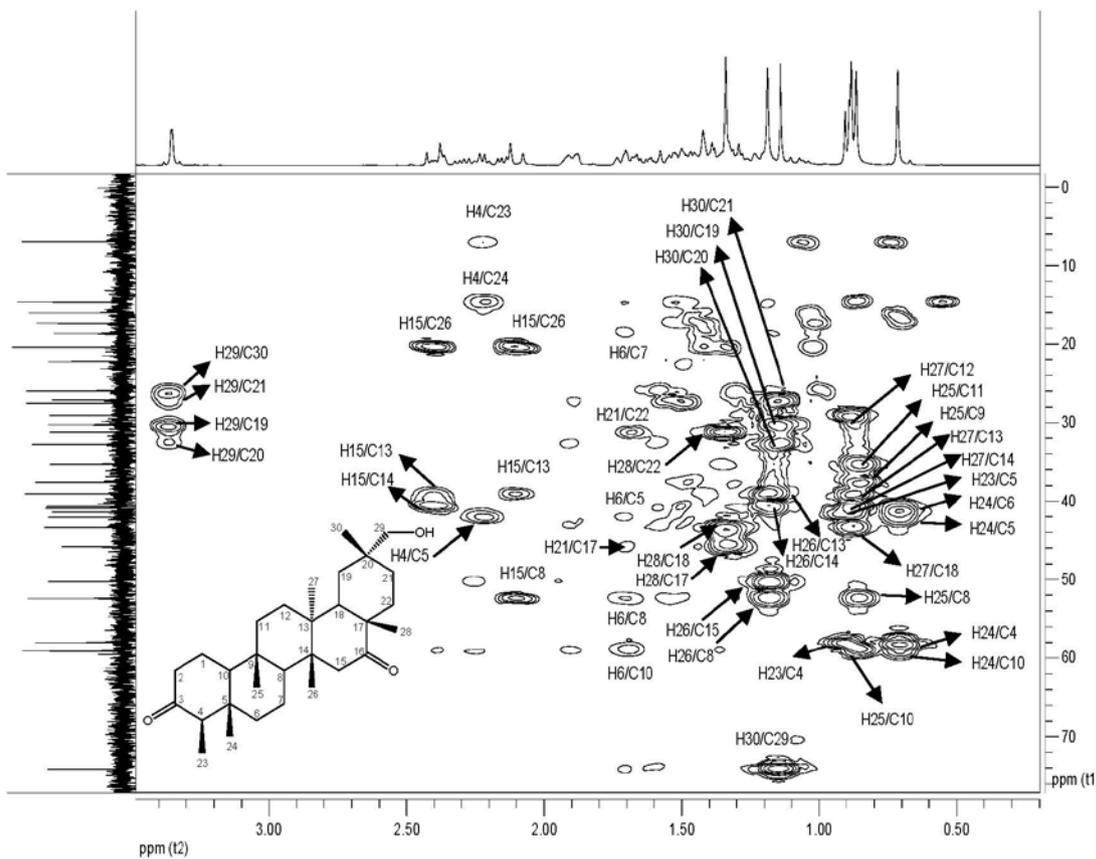


Figure S6. HMBC correlation of compound **1** ( $\text{CDCl}_3 + \text{Py}-d_5$ , 400 MHz).

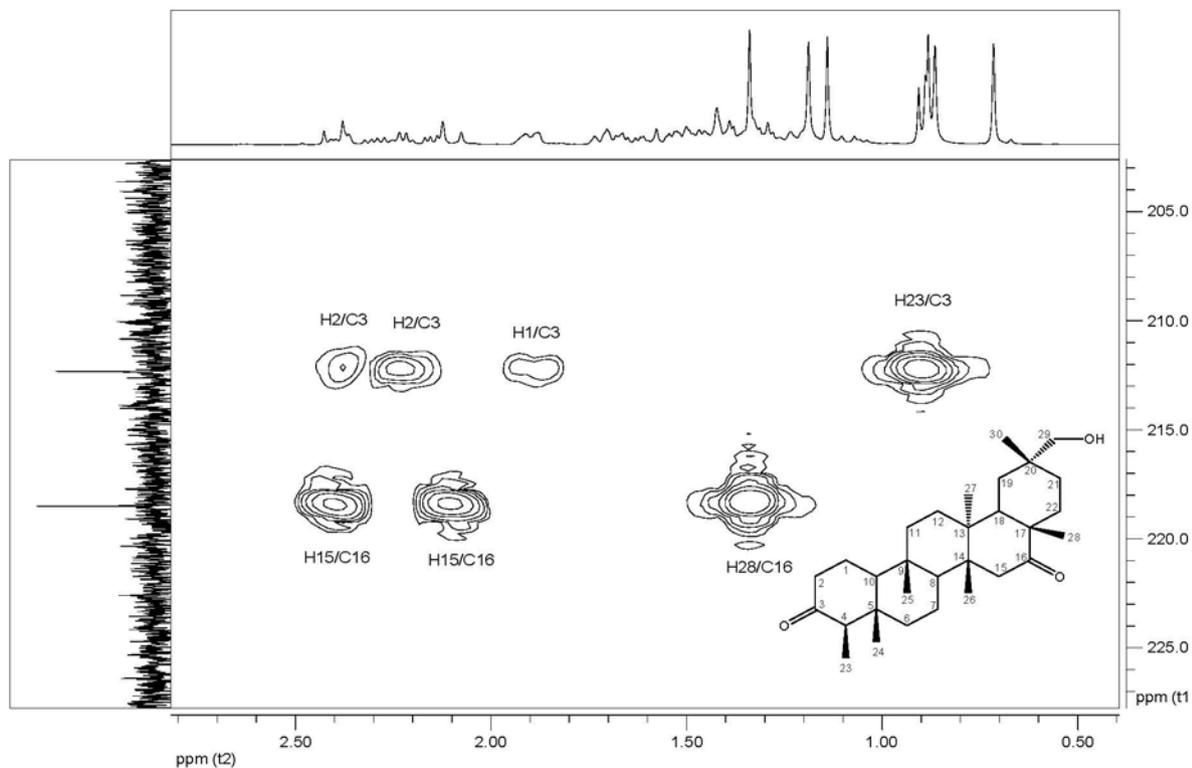


Figure S7. HMBC correlation of compound **1** (region of 2.8 to 0.5 ppm,  $\text{CDCl}_3 + \text{Py}-d_5$ , 400 MHz).



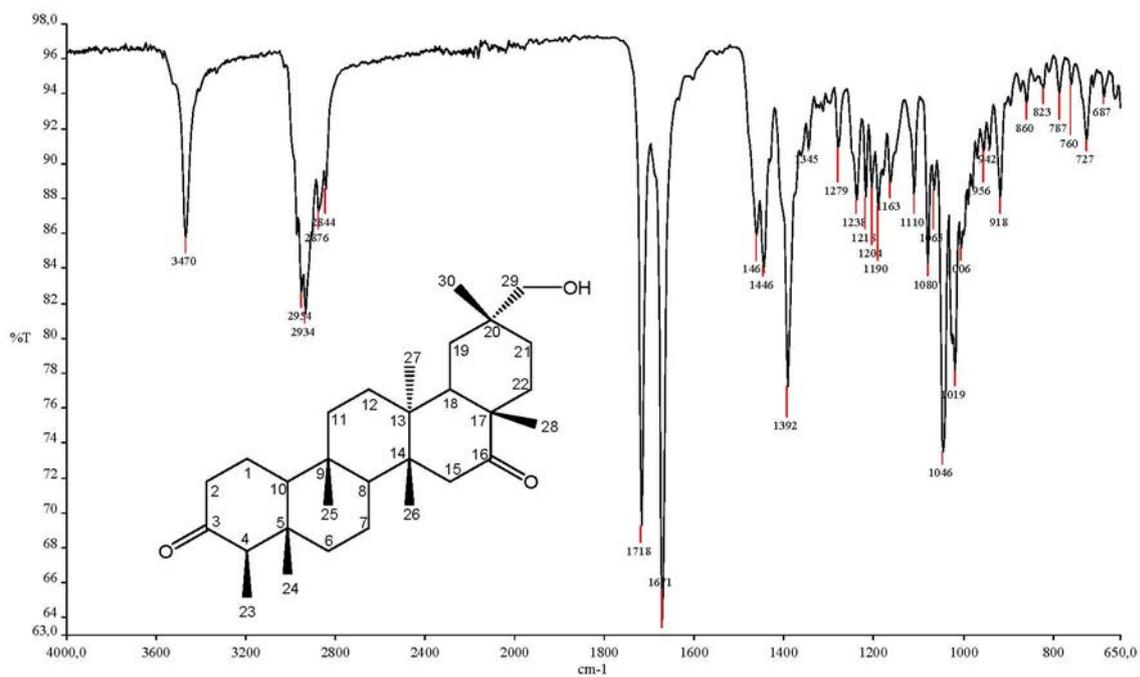


Figure S10. IR spectrum of compound 1 (ATR).

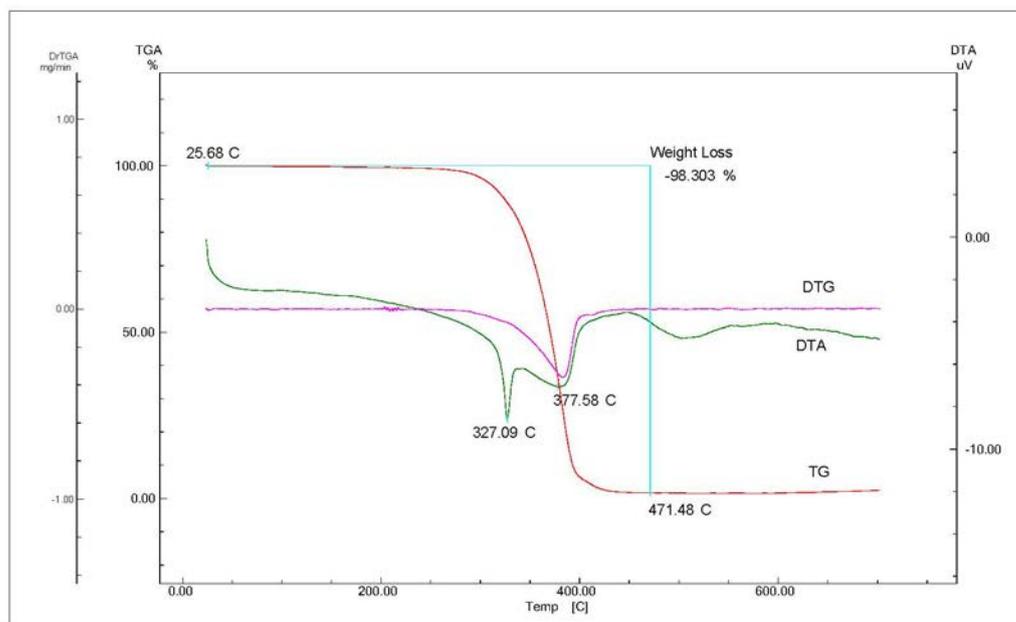


Figure S11. TG, DTG and DTA thermal curves of 1.

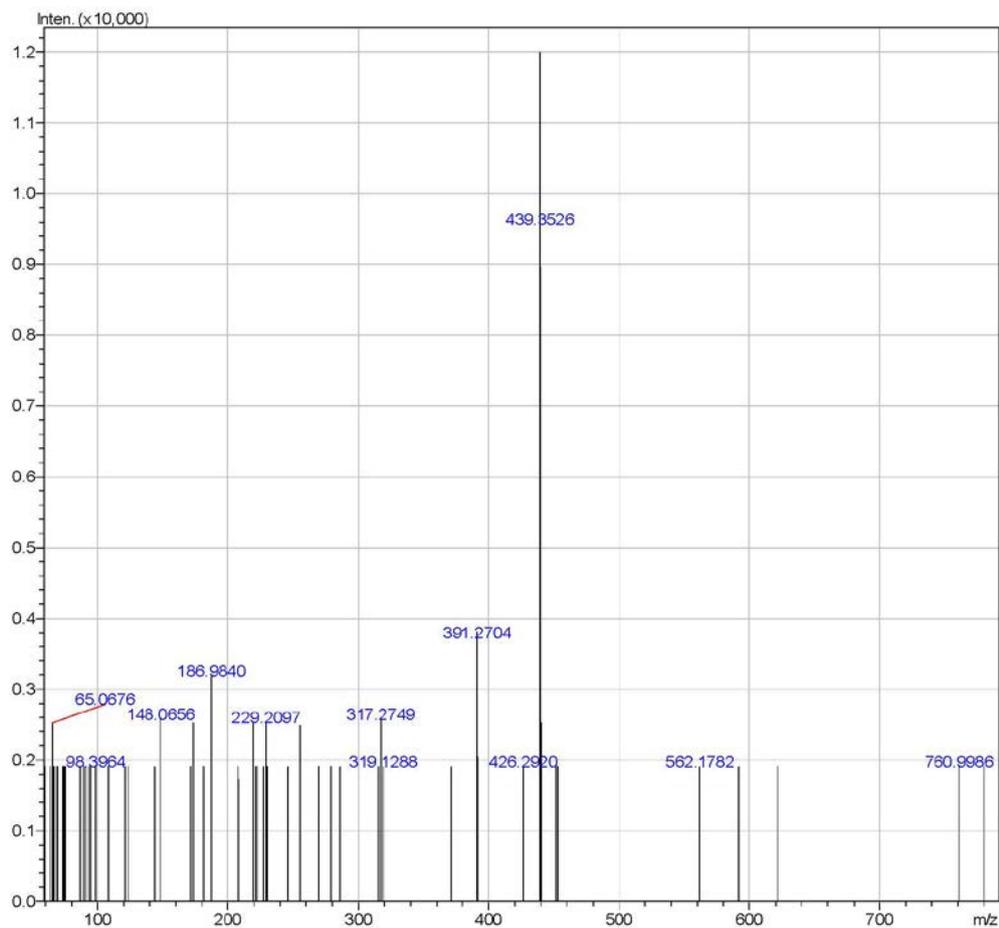


Figure S12. HR-APCIMS (positive-ion mode) spectrum of compound 1.

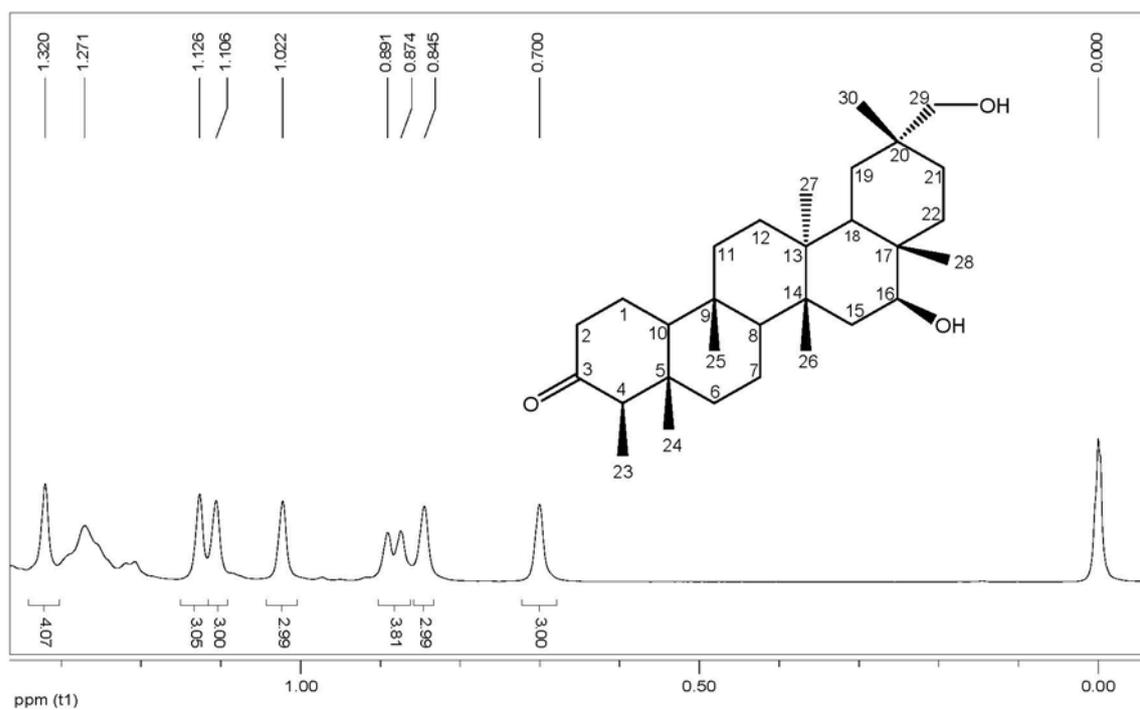


Figure S13. <sup>1</sup>H NMR spectrum of compound 2 (CDCl<sub>3</sub> + Py-d<sub>5</sub>, 400 MHz).

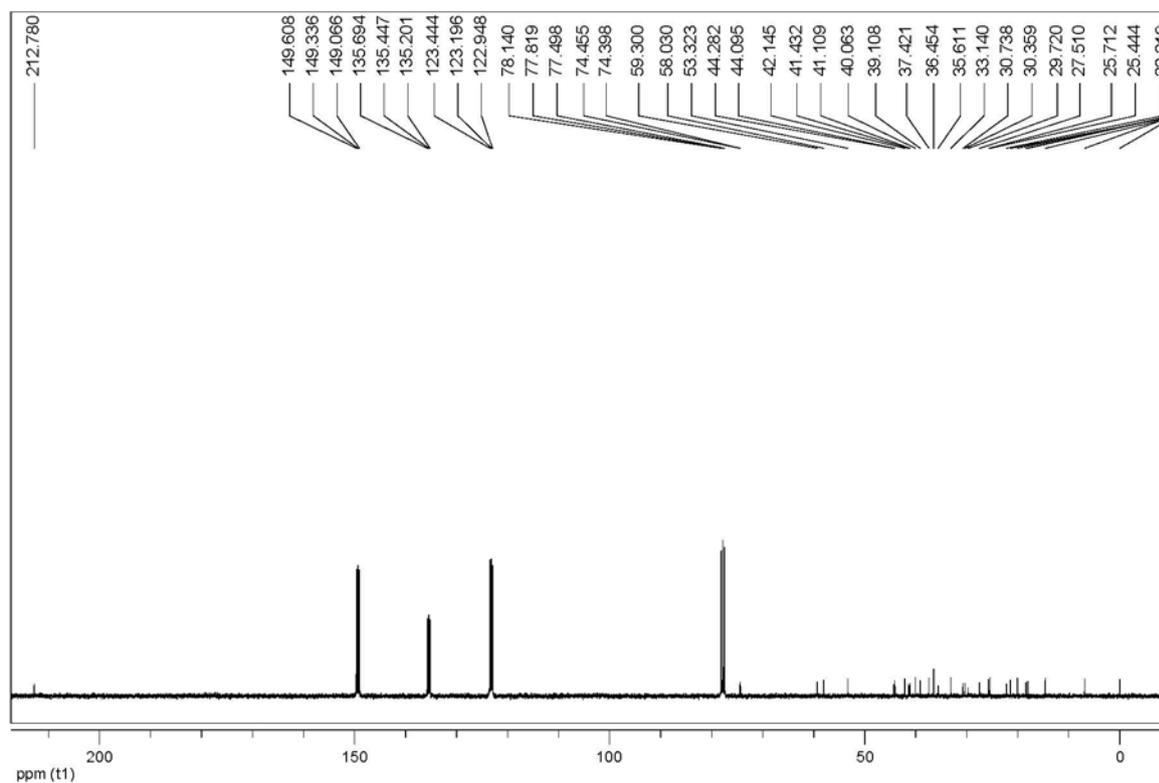


Figure S14.  $^1\text{H}$  NMR spectrum of compound **2** (region of 1.32 to 0 ppm,  $\text{CDCl}_3 + \text{Py}-d_5$ , 400 MHz).

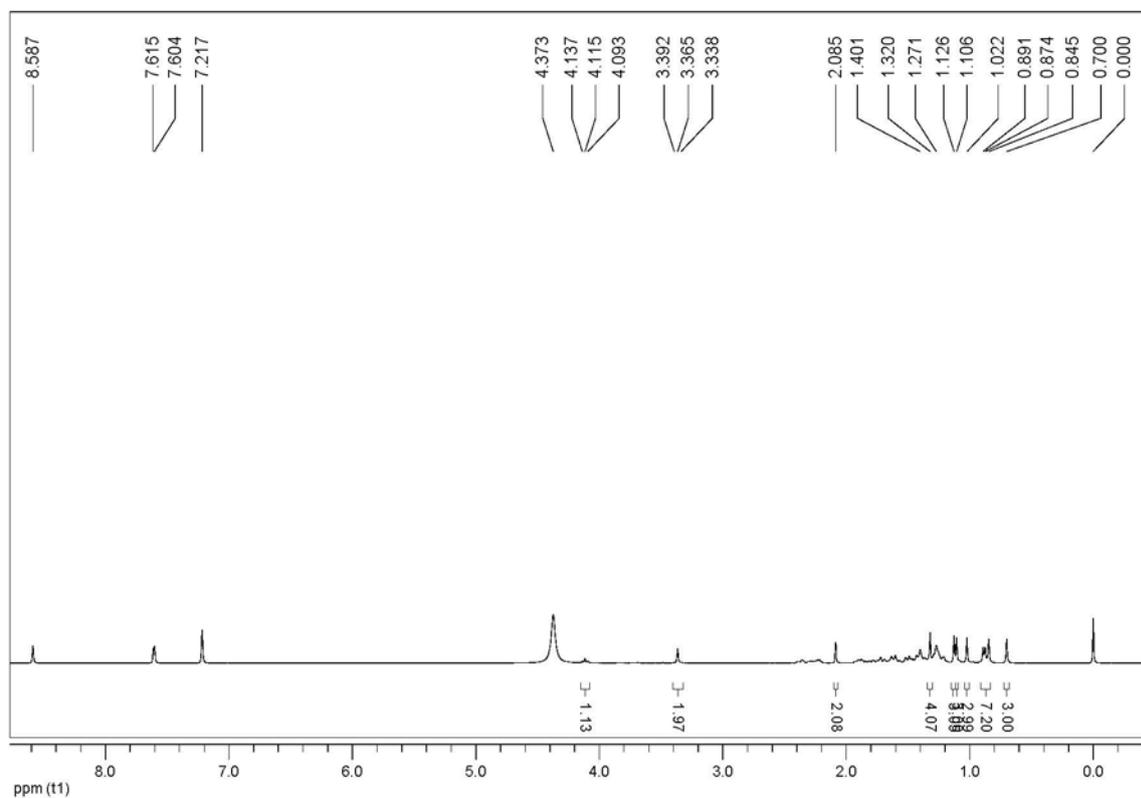
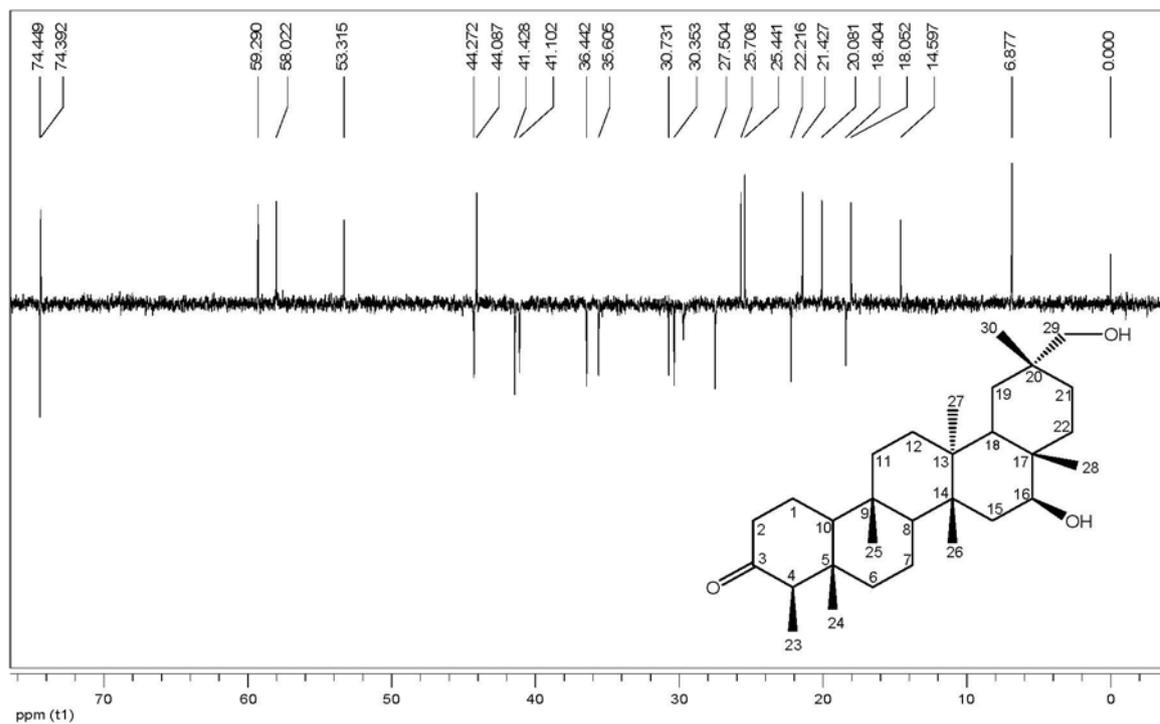
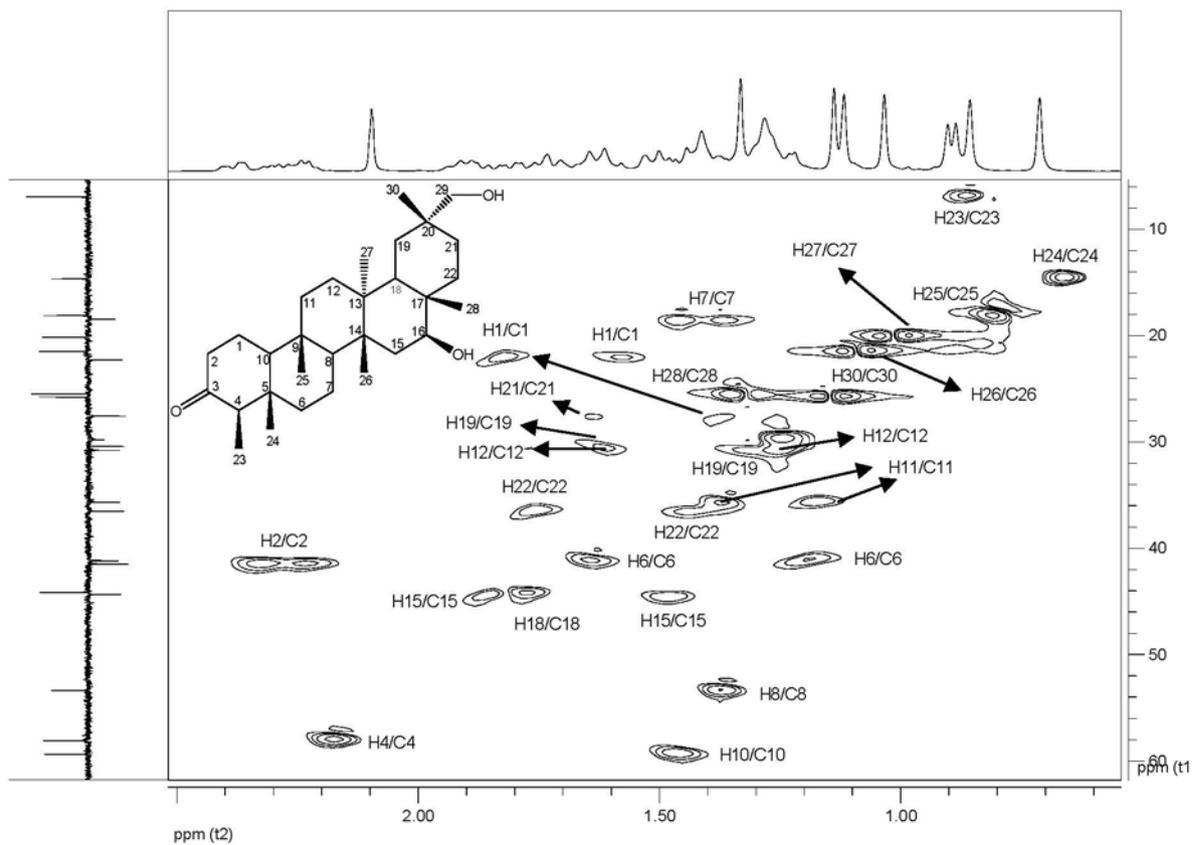


Figure S15.  $^{13}\text{C}$  NMR spectrum of compound **2** ( $\text{CDCl}_3 + \text{Py}-d_5$ , 100 MHz).



**Figure S16.** Subspectrum DEPT135 of compound **2** ( $\text{CDCl}_3 + \text{Py}-d_5$ , 100 MHz).



**Figure S17.** HSQC correlation of compound **2** ( $\text{CDCl}_3 + \text{Py}-d_5$ , 400 MHz).

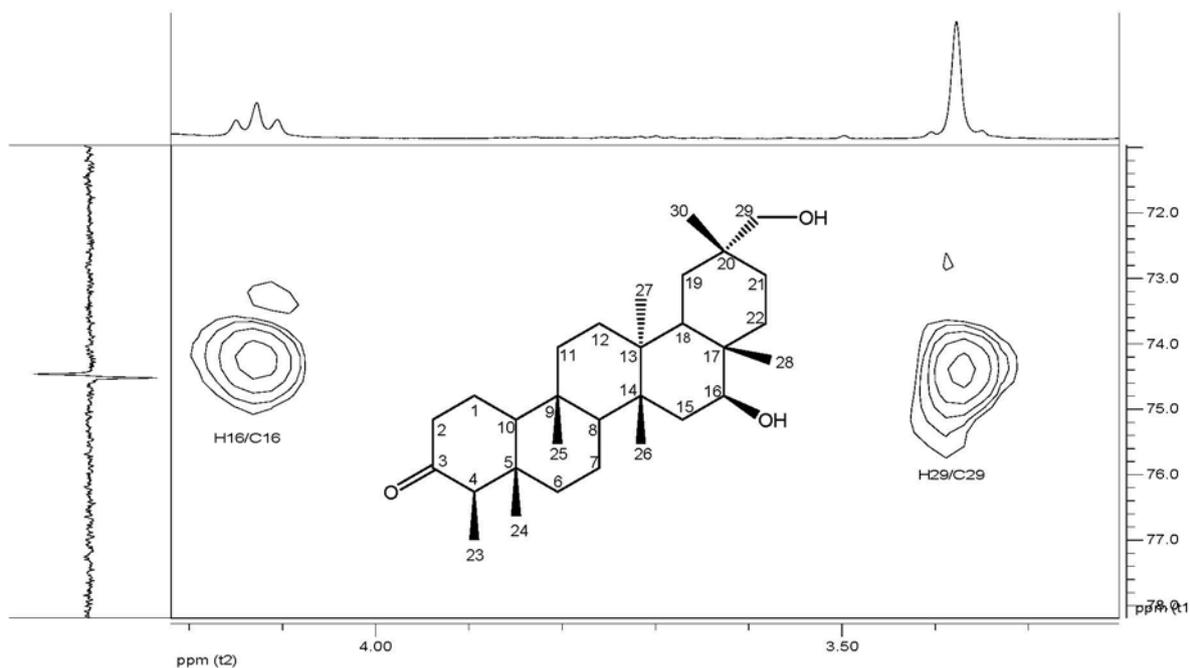


Figure S18. HSQC correlation of compound 2 (region of 4.2 to 3.3 ppm  $\text{CDCl}_3$  +  $\text{Py}-d_5$ , 400 MHz).

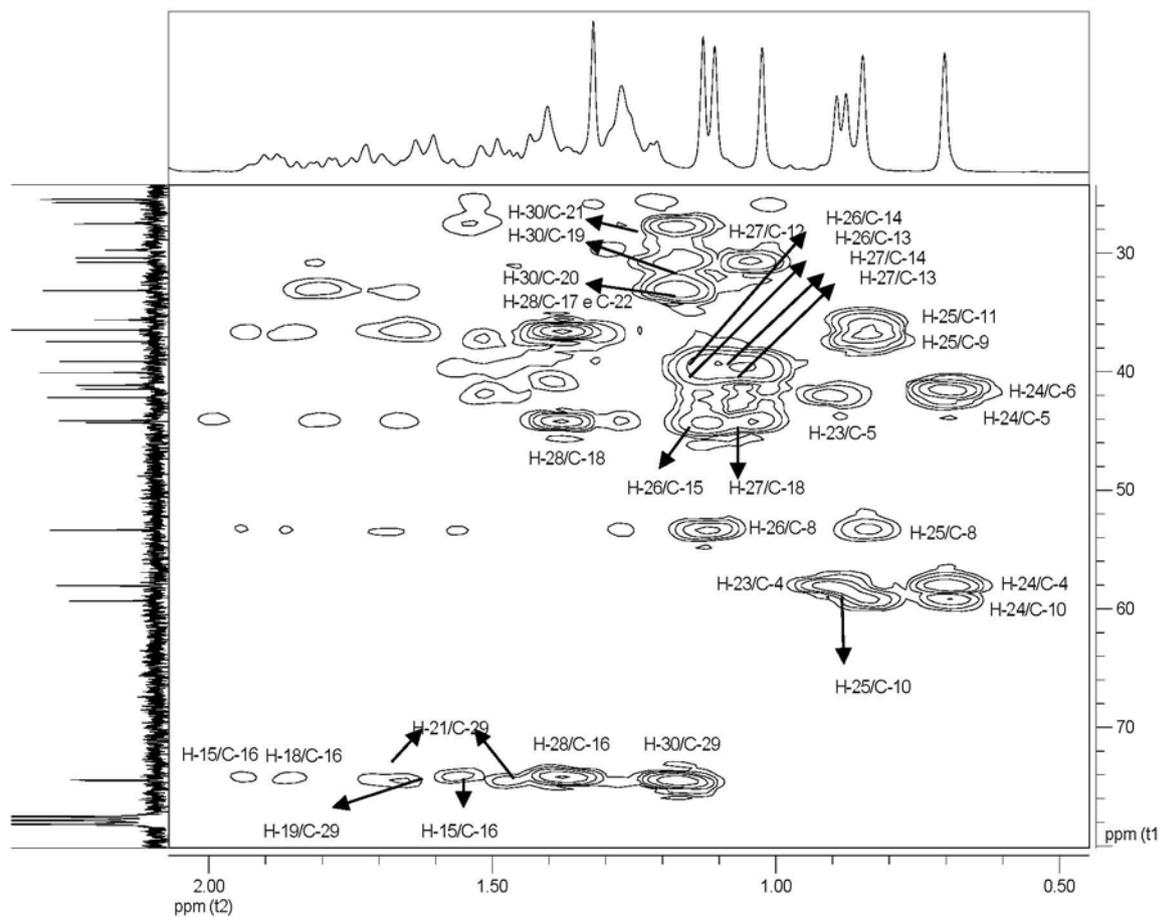
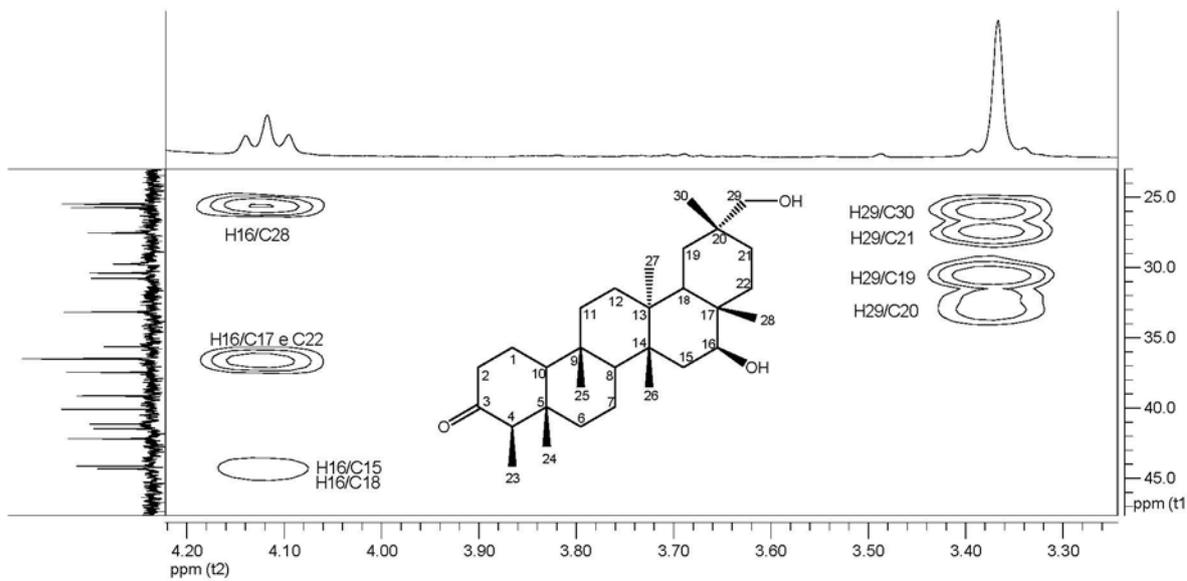
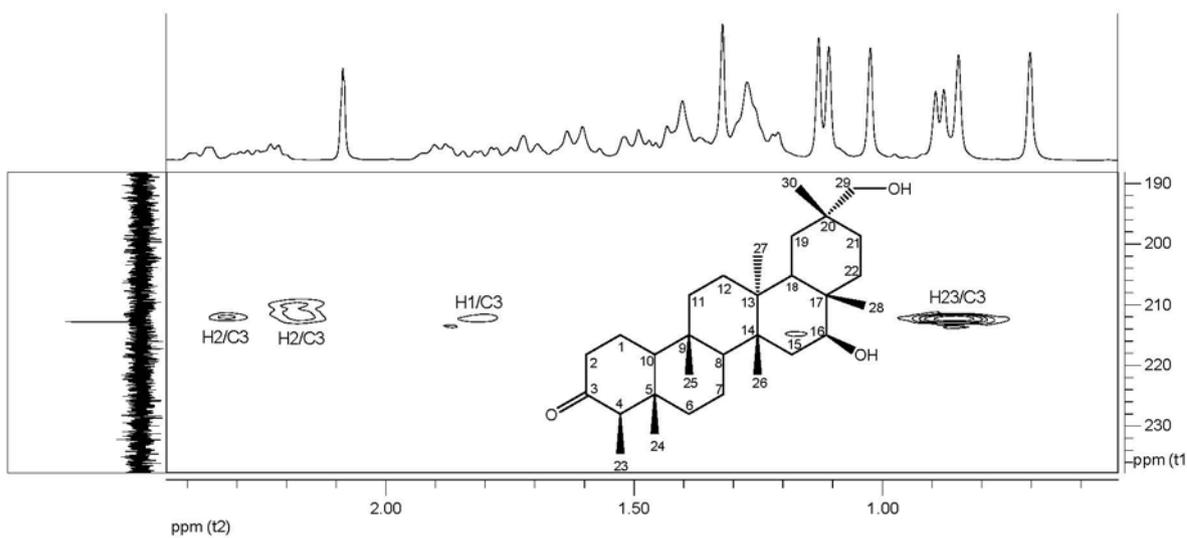


Figure S19. HMBC correlation of compound 2 ( $\text{CDCl}_3$  +  $\text{Py}-d_5$ , 400 MHz).



**Figure S20.** HMBC correlation of compound **2** (region of 4.2 to 3.3 ppm  $\text{CDCl}_3 + \text{Py}-d_5$ , 400 MHz).



**Figure S21.** HMBC correlation of compound **2** (region of 2.4 to 0.6 ppm  $\text{CDCl}_3 + \text{Py}-d_5$ , 400 MHz).

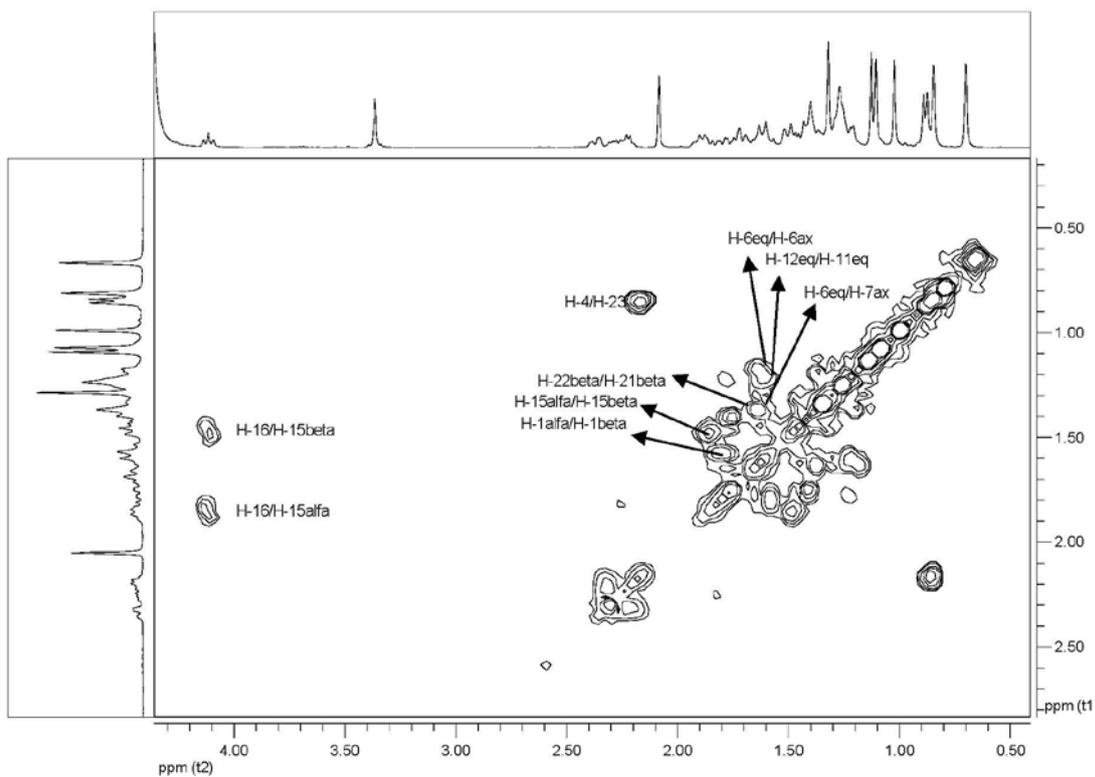


Figure S22. COSY correlation of compound 2 (CDCl<sub>3</sub> + Py-*d*<sub>5</sub>, 400 MHz).

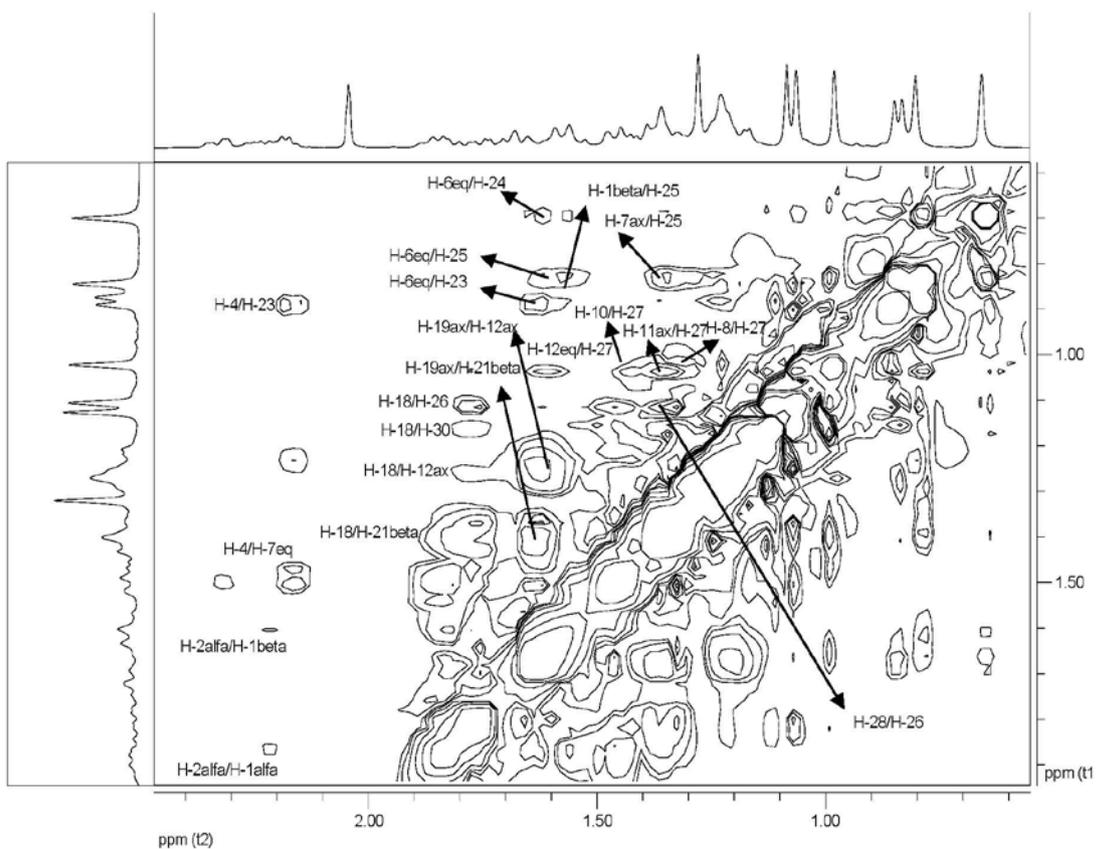
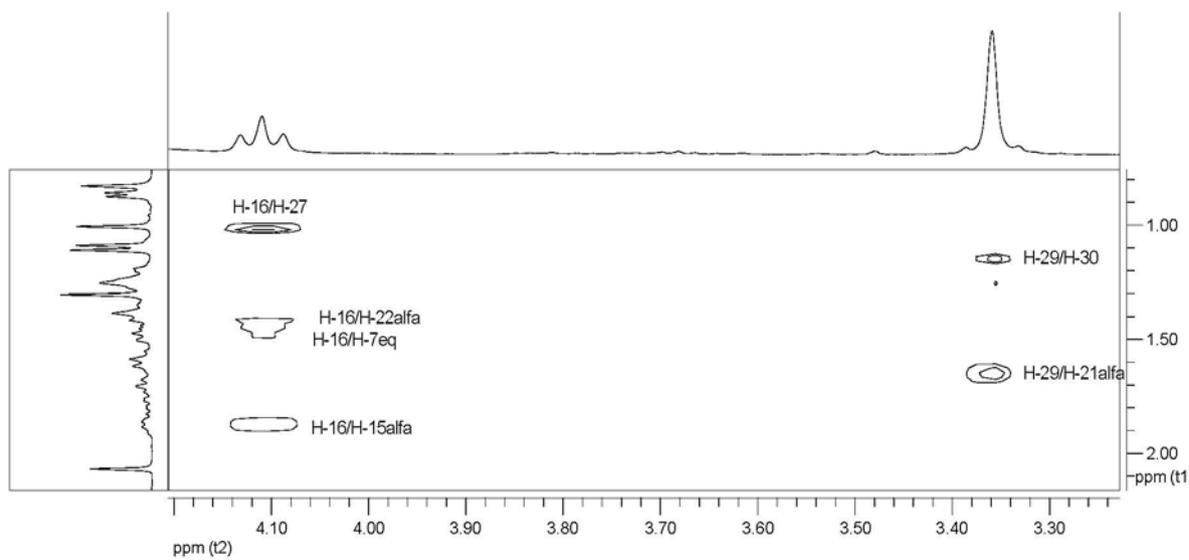
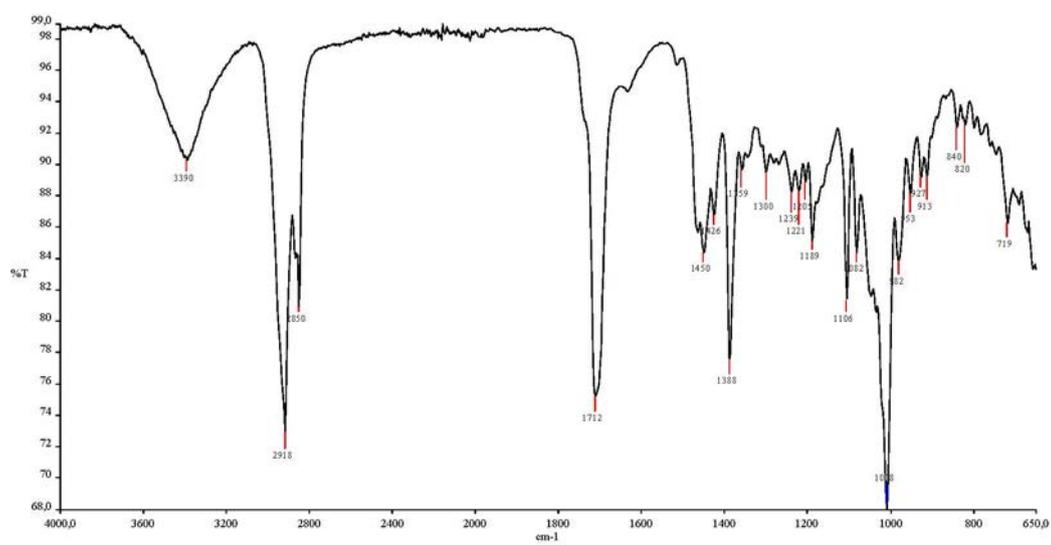


Figure S23. NOESY correlation of compound 2 (CDCl<sub>3</sub> + Py-*d*<sub>5</sub>, 400 MHz).



**Figure S24.** NOESY correlation of compound **2** (region of 4.2 to 3.3 ppm,  $\text{CDCl}_3 + \text{Py}-d_5$ , 400 MHz).



**Figure S25.** IR spectrum of compound **2** (ATR).

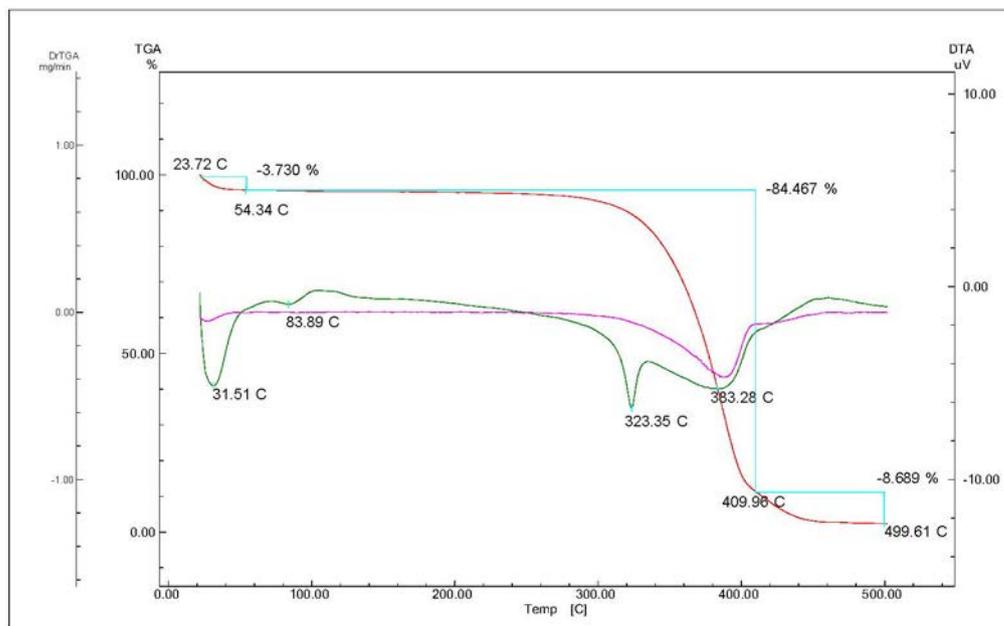


Figure S26. TG, DTG and DTA thermal curves of **2**.

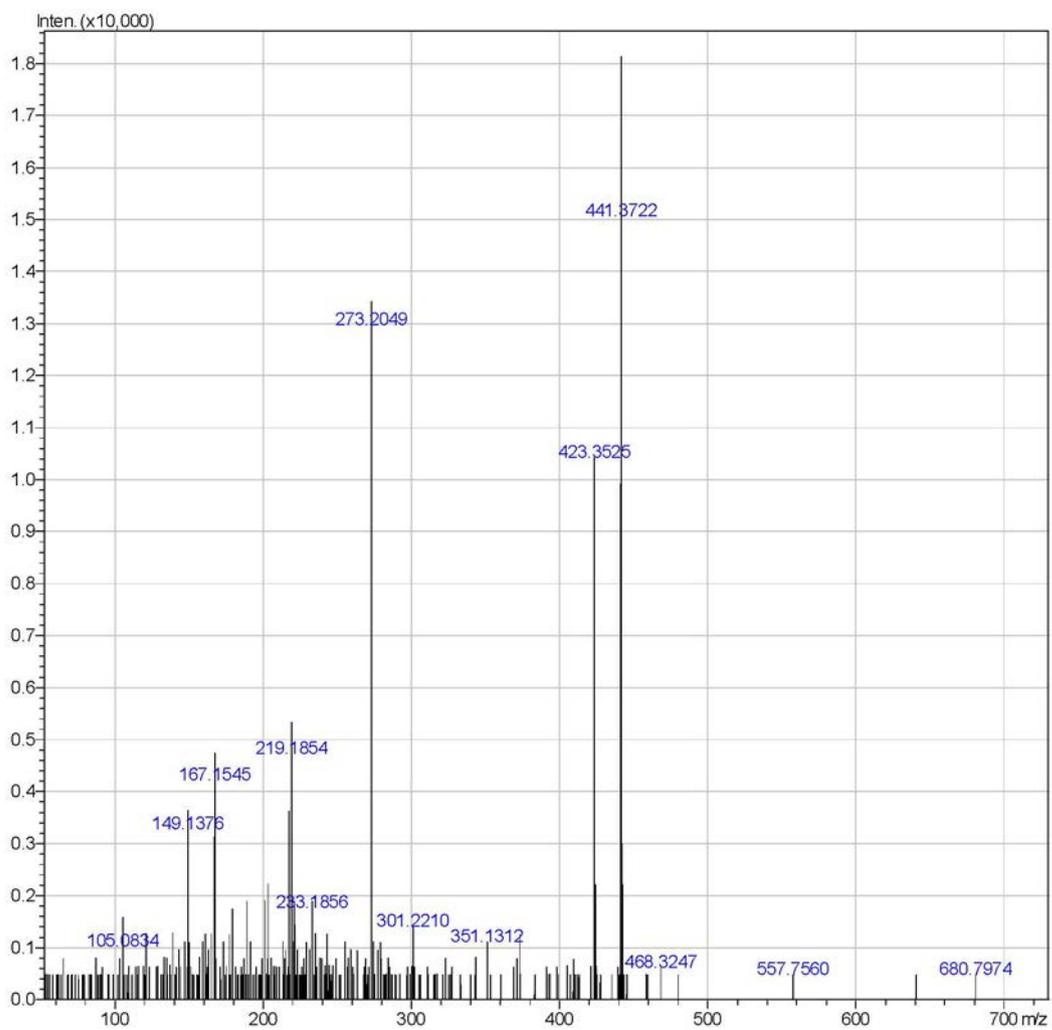


Figure S27. HR-APCIMS (positive-ion mode) spectrum of compound **2**.