

## Supplementary Information

### Synthesis and Evaluation of Cytotoxic Effects of Amino-ester Derivatives of Natural $\alpha,\beta$ -Amyrin Mixture

Mauricio M. Victor,<sup>\*a,b</sup> Jorge M. David,<sup>a,b</sup> Marcelo A. S. dos Santos,<sup>a,c</sup> André L. B. S. Barreiros,<sup>d</sup> Marizeth L. Barreiros,<sup>d</sup> Fernanda S. Andrade,<sup>d</sup> Adriana A. Carvalho,<sup>e</sup> Maria Claudia S. Luciano,<sup>f</sup> Manoel O. de Moraes,<sup>f</sup> Francisco W. A. Barros-Nepomuceno<sup>g</sup> and Claudia Pessoa<sup>f,h</sup>

<sup>a</sup>Departamento de Química Orgânica, Instituto de Química, Universidade Federal da Bahia and  
<sup>b</sup>Instituto Nacional de Ciência e Tecnologia de Energia e Meio Ambiente, 40170-115 Salvador-BA, Brazil

<sup>c</sup>Instituto Federal de Educação, Ciência e Tecnologia da Bahia (IFBA),  
44096-486 Feira de Santana-BA, Brazil

<sup>d</sup>Departamento de Química and <sup>e</sup>Departamento de Fisiologia, Universidade Federal do Sergipe,  
49000-100 São Cristóvão-SE, Brazil

<sup>f</sup>Núcleo de Pesquisa e Desenvolvimento de Medicamentos (NPDM), Universidade Federal do Ceará,  
60430-275 Fortaleza-CE, Brazil

<sup>g</sup>Universidade da Integração Internacional da Lusofonia Afro-Brasileira (UNILAB),  
62785-000 Acarape-CE, Brazil

<sup>h</sup>Fundação Oswaldo Cruz, 60176-032 Fortaleza-CE, Brazil

#### Compound 2a,b

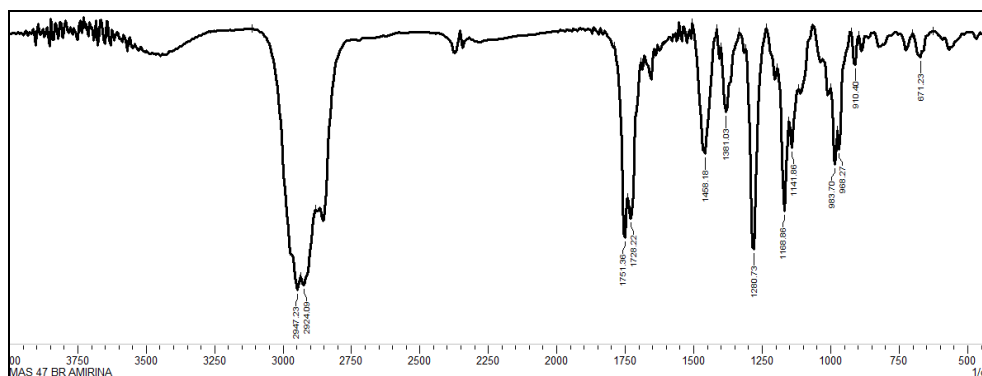
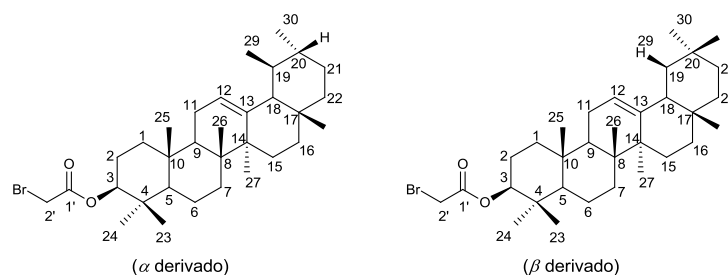
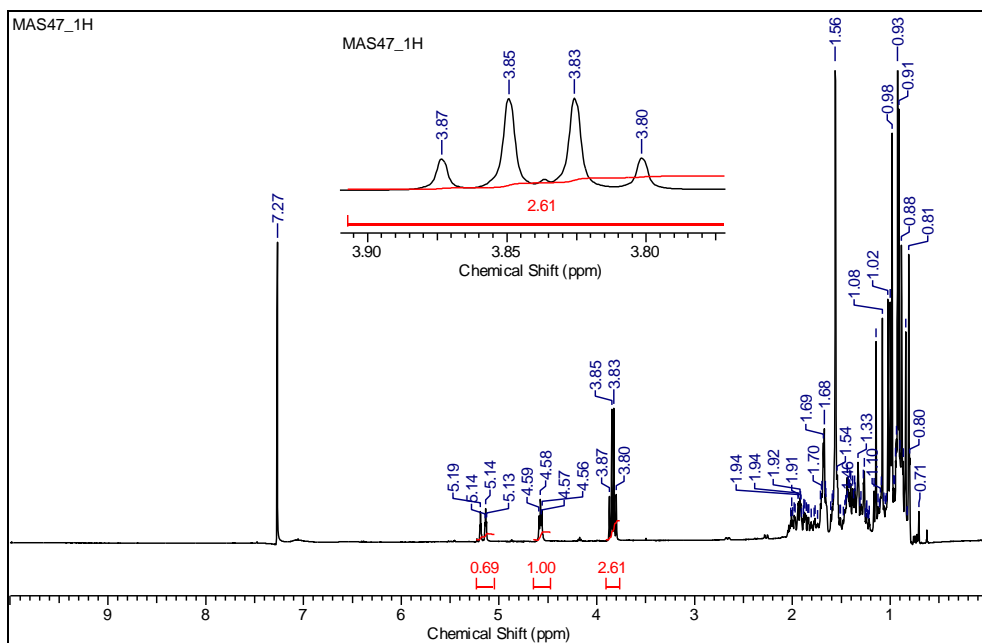
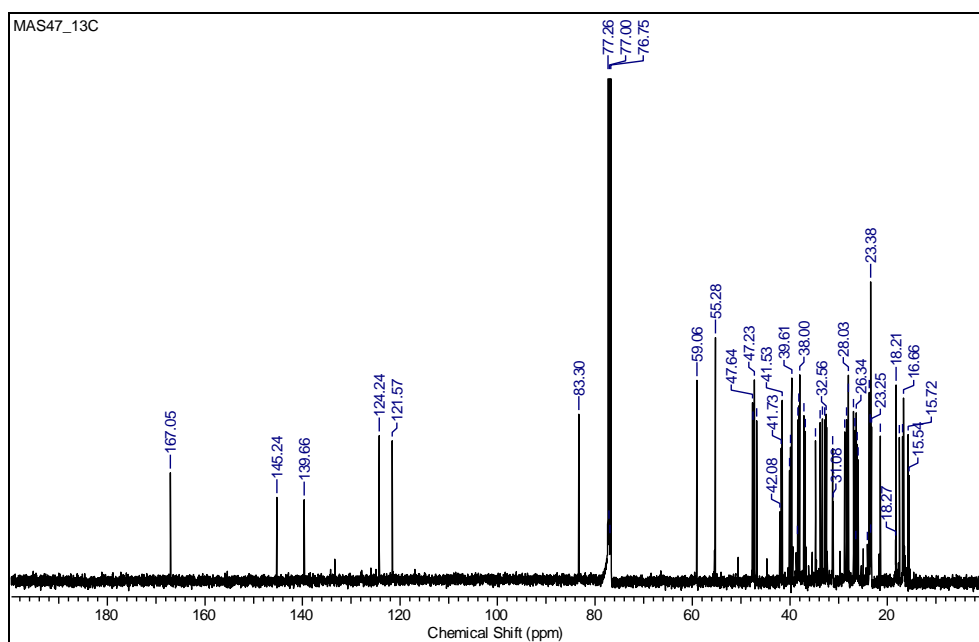


Figure S1. FTIR spectrum (KBr) of 3-bromoacetyl- $\alpha,\beta$ -amyrin esters (2a,b).

\*e-mail: mmvictor@ufba.br

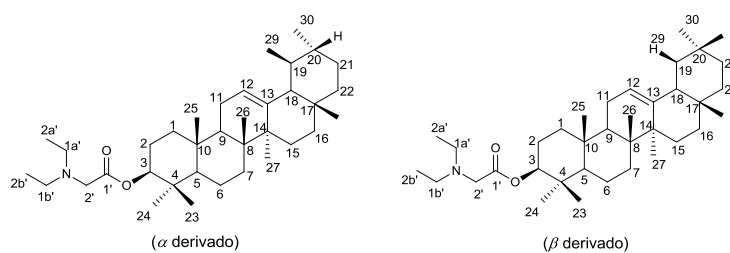


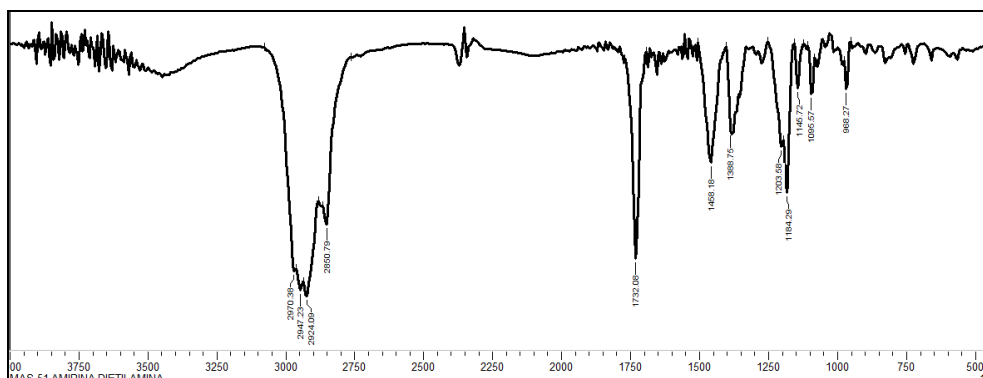
**Figure S2.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CDCl}_3$ ) of 3-bromoacetyl- $\alpha,\beta$ -amyrin esters (**2a,b**).



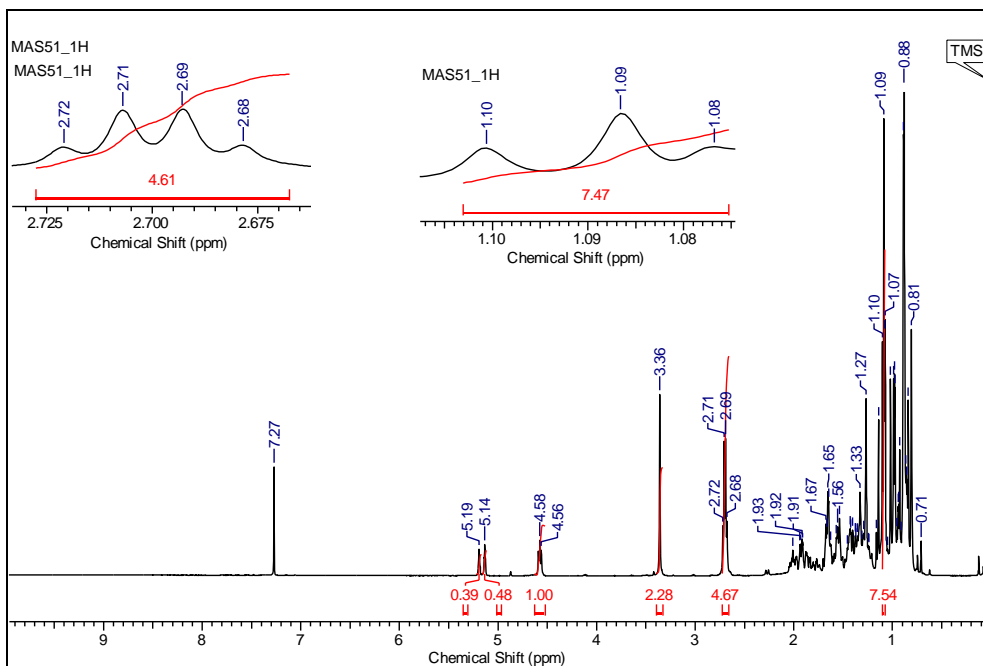
**Figure S3.**  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CDCl}_3$ ) of 3-bromoacetyl- $\alpha,\beta$ -amyrin esters (**2a,b**).

**Compound 3a,b**

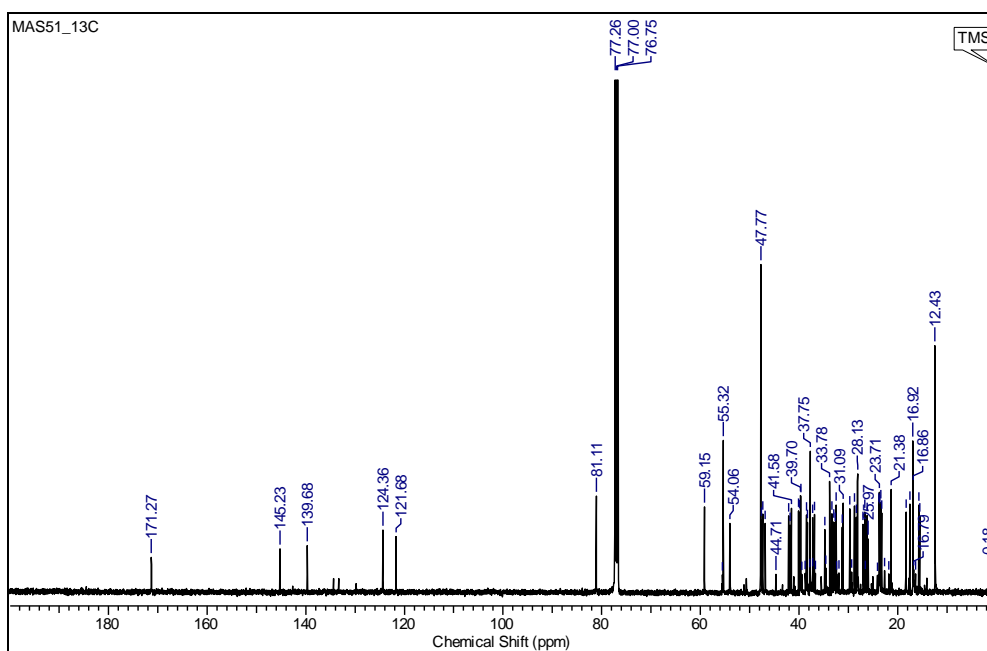




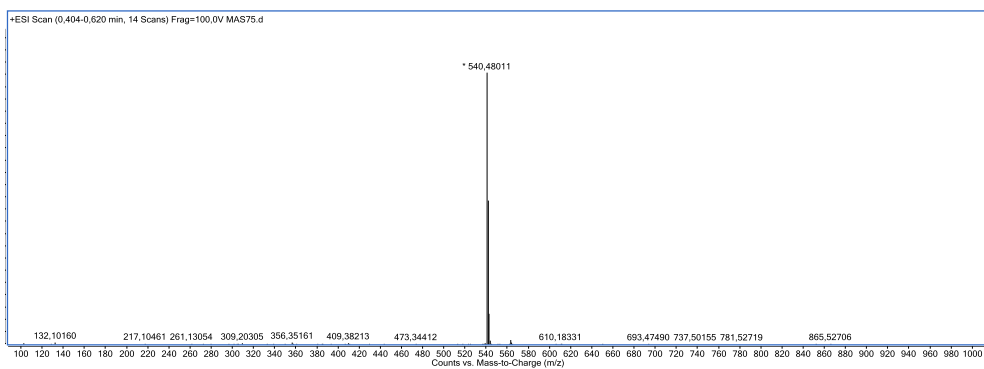
**Figure S4.** FTIR spectrum (KBr) of  $\alpha$ -diethylaminoacetyl- $\alpha,\beta$ -amyrin esters (**3a,b**).



**Figure S5.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CDCl}_3$ ) of  $\alpha$ -diethylaminoacetyl- $\alpha,\beta$ -amyrin esters (**3a,b**).

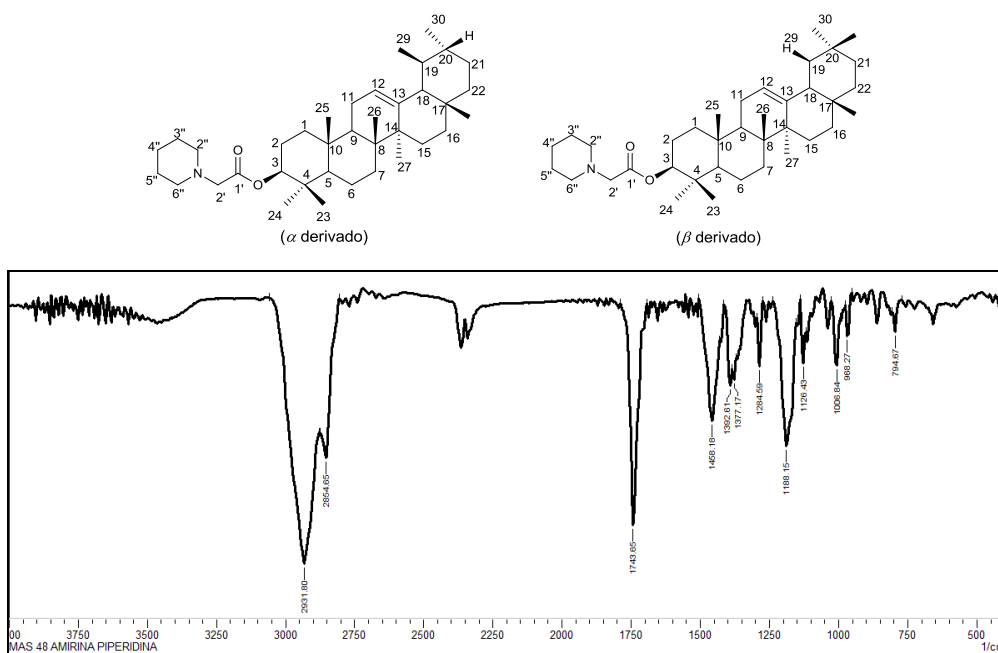


**Figure S6.**  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CDCl}_3$ ) of  $\alpha$ -diethylaminoacetyl- $\alpha,\beta$ -amyrin esters (**3a,b**).

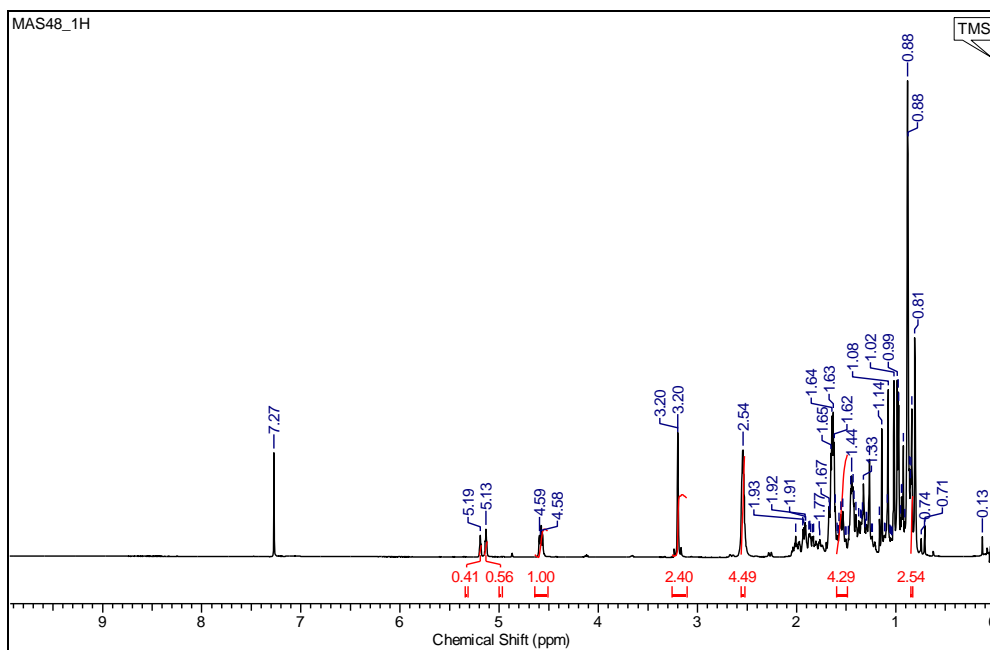


**Figure S7.** ESI-HRMS spectrum of  $\alpha$ -diethylaminoacetyl- $\alpha,\beta$ -amyryn esters (**3a,b**).

Compound **4a,b**



**Figure S8.** FTIR spectrum (KBr) of  $\alpha$ -piperidinoacetyl- $\alpha,\beta$ -amyryn esters (**4a,b**).



**Figure S9.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CDCl}_3$ ) of  $\alpha$ -piperidinoacetyl- $\alpha,\beta$ -amyryn esters (**4a,b**).

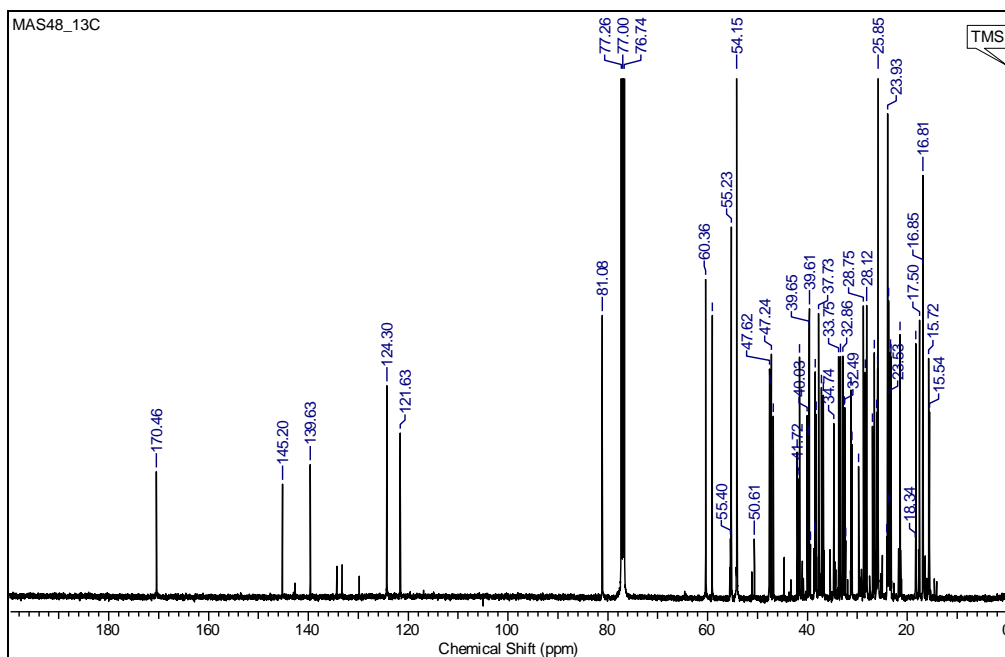


Figure S10.  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CDCl}_3$ ) of  $\alpha$ -piperidinoacetyl- $\alpha,\beta$ -amyryn esters (**4a,b**).

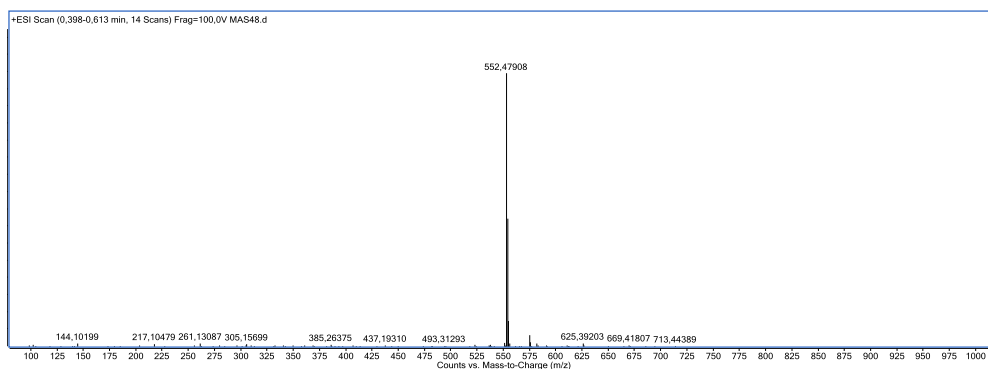


Figure S11. ESI-HRMS spectrum of  $\alpha$ -piperidinoacetyl- $\alpha,\beta$ -amyryn esters (**4a,b**).

Compound **5a,b**

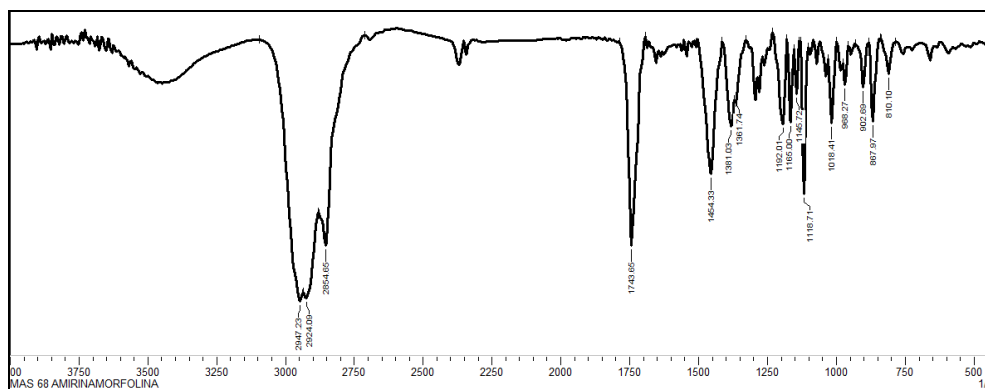
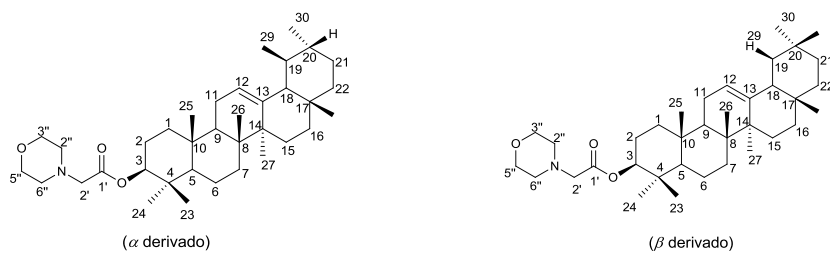
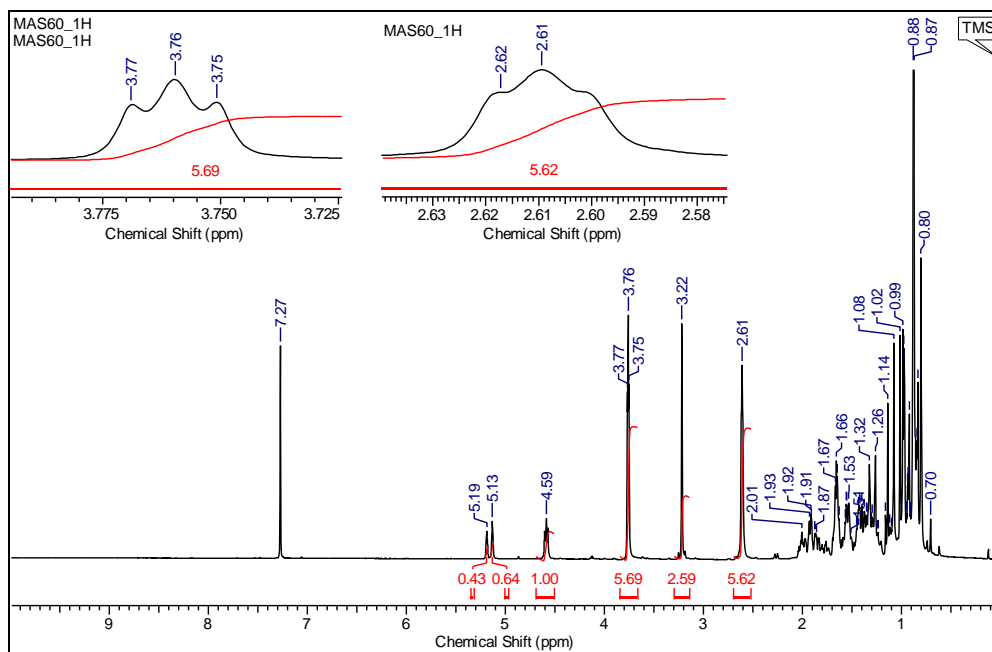
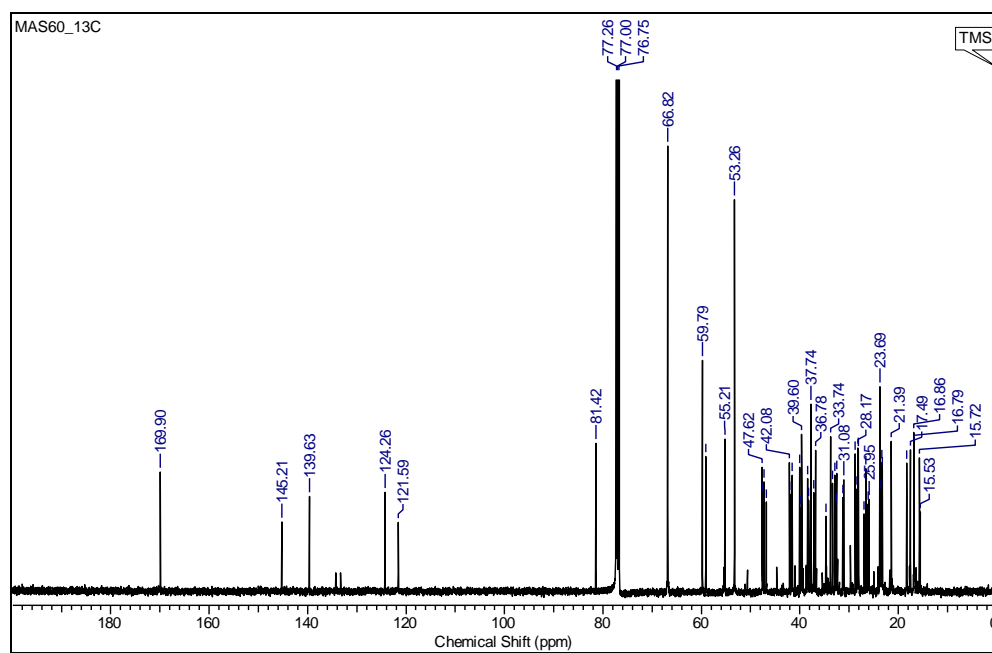


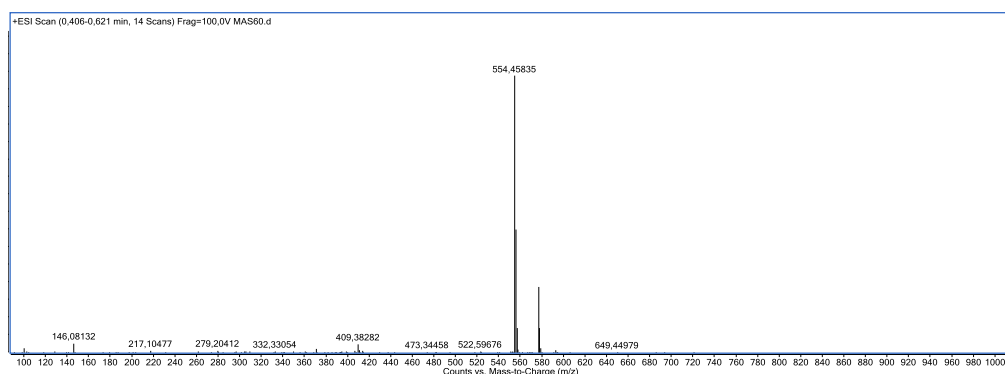
Figure S12. FTIR spectrum (KBr) of  $\alpha$ -morpholinoacetyl- $\alpha,\beta$ -amyryn esters (**5a,b**).



**Figure S13.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CDCl}_3$ ) of  $\alpha$ -morpholinoacetyl- $\alpha,\beta$ -amyrin esters (**5a,b**).



**Figure S14.**  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CDCl}_3$ ) of  $\alpha$ -morpholinoacetyl- $\alpha,\beta$ -amyrin esters (**5a,b**).



**Figure S15.** ESI-HRMS spectrum of  $\alpha$ -morpholinoacetyl- $\alpha,\beta$ -amyrin esters (**5a,b**).

Compound **6a,b**

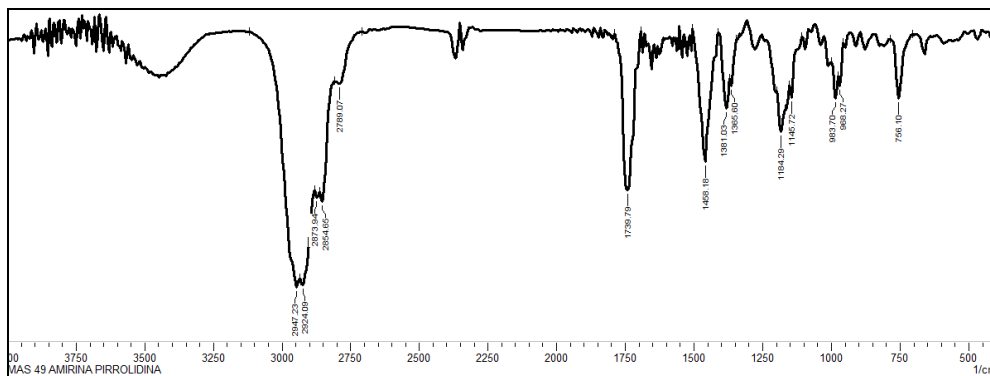
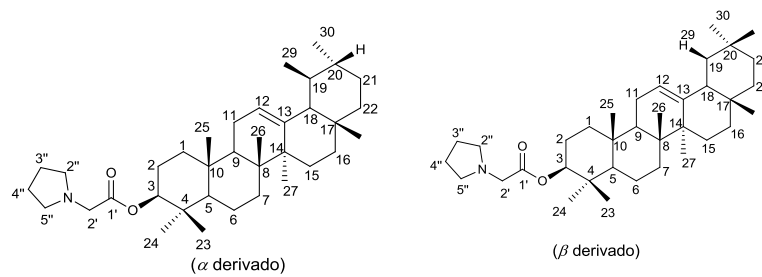


Figure S16. FTIR spectrum (KBr) of  $\alpha$ -pyrrolidinoacetyl- $\alpha,\beta$ -amyirin esters (**6a,b**).

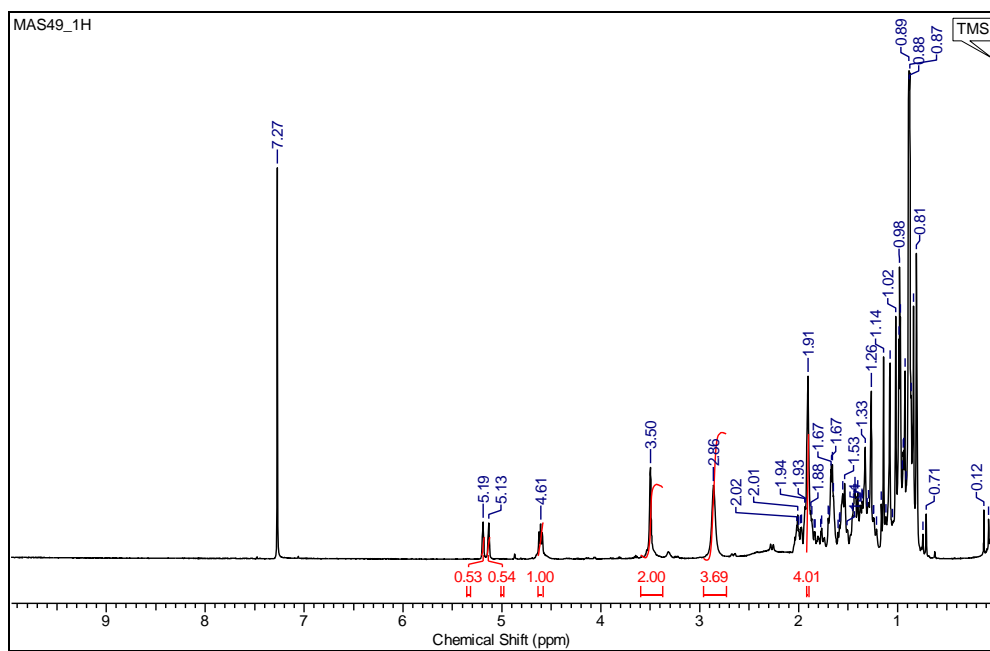
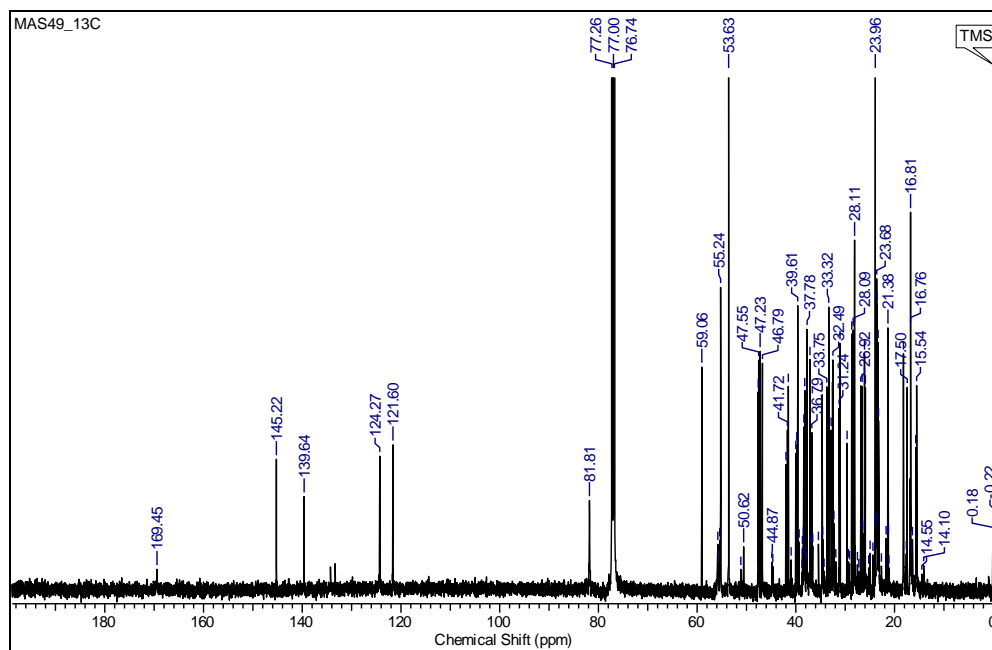
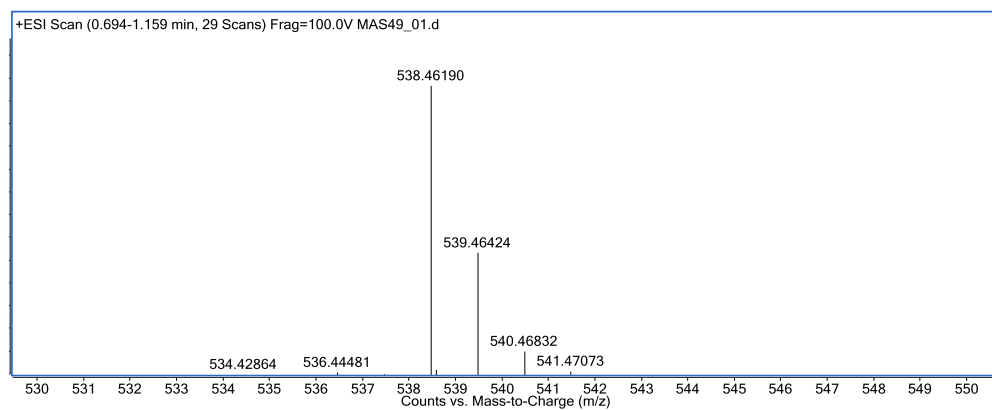


Figure S17.  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CDCl}_3$ ) of  $\alpha$ -pyrrolidinoacetyl- $\alpha,\beta$ -amyirin esters (**6a,b**).

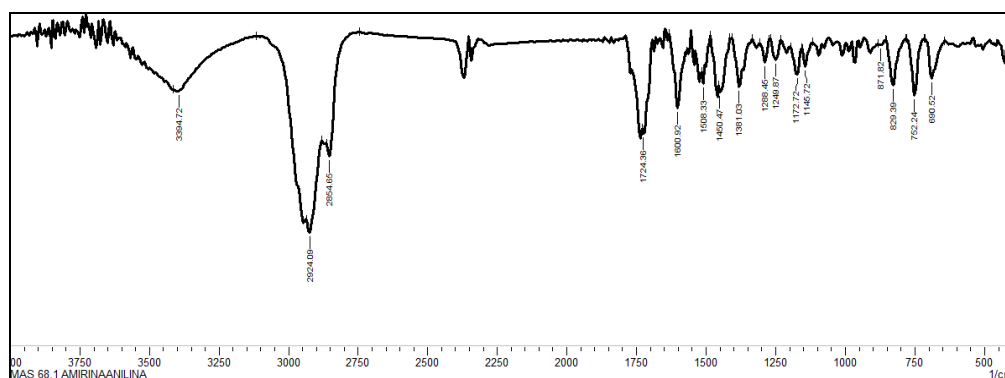
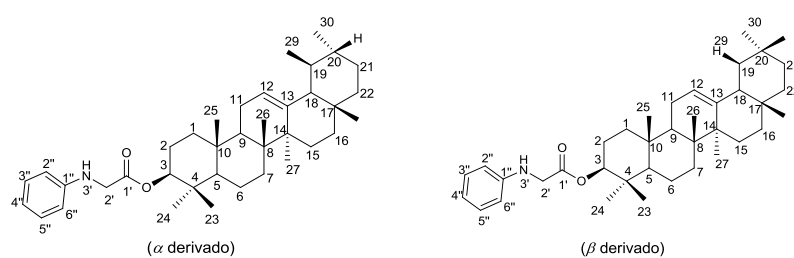


**Figure S18.**  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CDCl}_3$ ) of  $\alpha$ -pyrrolidinoacetyl- $\alpha,\beta$ -amyrin esters (**6a,b**).



**Figure S19.** ESI-HRMS spectrum of  $\alpha$ -pyrrolidinoacetyl- $\alpha,\beta$ -amyrin esters (**6a,b**).

### Compound **7a,b**



**Figure S20.** FTIR spectrum (KBr) of  $\alpha$ -anilinoacetyl- $\alpha,\beta$ -amyrin esters (**7a,b**).



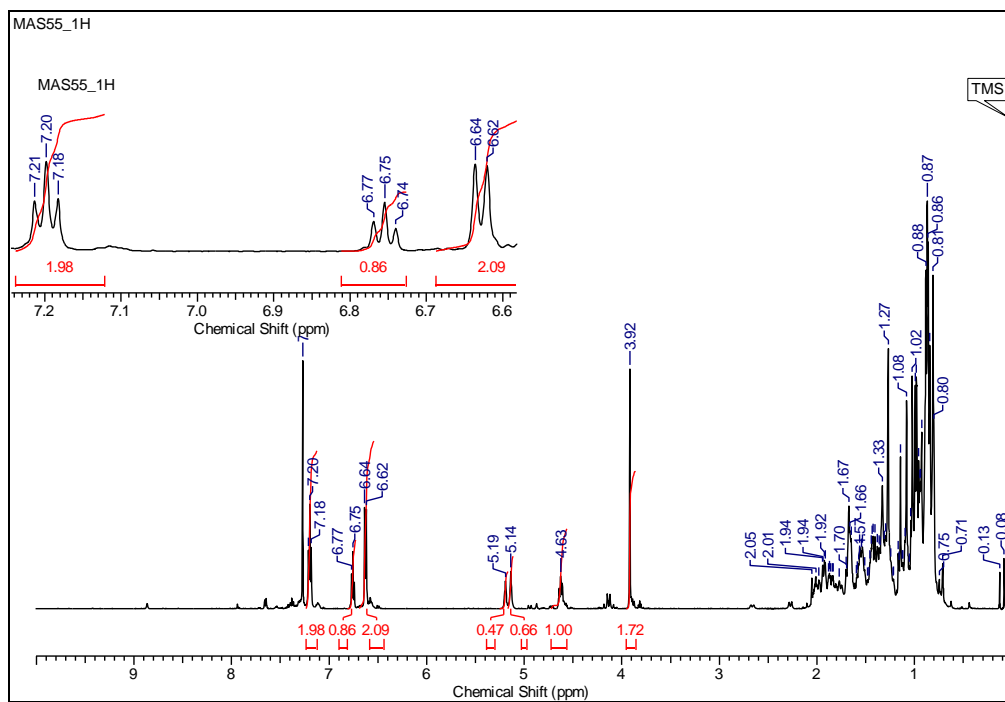


Figure S21.  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CDCl}_3$ ) of  $\alpha$ -anilinoacetyl- $\alpha,\beta$ -amyrin esters (**7a,b**).

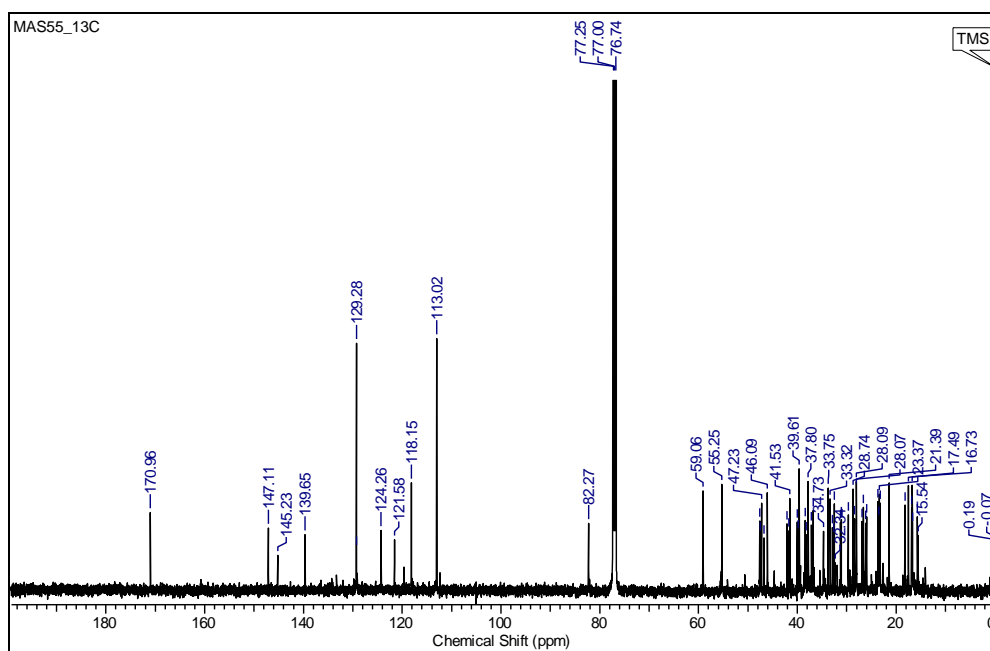


Figure S22.  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CDCl}_3$ ) of  $\alpha$ -anilinoacetyl- $\alpha,\beta$ -amyrin esters (**7a,b**).

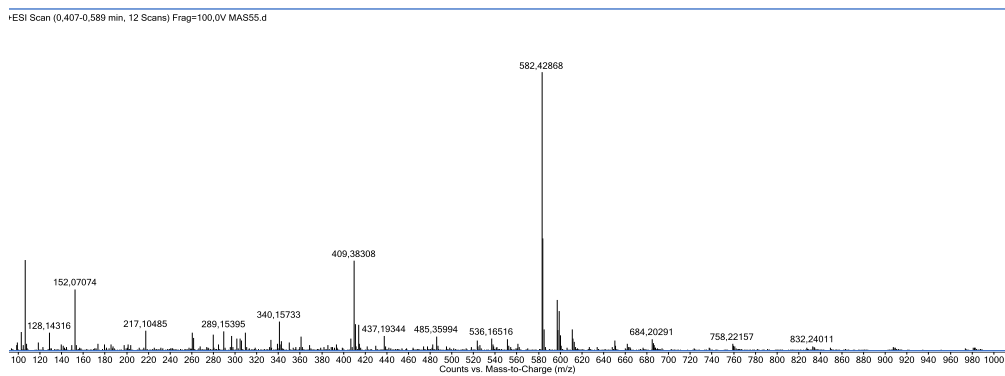


Figure S23. ESI-HRMS spectrum of  $\alpha$ -anilinoacetyl- $\alpha,\beta$ -amyrin esters (**7a,b**).

Compound **8a,b**

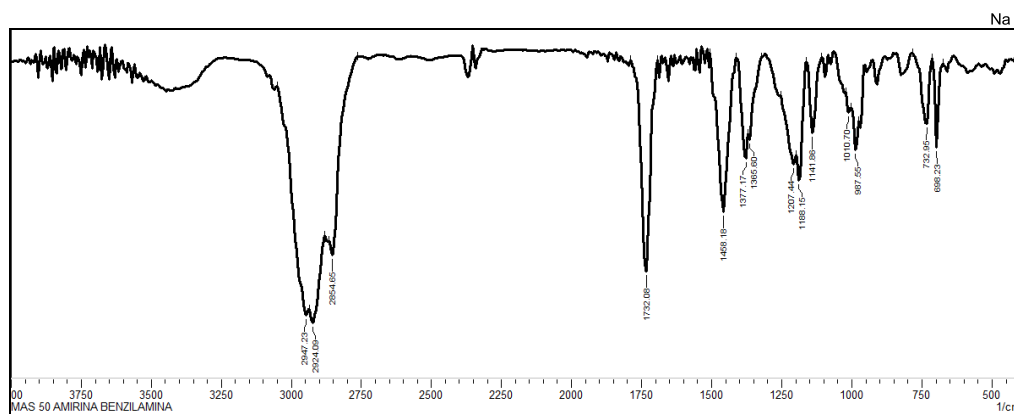
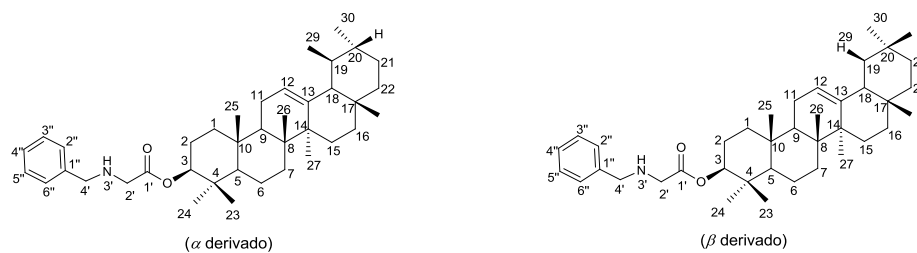


Figure S24. FTIR spectrum (KBr) of  $\alpha$ -benzylaminoacetyl- $\alpha,\beta$ -amyrin esters (**8a,b**).

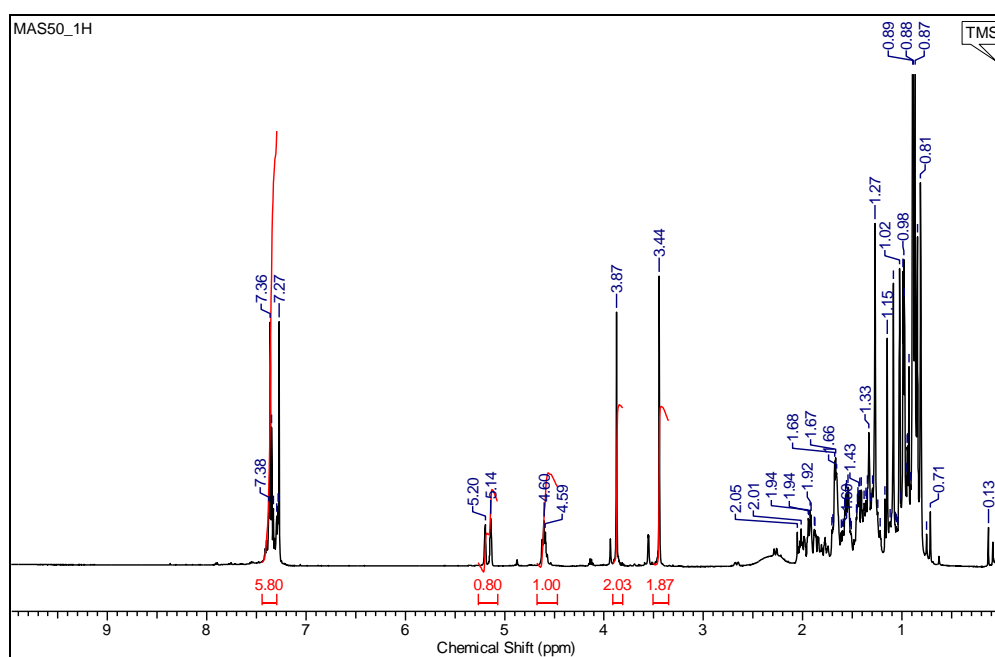
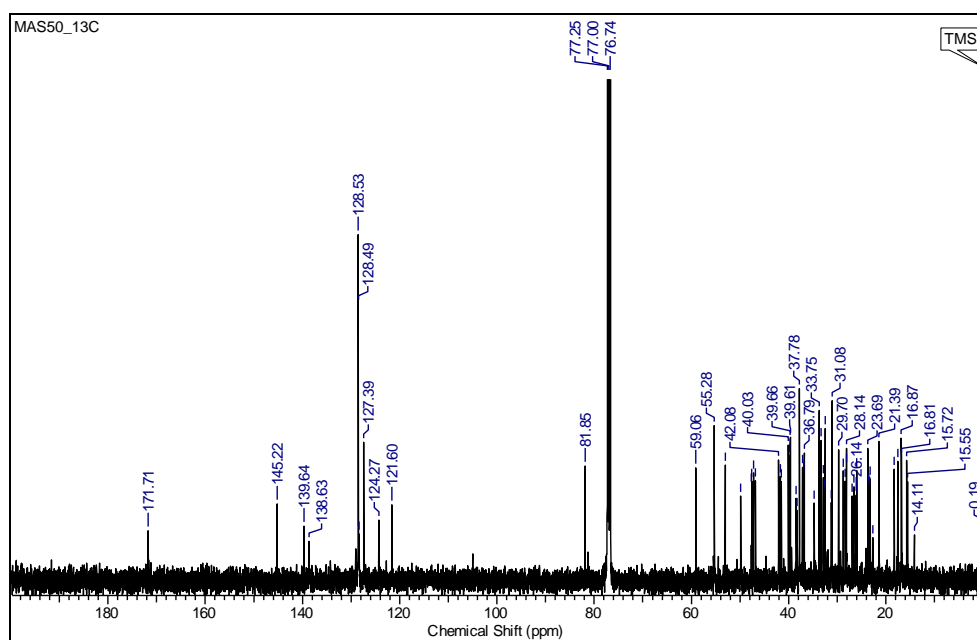
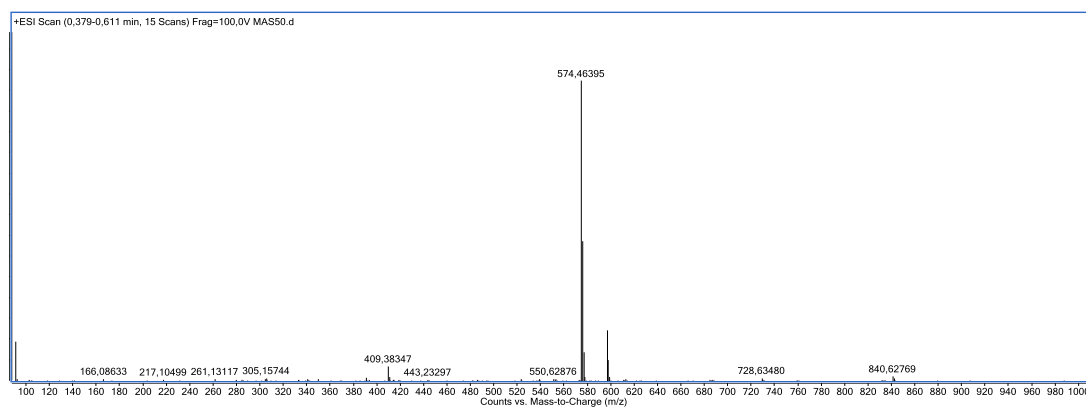


Figure S25.  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CDCl}_3$ ) of  $\alpha$ -benzylaminoacetyl- $\alpha,\beta$ -amyrin esters (**8a,b**).

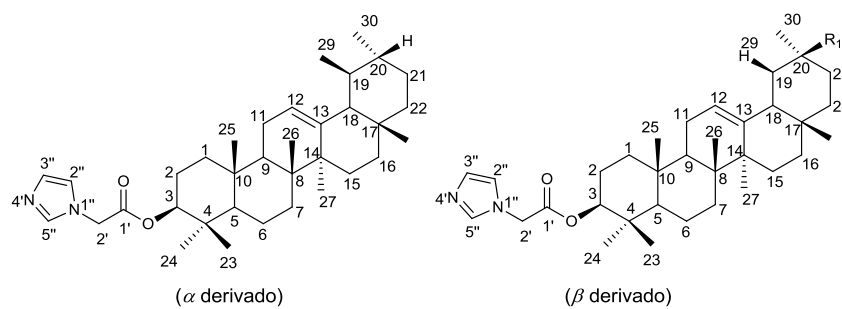


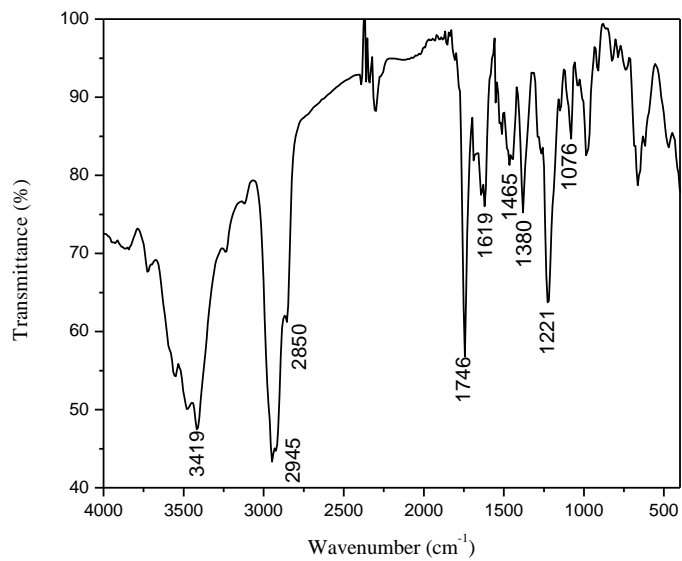
**Figure S26.**  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CDCl}_3$ ) of  $\alpha$ -benzylaminoacetyl- $\alpha,\beta$ -amyrin esters (**8a,b**).



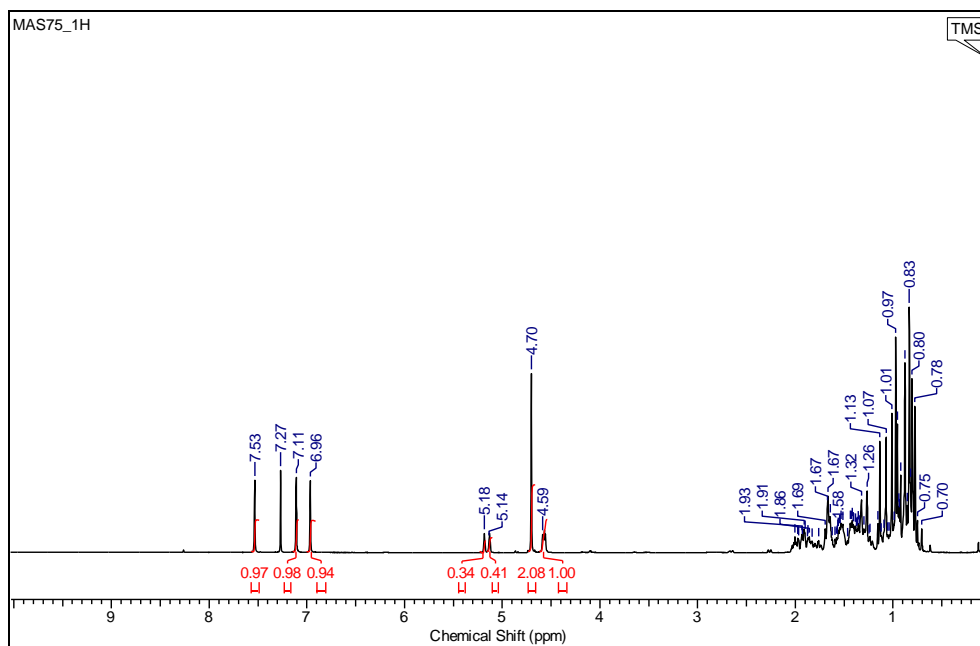
**Figure S27.** ESI-HRMS spectrum of  $\alpha$ -benzylaminoacetyl- $\alpha,\beta$ -amyrin esters (**8a,b**).

Compound **9a,b**





**Figure S28.** FTIR spectrum (KBr) of  $\alpha$ -imidazoacetyl- $\alpha,\beta$ -amyrin esters (**9a,b**).



**Figure S29.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CDCl}_3$ ) of  $\alpha$ -imidazoacetyl- $\alpha,\beta$ -amyrin esters (**9a,b**).

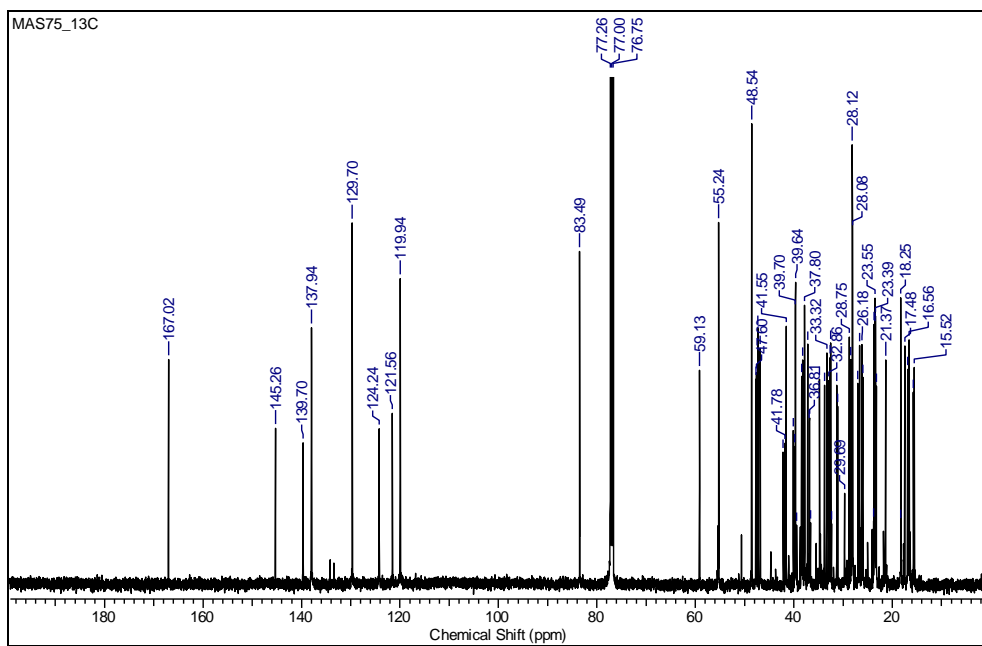


Figure S30.  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CDCl}_3$ ) of  $\alpha$ -imidazoacetyl- $\alpha,\beta$ -amyrin esters (**9a,b**).

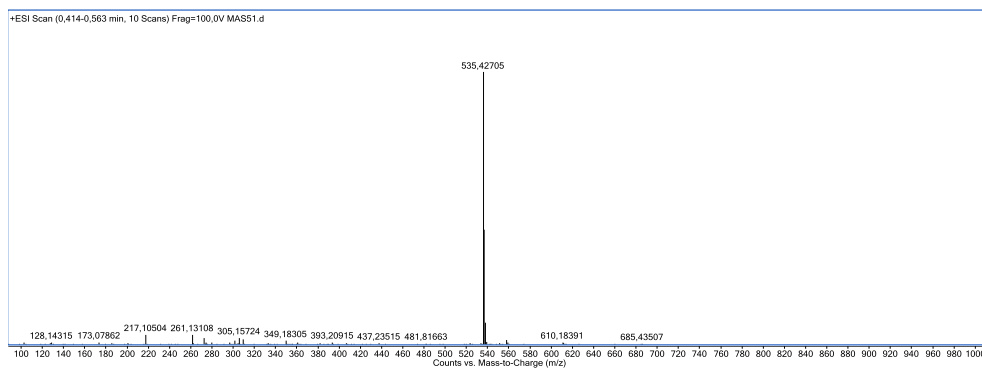


Figure S31. ESI-HRMS spectrum of  $\alpha$ -imidazoacetyl- $\alpha,\beta$ -amyrin esters (**9a,b**).