

# Supplementary Information

## PAMPA Permeability, Acetylcholinesterase Inhibition and Antioxidant Activity of Pyranoisoflavones from *Polygala molluginifolia* (Polygalaceae)

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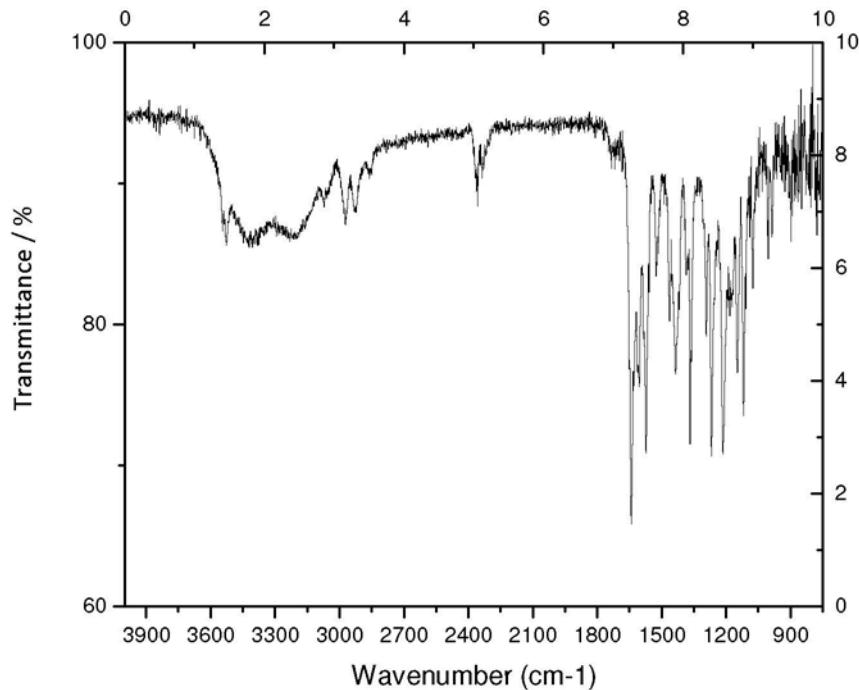
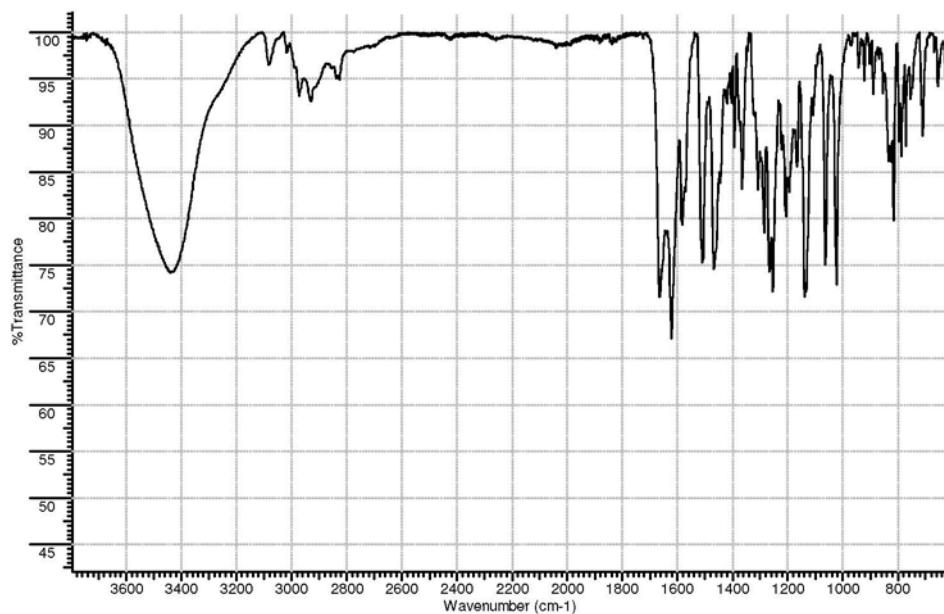
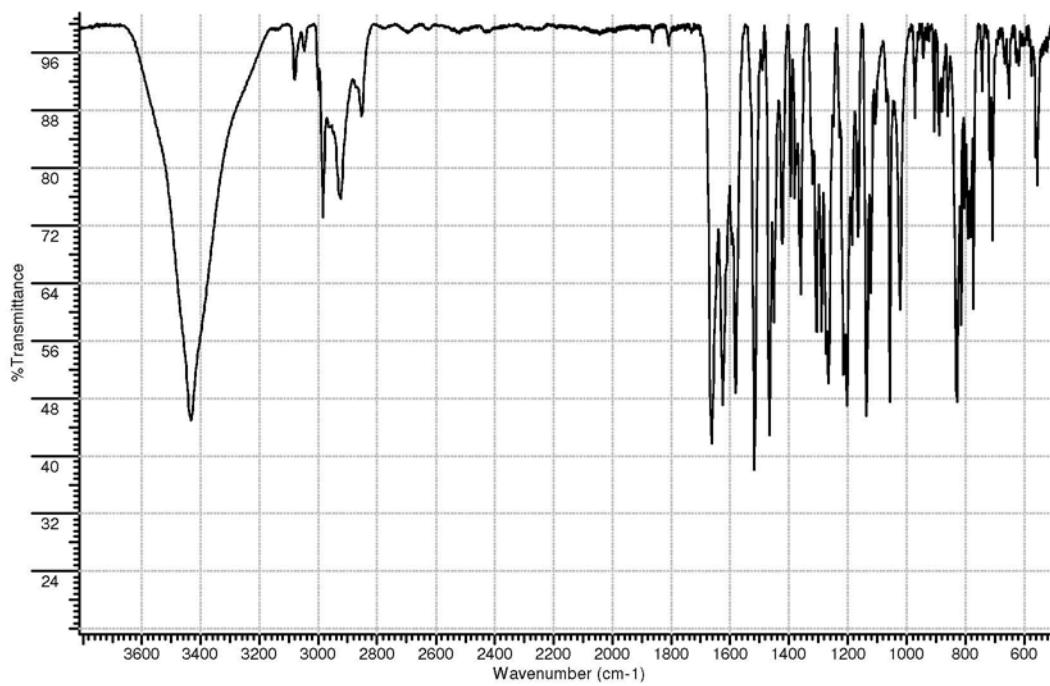


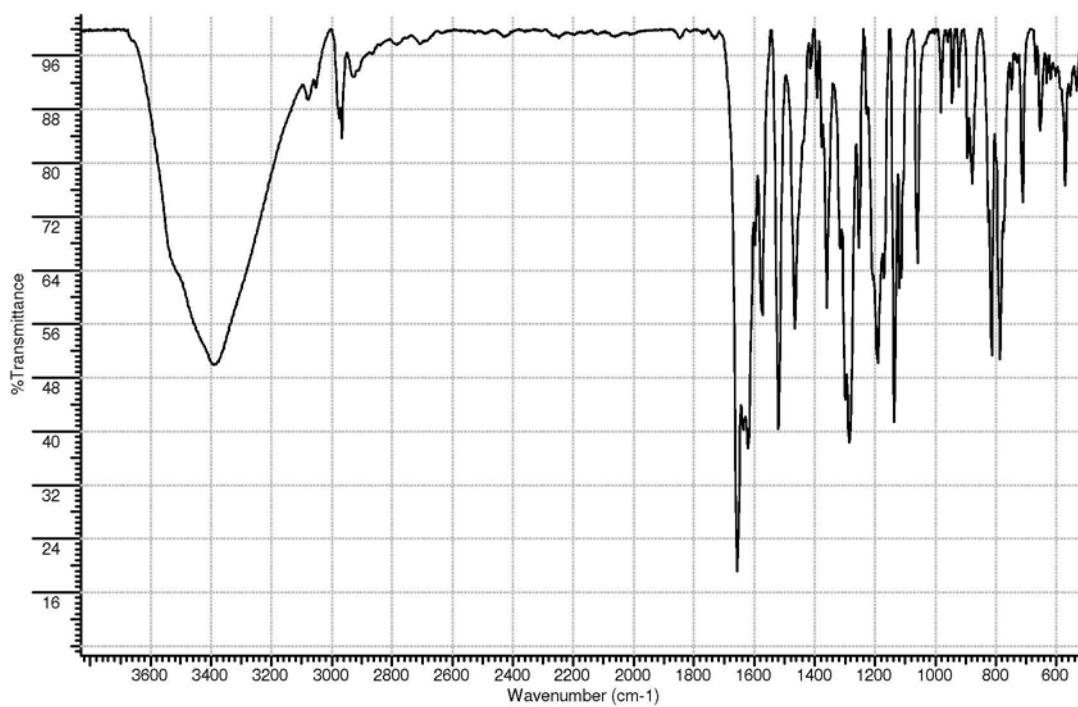
Figure S1. IR spectrum (KBr disks) of isoflavone 1.



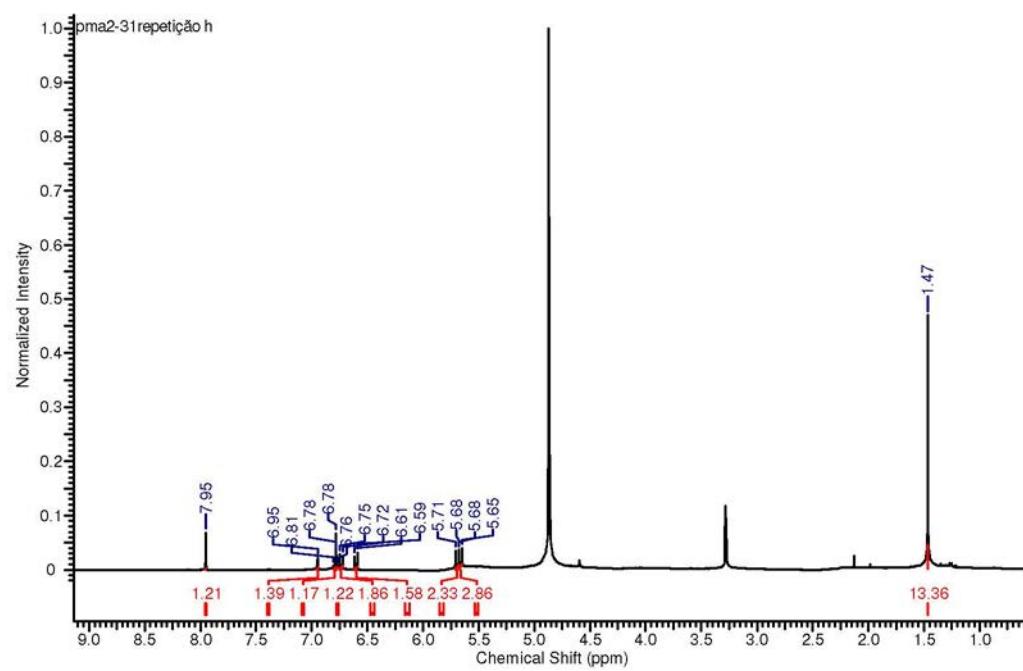
**Figure S2.** IR spectrum (KBr disks) of isoflavone 2.



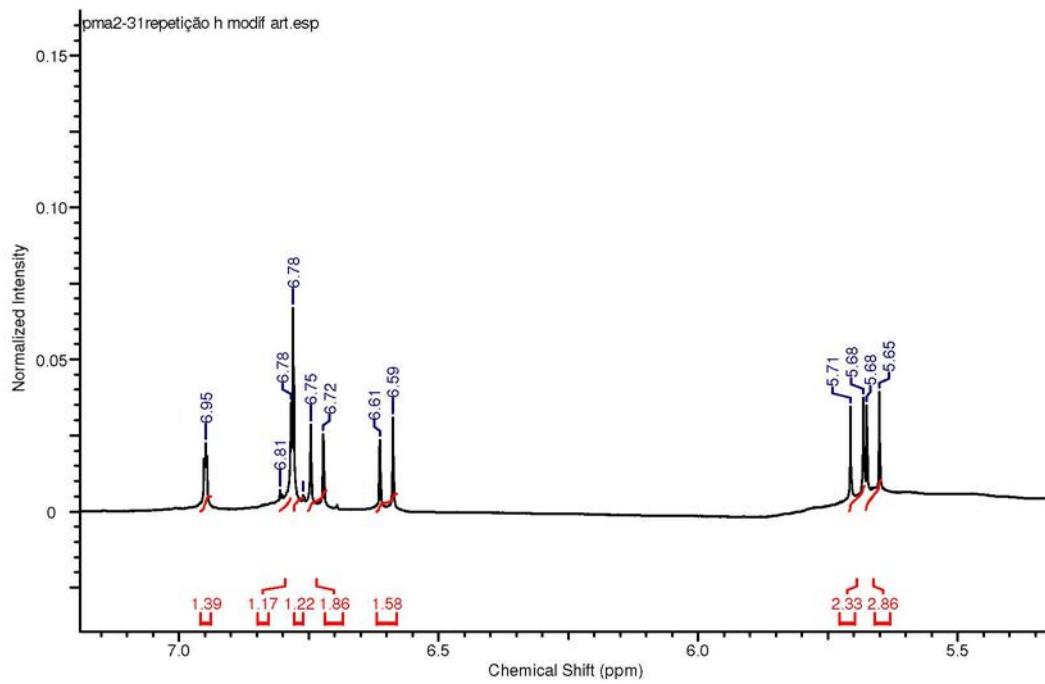
**Figure S3.** IR spectrum (KBr disks) of isoflavone 3.



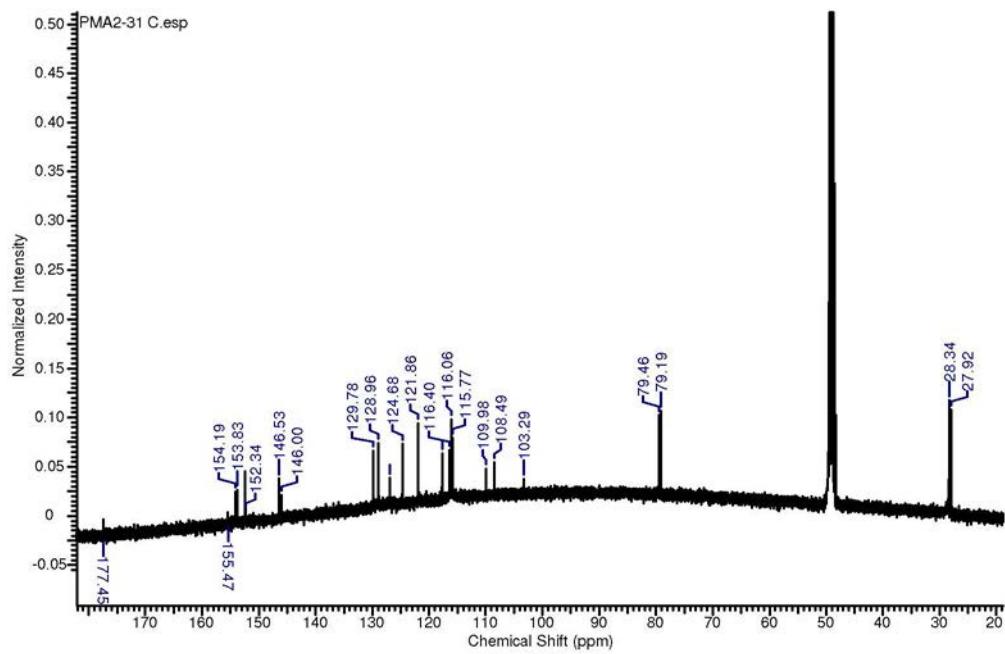
**Figure S4.** IR spectrum (KBr disks) of isoflavone **4**.



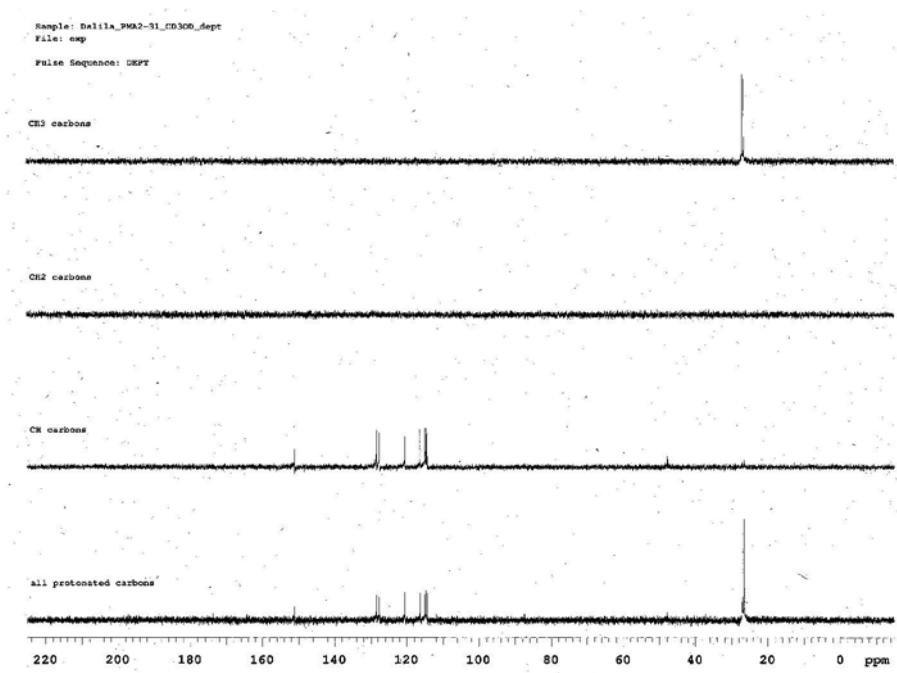
**Figure S5.** <sup>1</sup>H NMR spectrum (400 MHz, CD<sub>3</sub>OD) of isoflavone **1**.



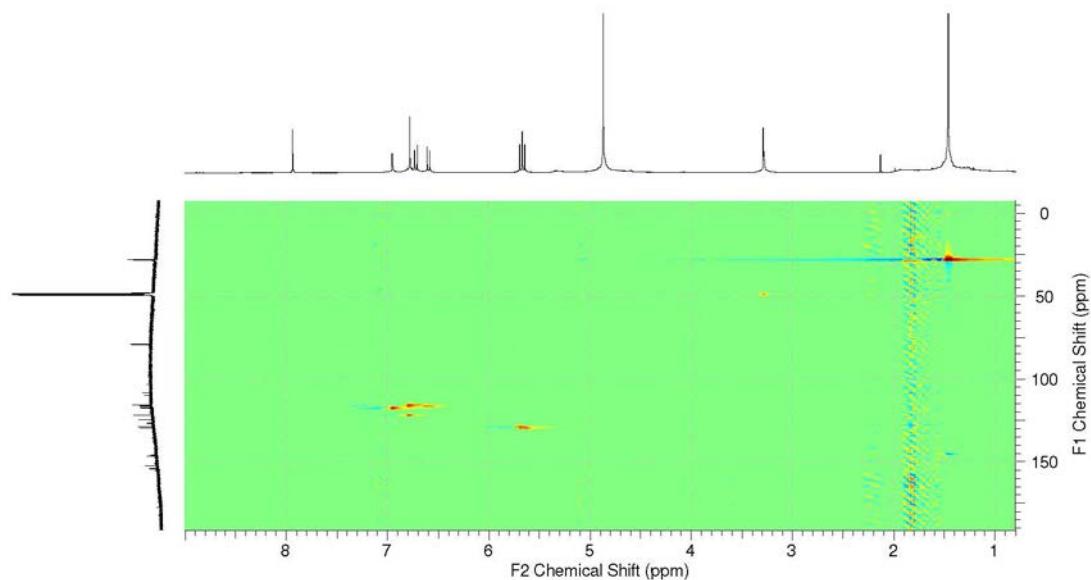
**Figure S6.** Expanded  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CD}_3\text{OD}$ ) of isoflavone **1**.



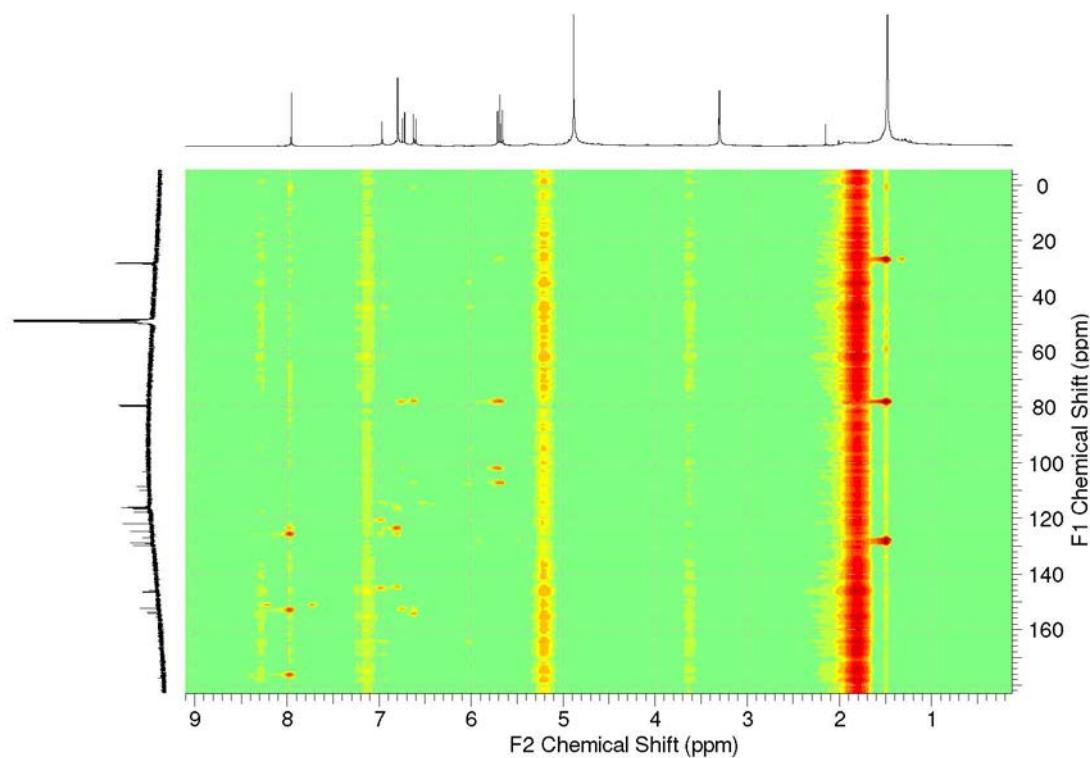
**Figure S7.**  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{CD}_3\text{OD}$ ) of isoflavone **1**.



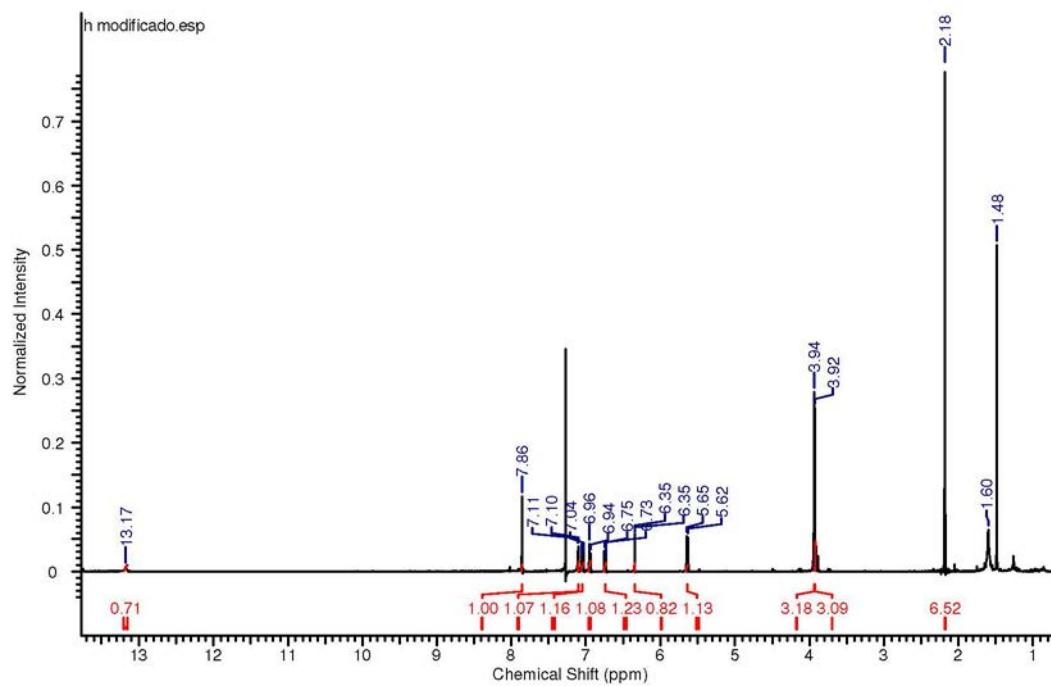
**Figure S8.** DEPT spectrum (100 MHz,  $\text{CD}_3\text{OD}$ ) of isoflavone **1**.



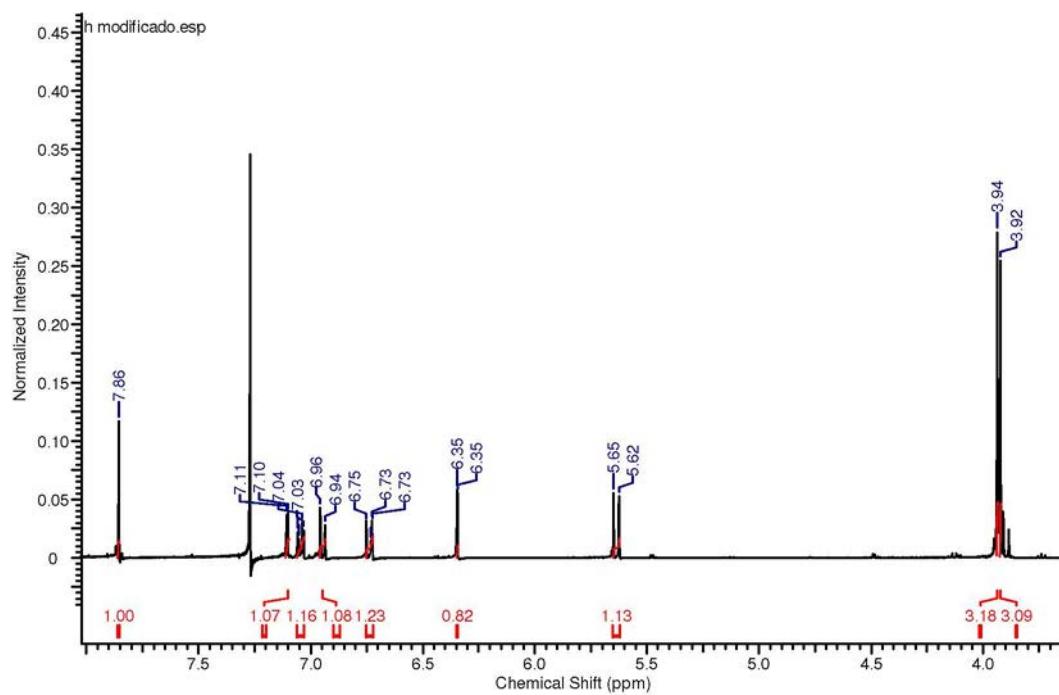
**Figure S9.** HMQC spectrum (400 MHz,  $\text{CD}_3\text{OD}$ ) of isoflavone **1**.



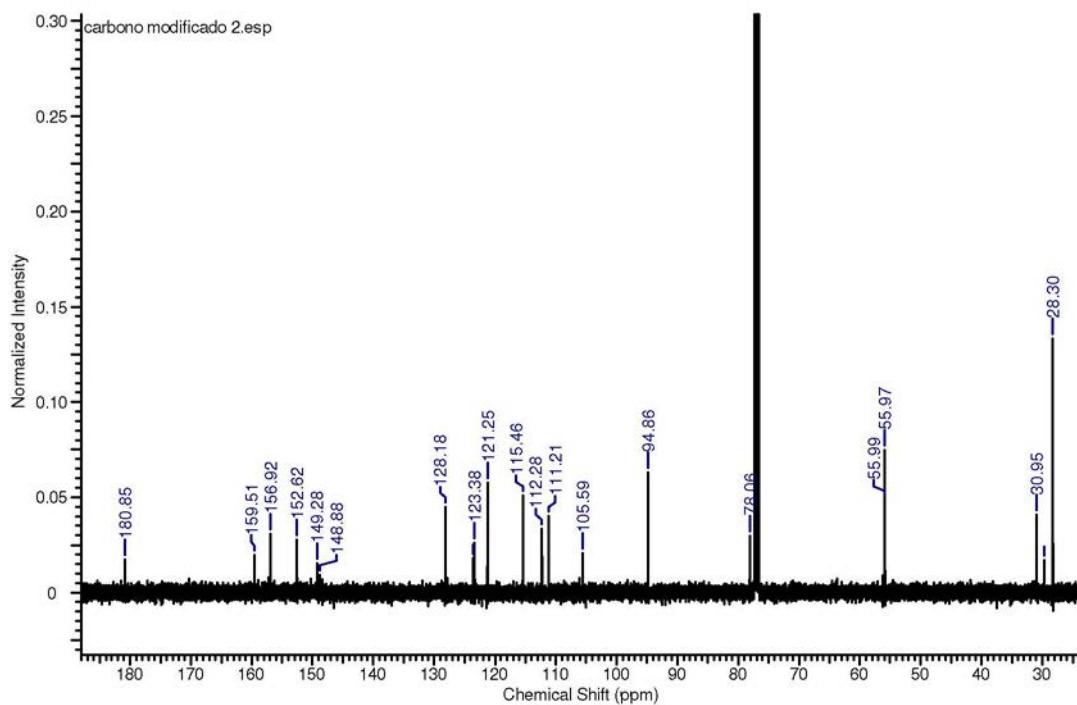
**Figure S10.** HMBC spectrum (400 MHz,  $\text{CD}_3\text{OD}$ ) of isoflavone **1**.



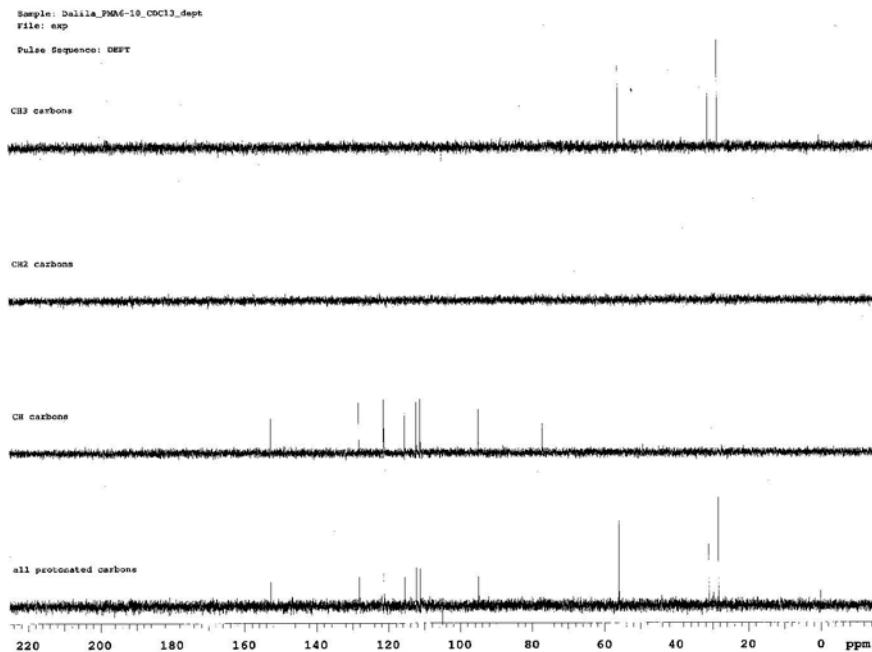
**Figure S11.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ ) of isoflavone **2**.



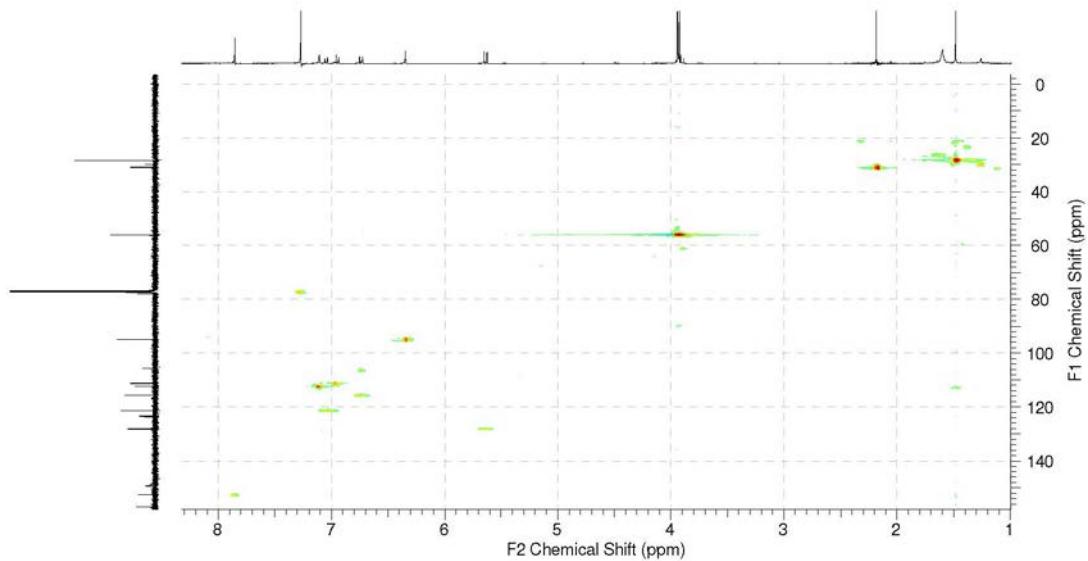
**Figure S12.** Expanded <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of isoflavone **2**.



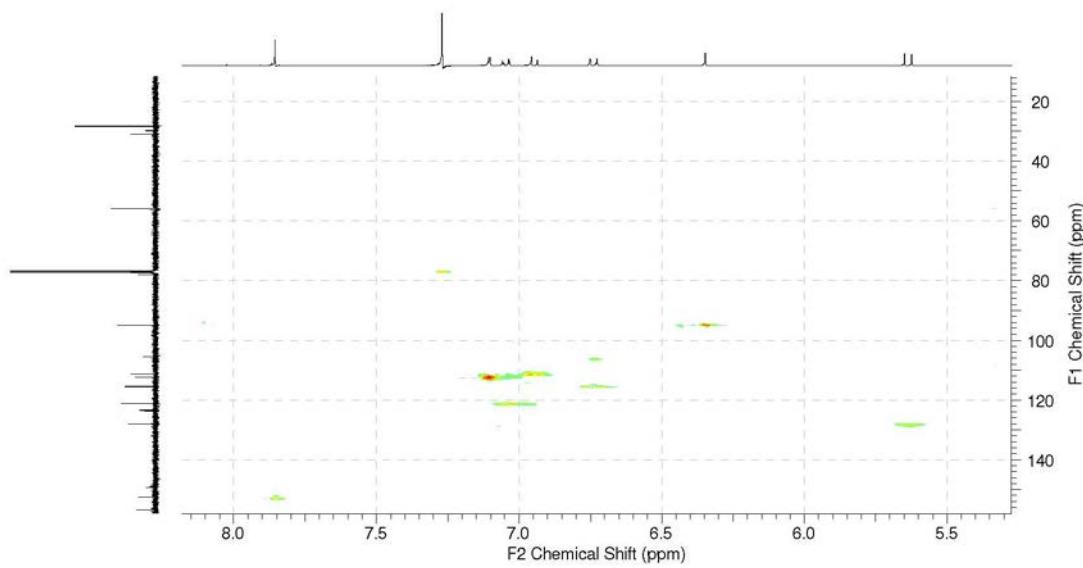
**Figure S13.** <sup>13</sup>C NMR spectrum (100 MHz, CDCl<sub>3</sub>) of isoflavone **2**.



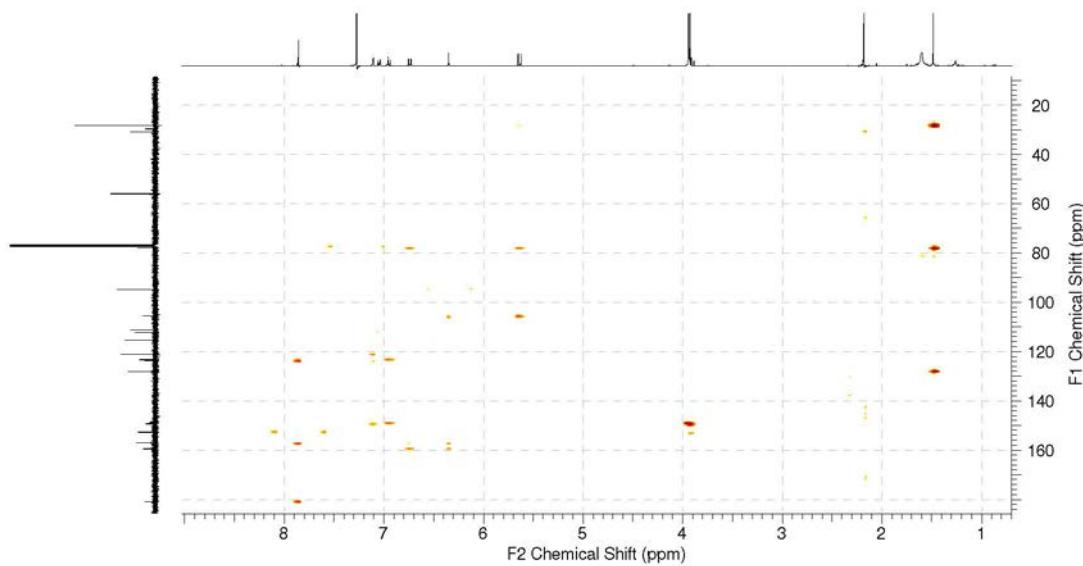
**Figure S14.** DEPT spectrum (100 MHz,  $\text{CDCl}_3$ ) of isoflavone **2**.



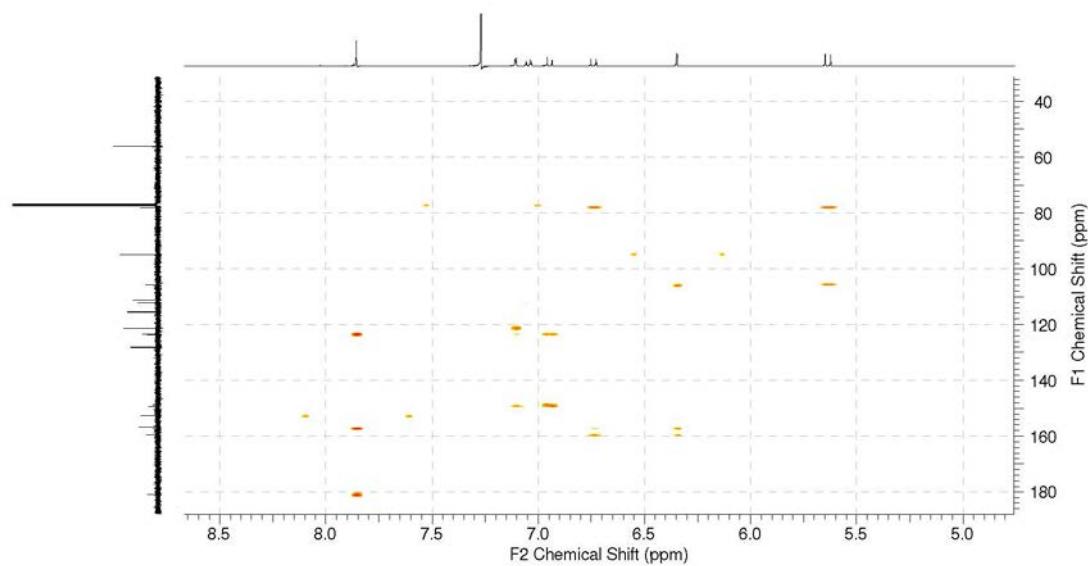
**Figure S15.** HMQC spectrum (400 MHz,  $\text{CDCl}_3$ ) of isoflavone **2**.



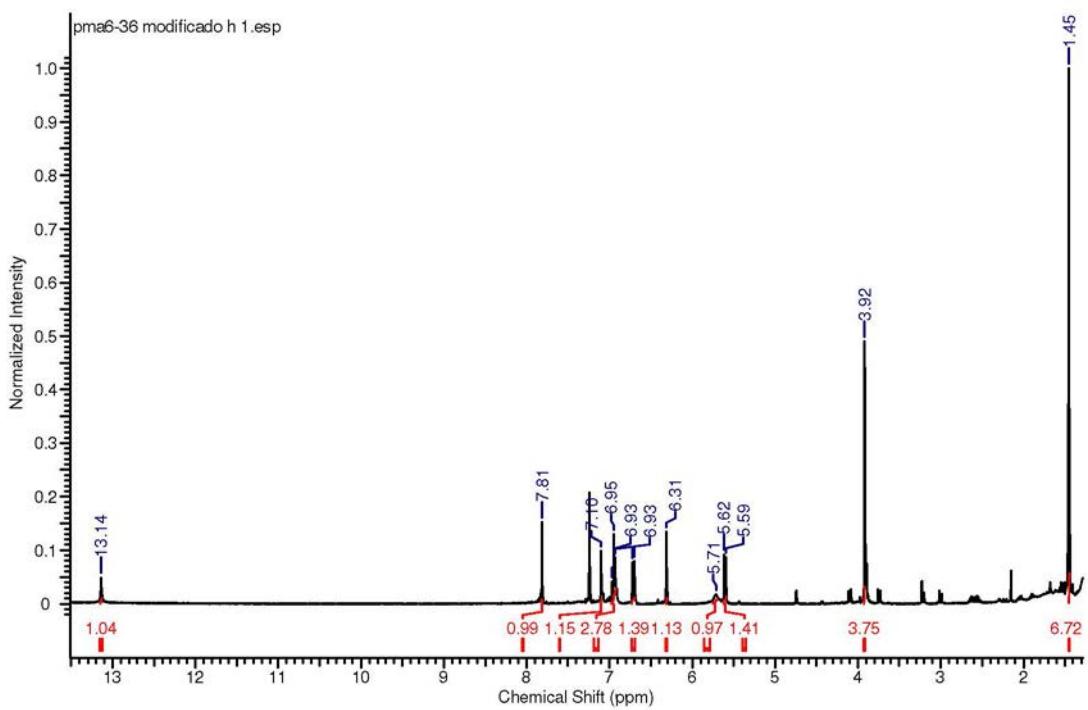
**Figure S16.** Expanded HMQC spectrum (400 MHz,  $\text{CDCl}_3$ ) of isoflavone **2**.



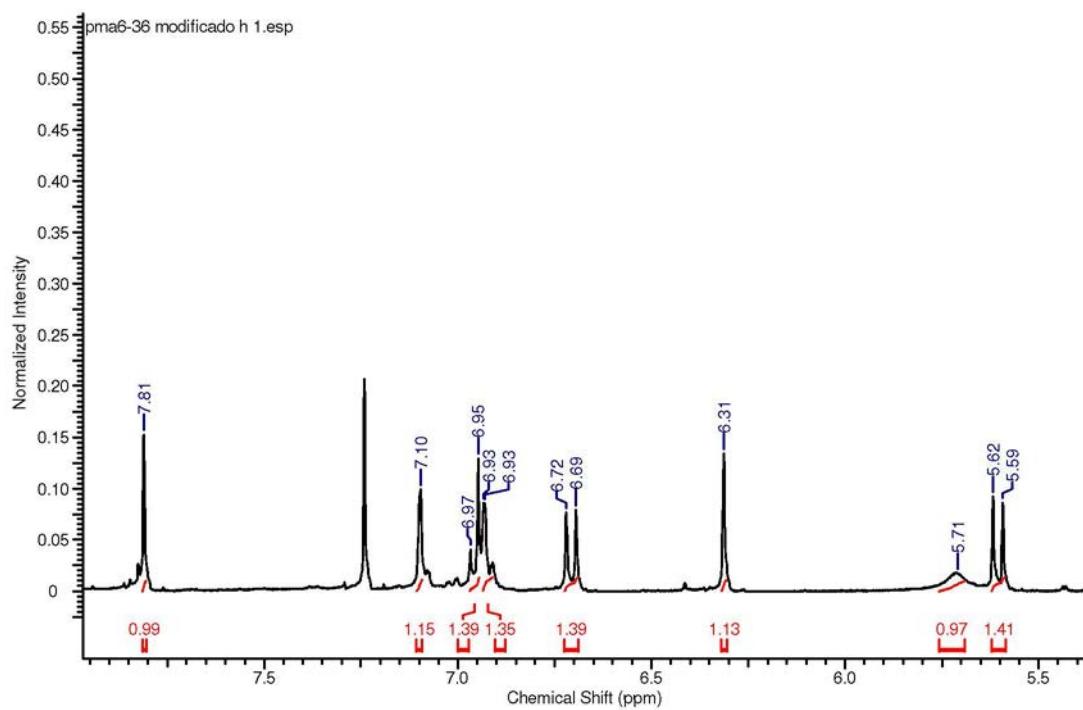
**Figure S17.** HMBC spectrum (400 MHz,  $\text{CDCl}_3$ ) of isoflavone **2**.



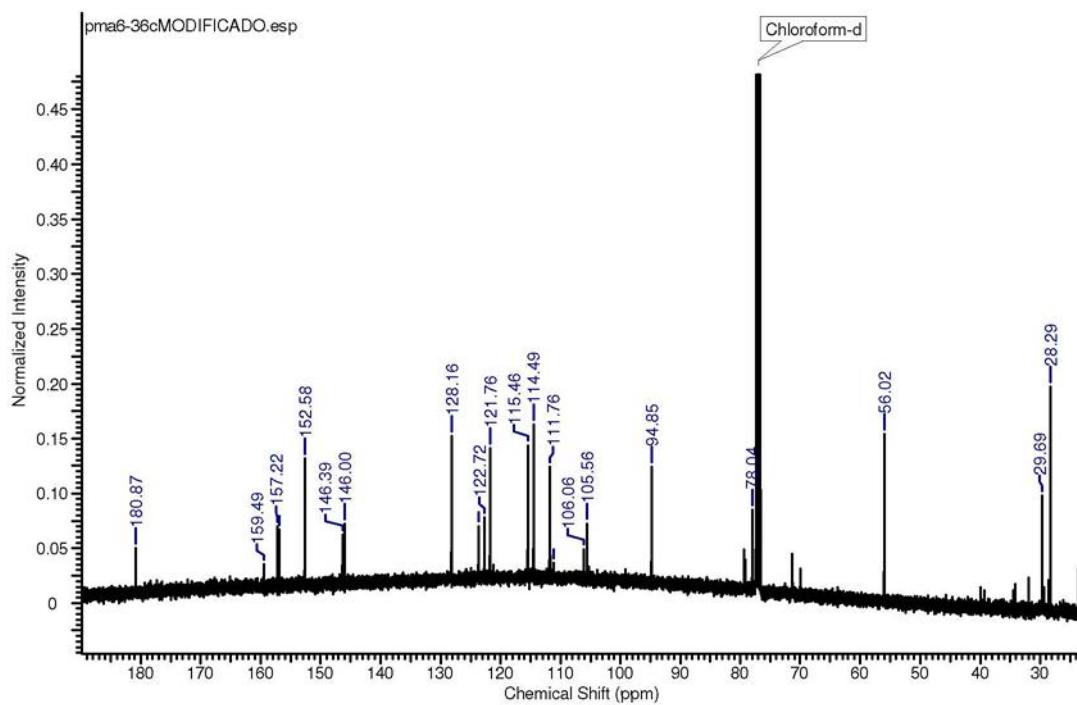
**Figure S18.** Expanded HMBC spectrum (400 MHz,  $\text{CDCl}_3$ ) of isoflavone **2**.



**FigureS 19.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ ) of isoflavone **3**.



**Figure S20.** Expanded <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of isoflavone **3**.



**Figure S21.** <sup>13</sup>C NMR spectrum (100 MHz, CDCl<sub>3</sub>) of isoflavone **3**.

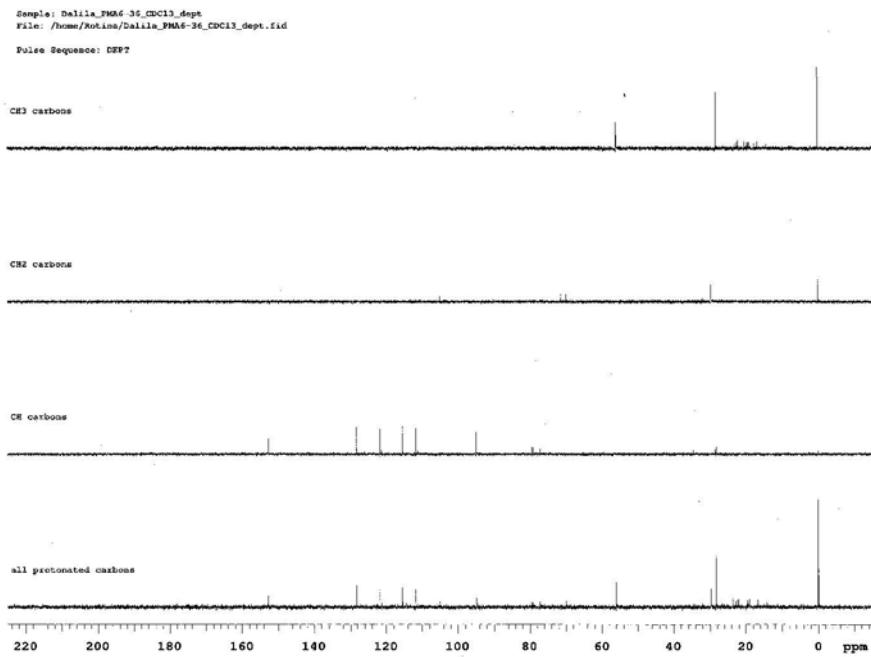


Figure S22. DEPT spectrum (100 MHz, CDCl<sub>3</sub>) of isoflavone 3.

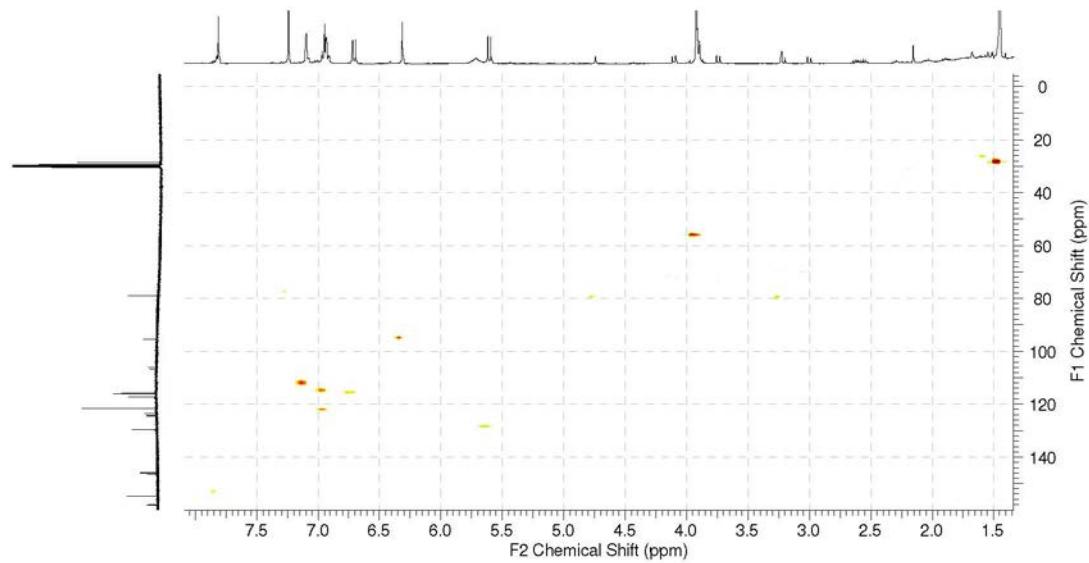
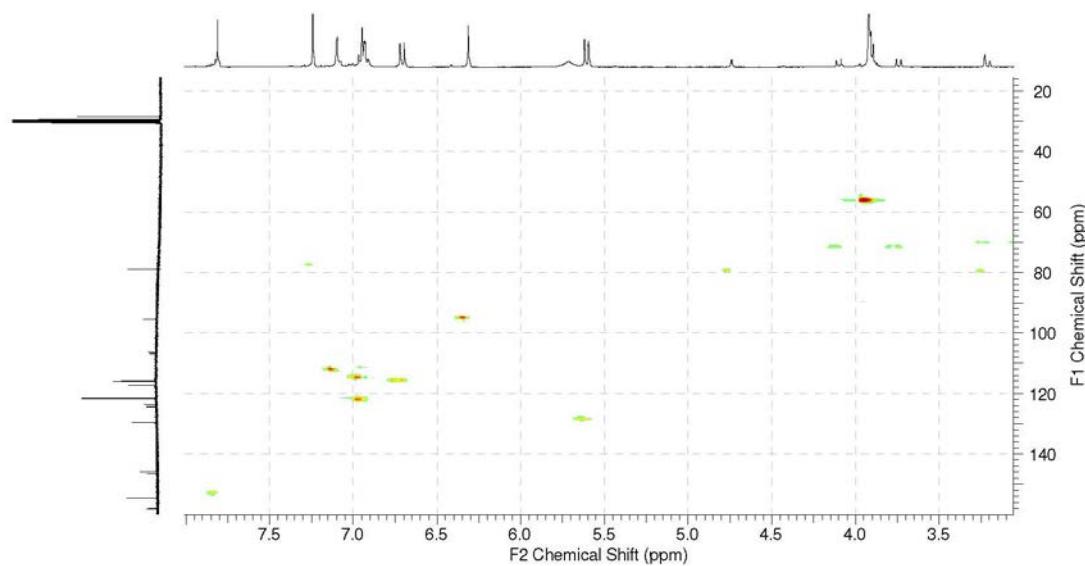
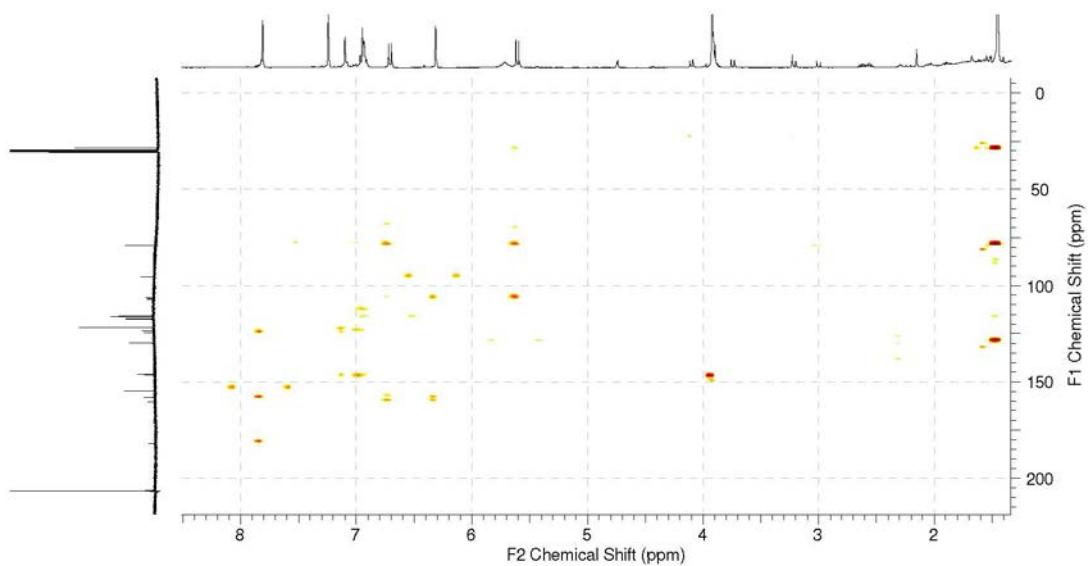


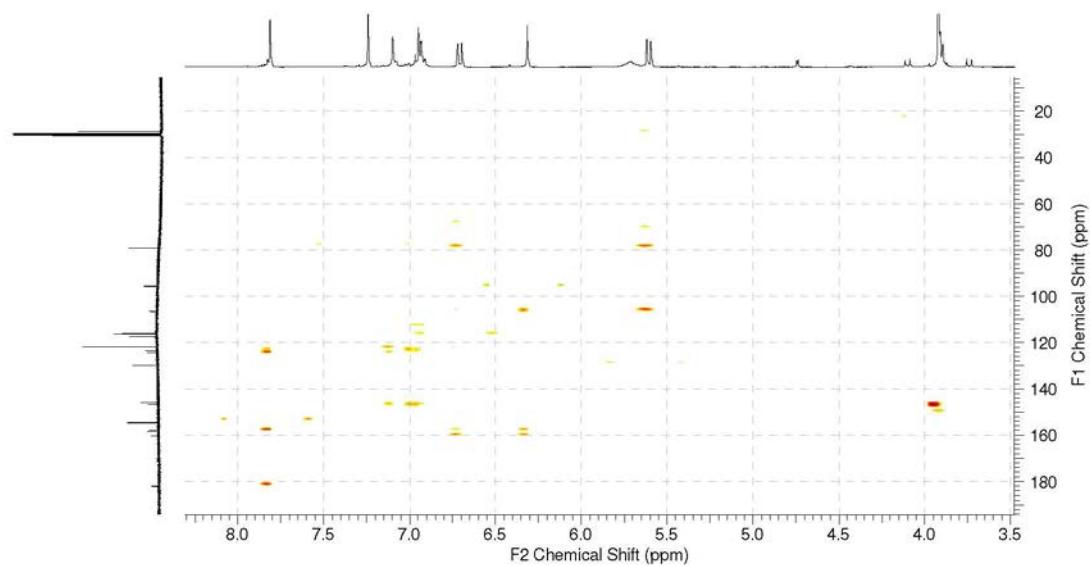
Figure S23. HMQC spectrum (400 MHz, CDCl<sub>3</sub>) of isoflavone 3.



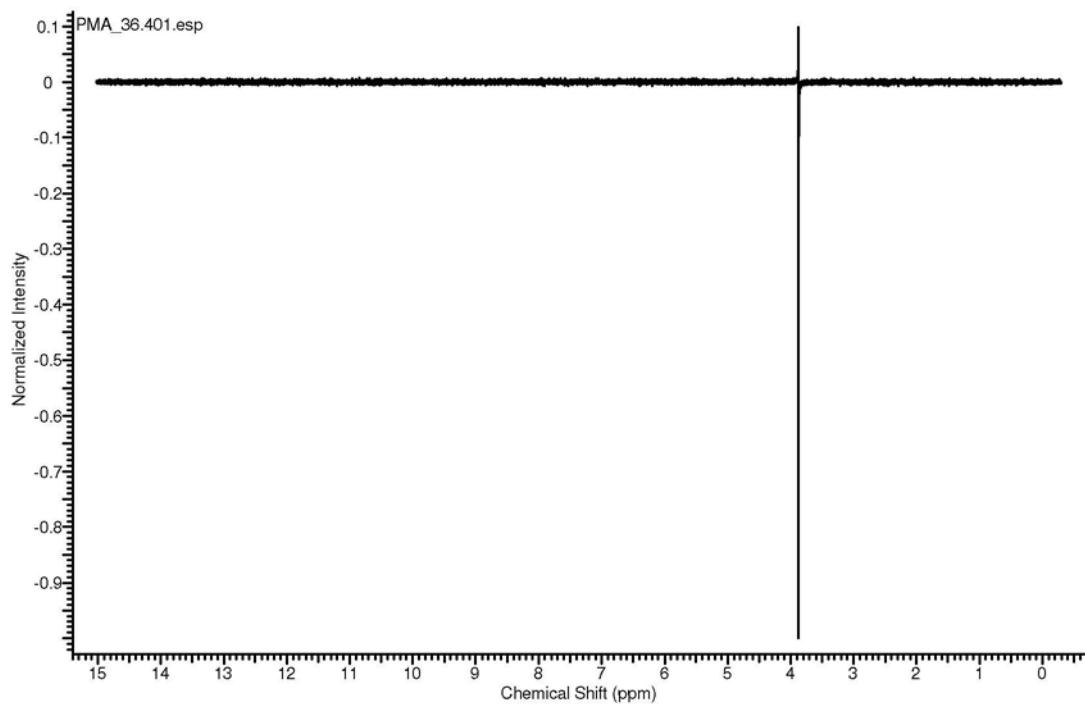
**Figure S24.** Expanded HMQC spectrum (400 MHz,  $\text{CDCl}_3$ ) of isoflavone **3**.



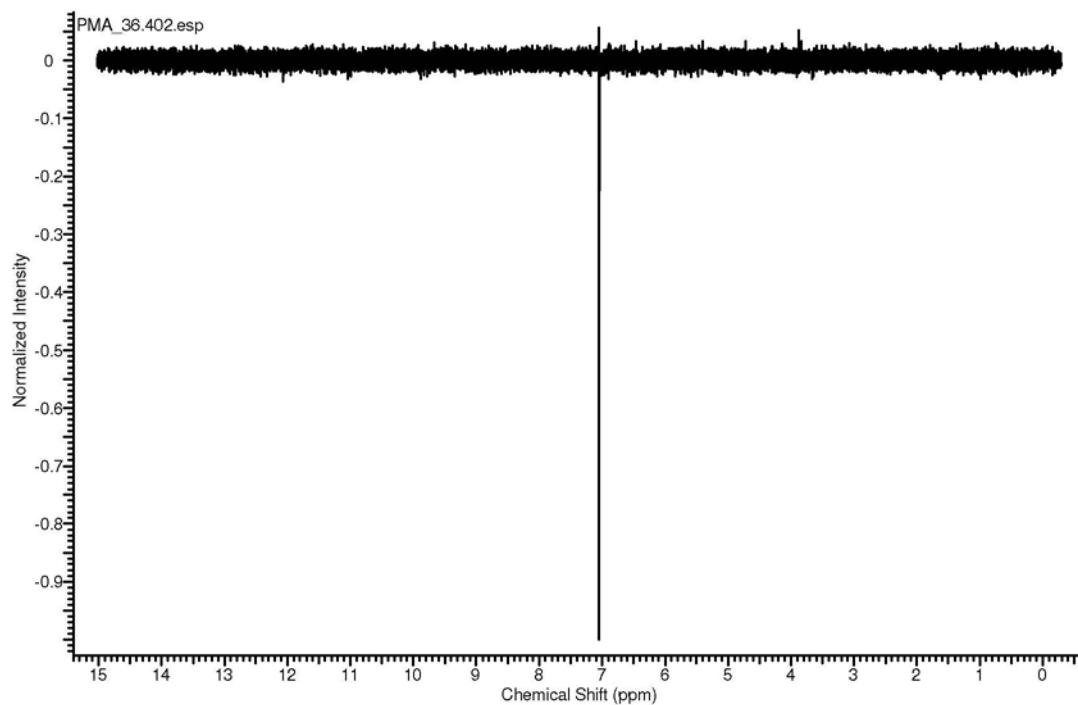
**Figure S25.** HMBC spectrum (400 MHz,  $\text{CDCl}_3$ ) of isoflavone **3**.



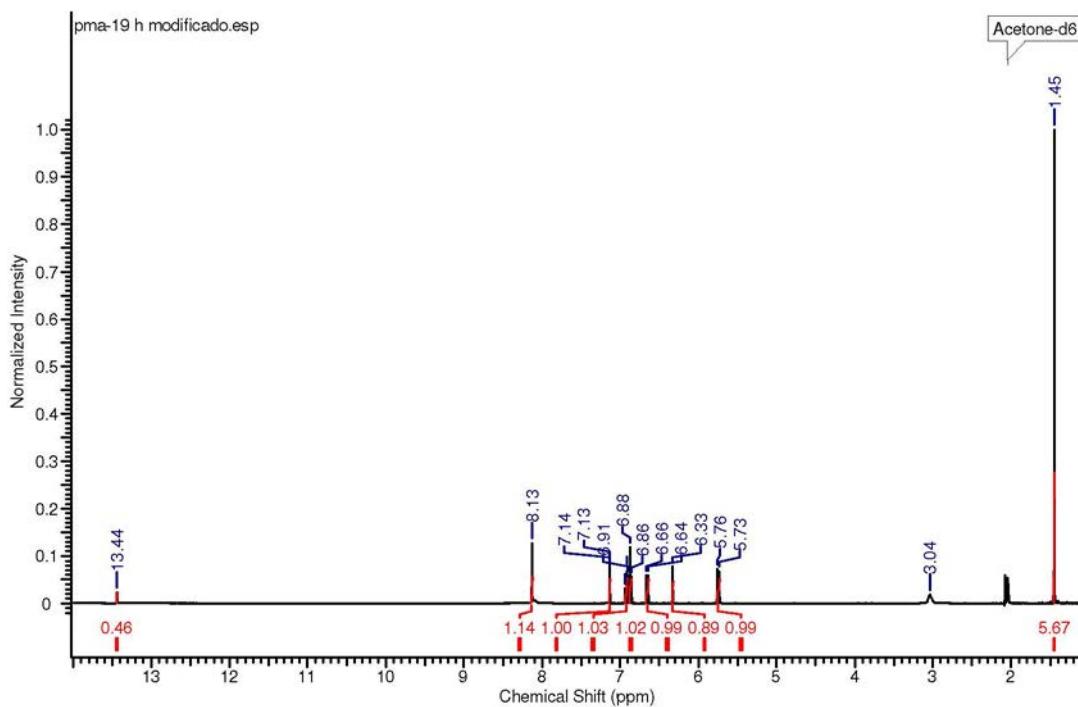
**Figure S26.** Expanded HMBC spectrum (400 MHz,  $\text{CDCl}_3$ ) of isoflavone **3**.



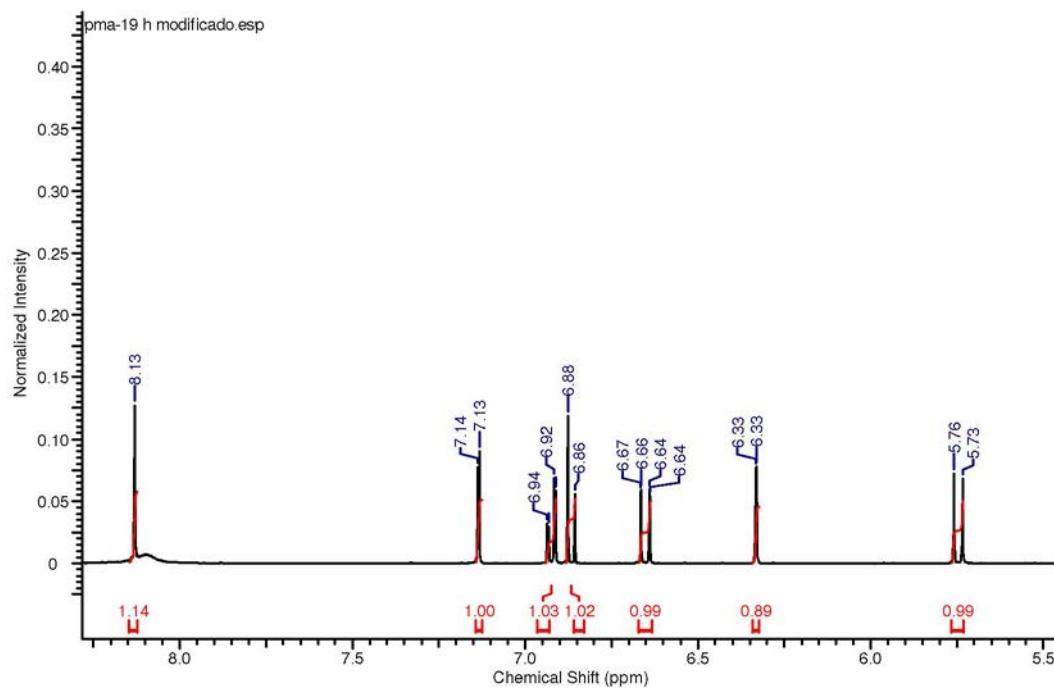
**Figure S27.** NOE spectrum (400 MHz,  $\text{CDCl}_3$ ) of isoflavone **3** ( $\text{H}-2'$  irradiated).



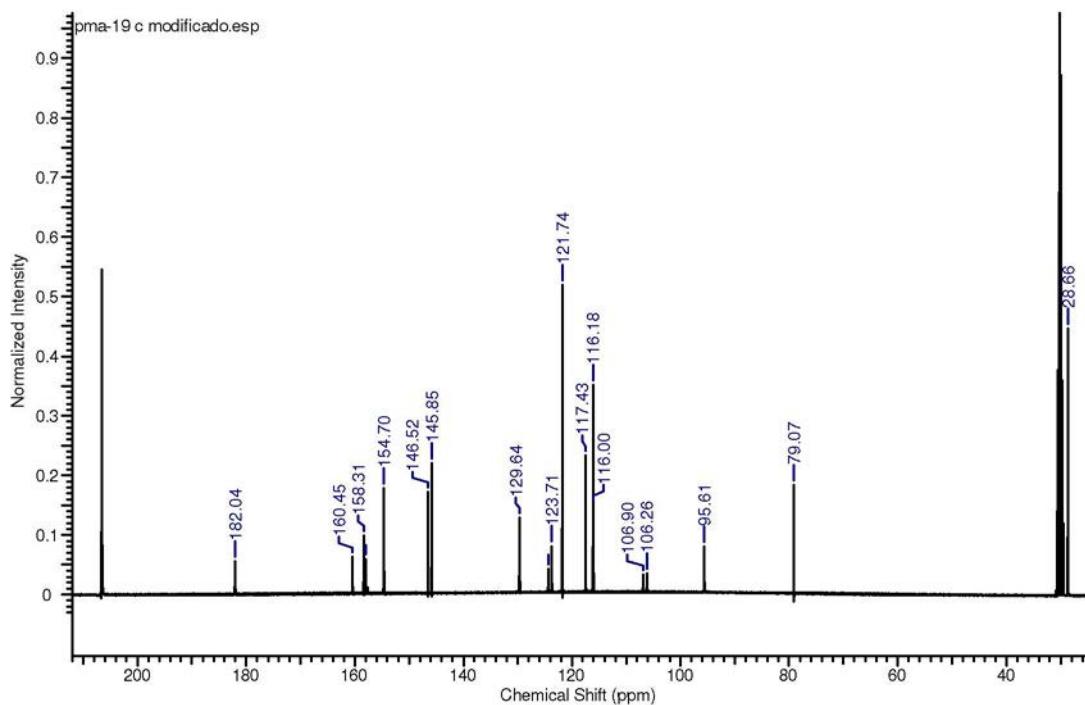
**Figure S28.** NOE spectrum (400 MHz,  $\text{CDCl}_3$ ) of isoflavone **3** (OME-3' irradiated).



**Figure S29.**  $^1\text{H}$  NMR spectrum (400MHz,  $\text{C}_3\text{D}_6\text{O}$ ) of isoflavone **4**.



**Figure S30.** Expanded  $^1\text{H}$  NMR spectrum (400MHz,  $\text{C}_3\text{D}_6\text{O}$ ) of isoflavone 4.



**Figure S31.**  $^{13}\text{C}$  NMR spectrum (100MHz,  $\text{C}_3\text{D}_6\text{O}$ ) of isoflavone 4.

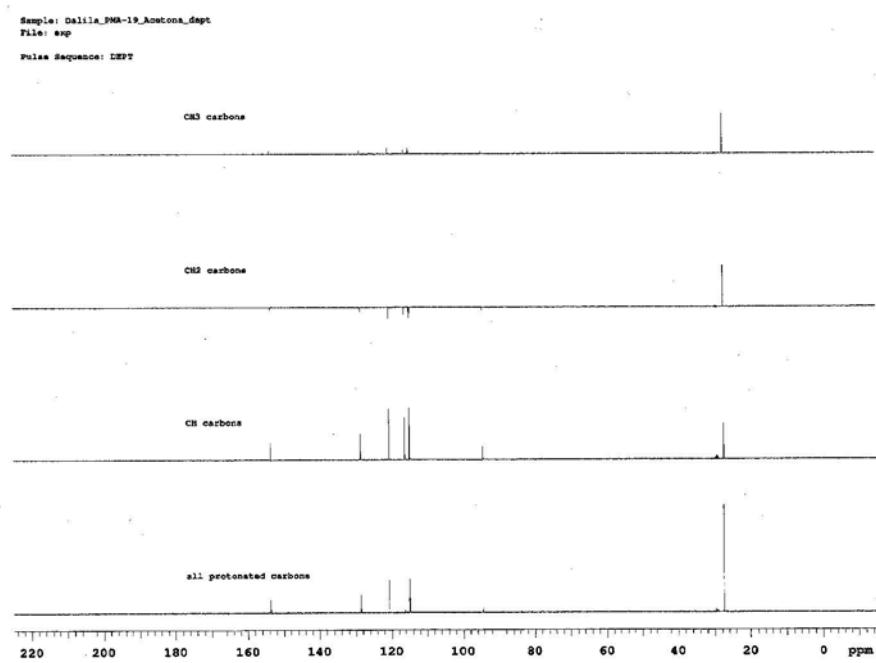


Figure S32. DEPT spectrum (100MHz, C<sub>3</sub>D<sub>6</sub>O) of isoflavone **4**.

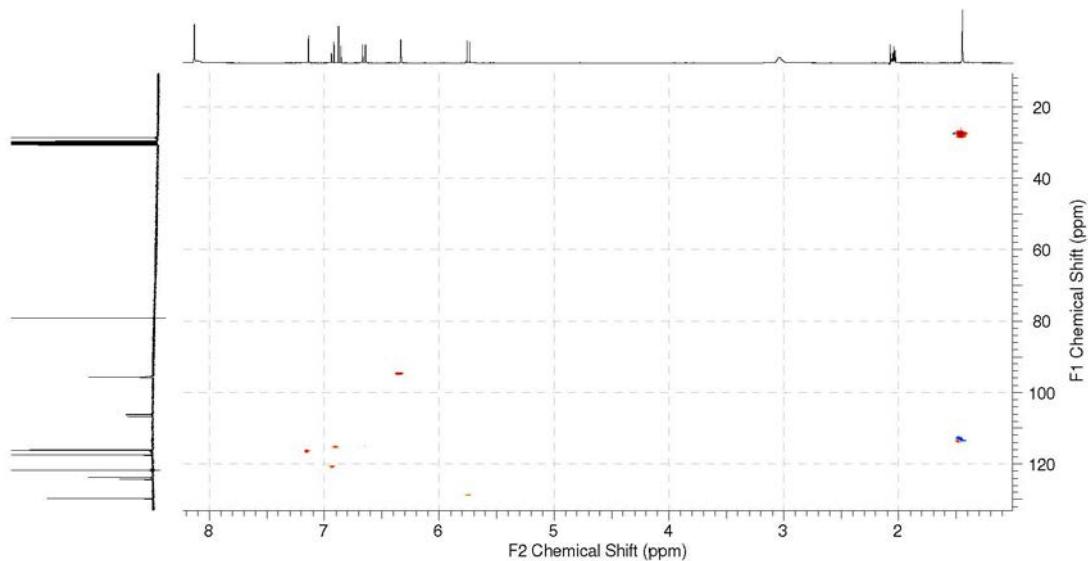


Figure S33. HMQC spectrum (400MHz, C<sub>3</sub>D<sub>6</sub>O) of isoflavone **4**.

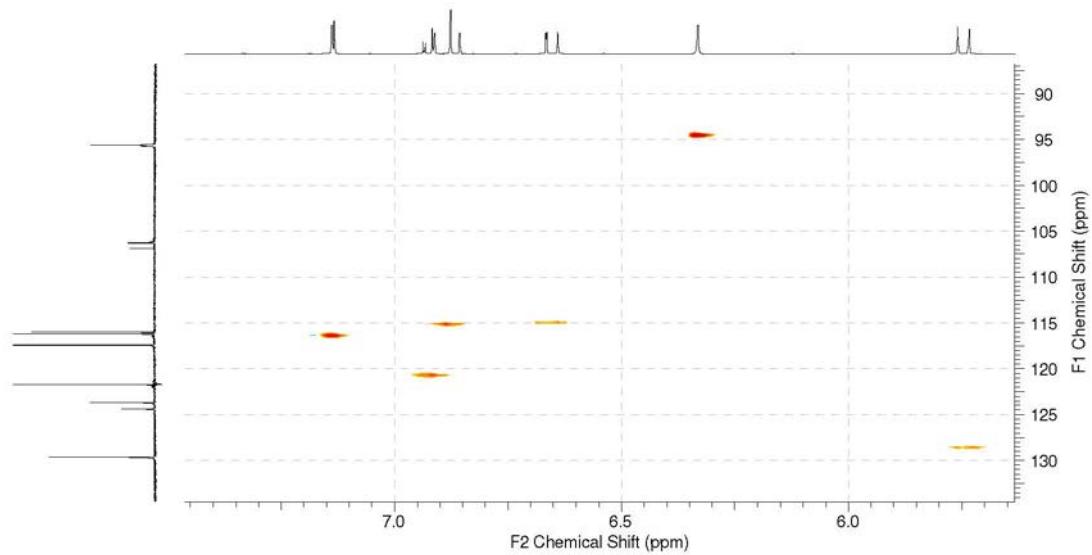


Figure S34. Expanded HMQC spectrum (400MHz, C<sub>6</sub>D<sub>6</sub>O) of isoflavone 4.

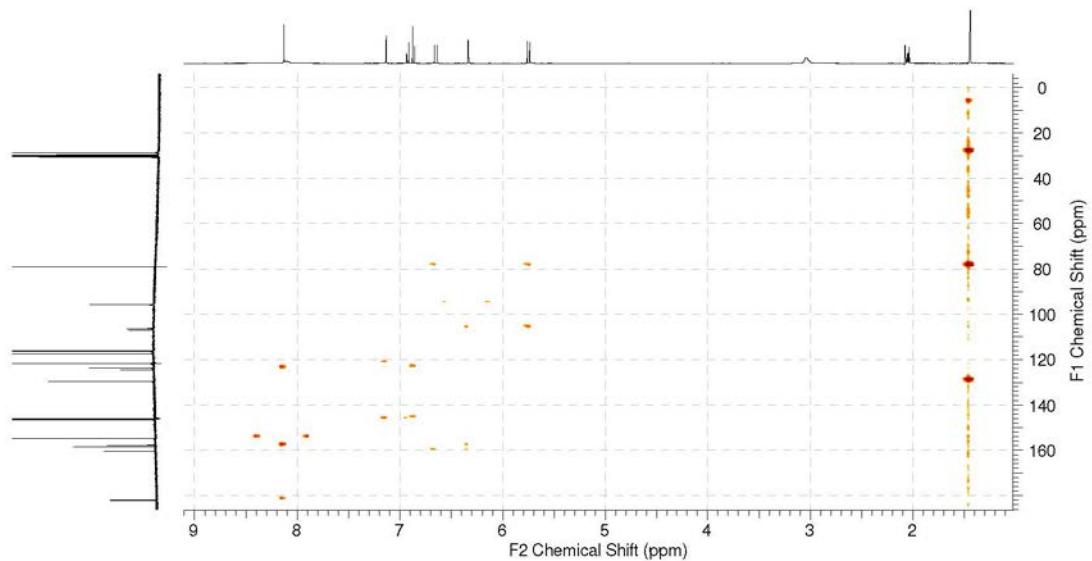
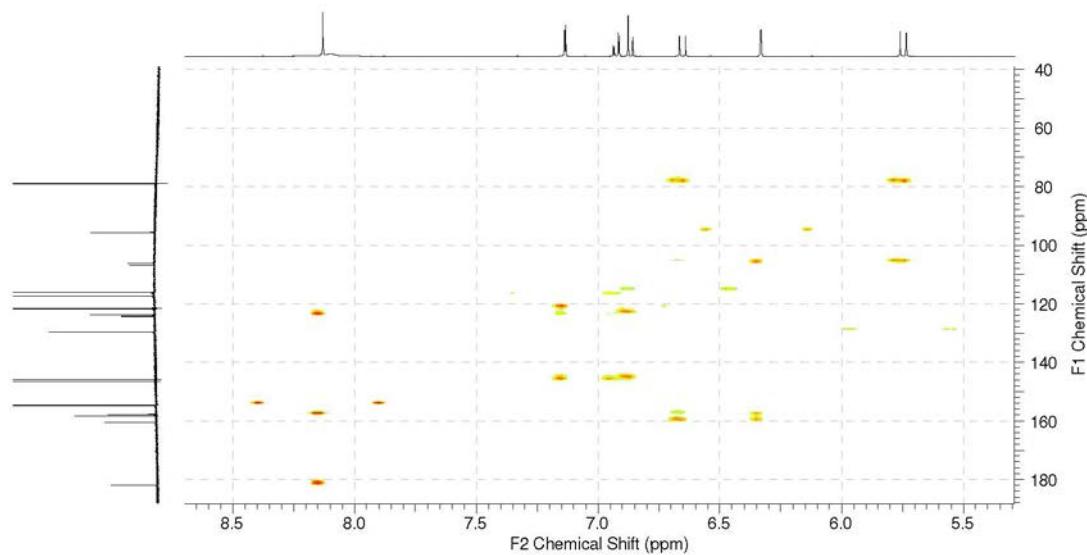
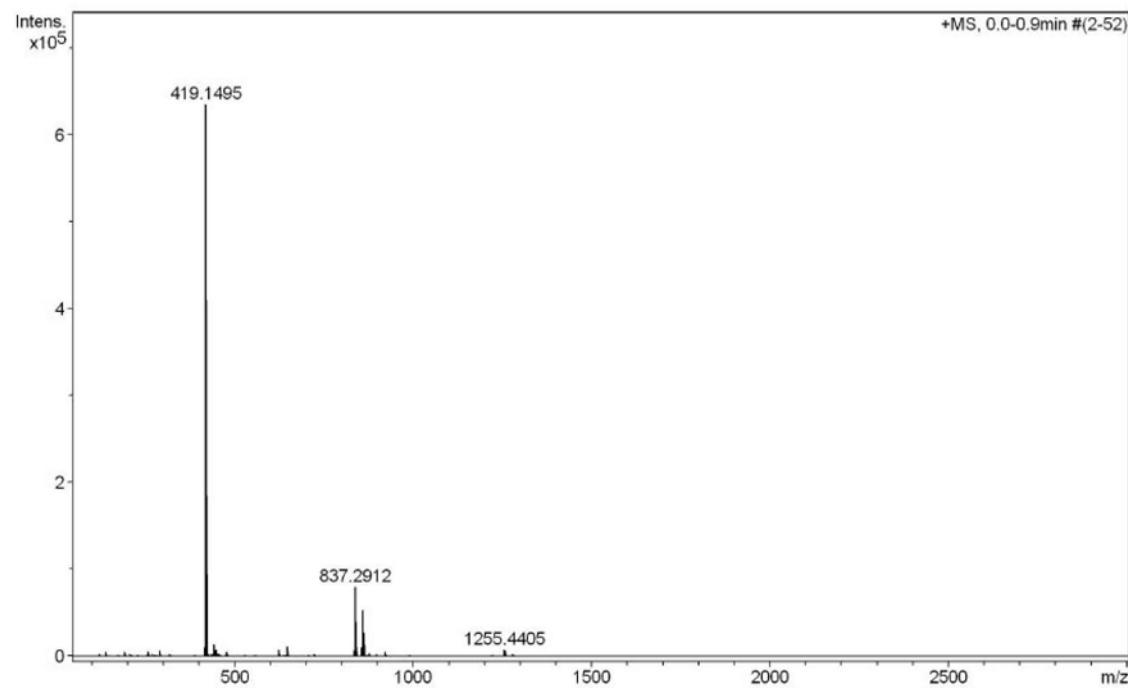


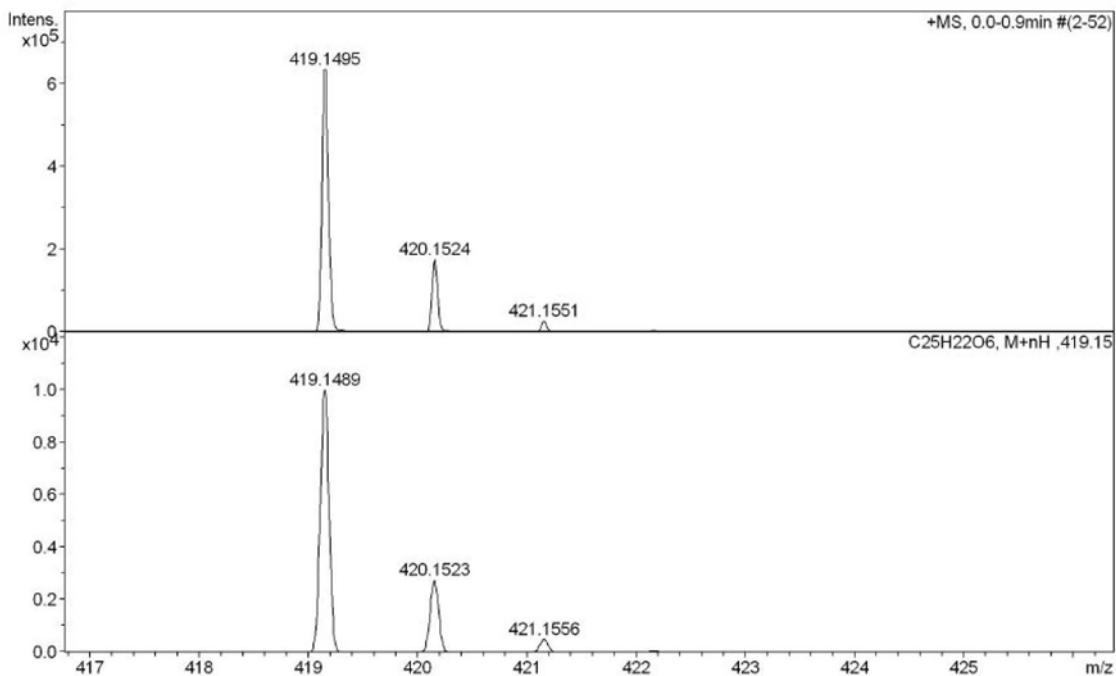
Figure S35. HMBC spectrum (400MHz, C<sub>6</sub>D<sub>6</sub>O) of isoflavone 4.



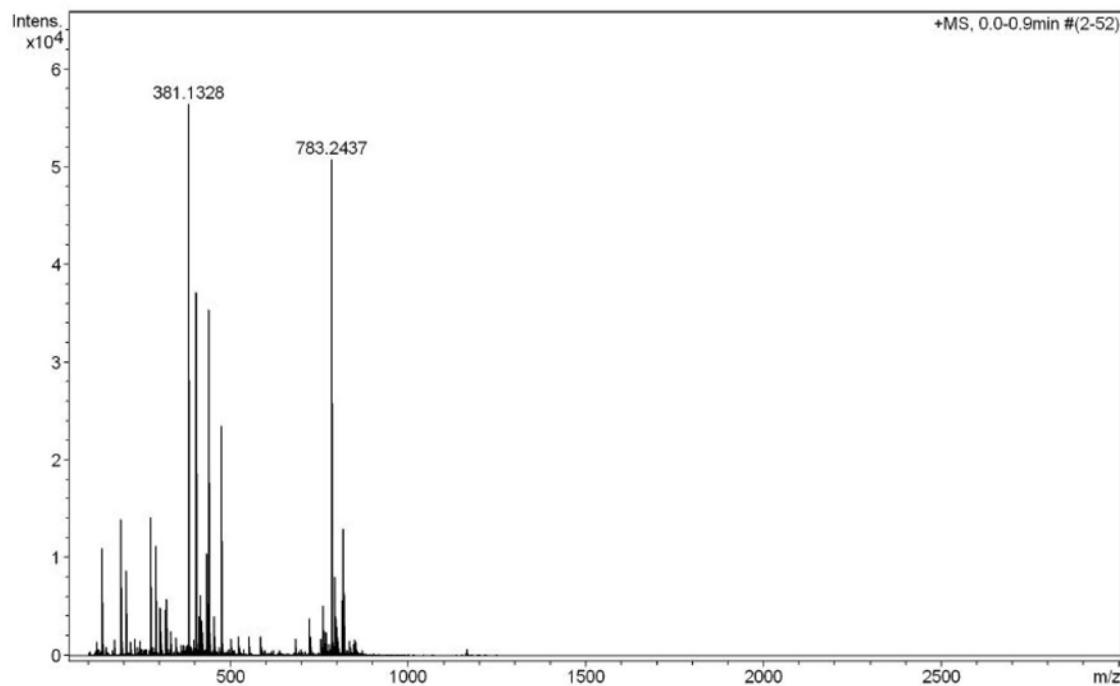
**Figure S36.** Expanded HMBC spectrum (400MHz, C<sub>3</sub>D<sub>6</sub>O) of isoflavone **4**.



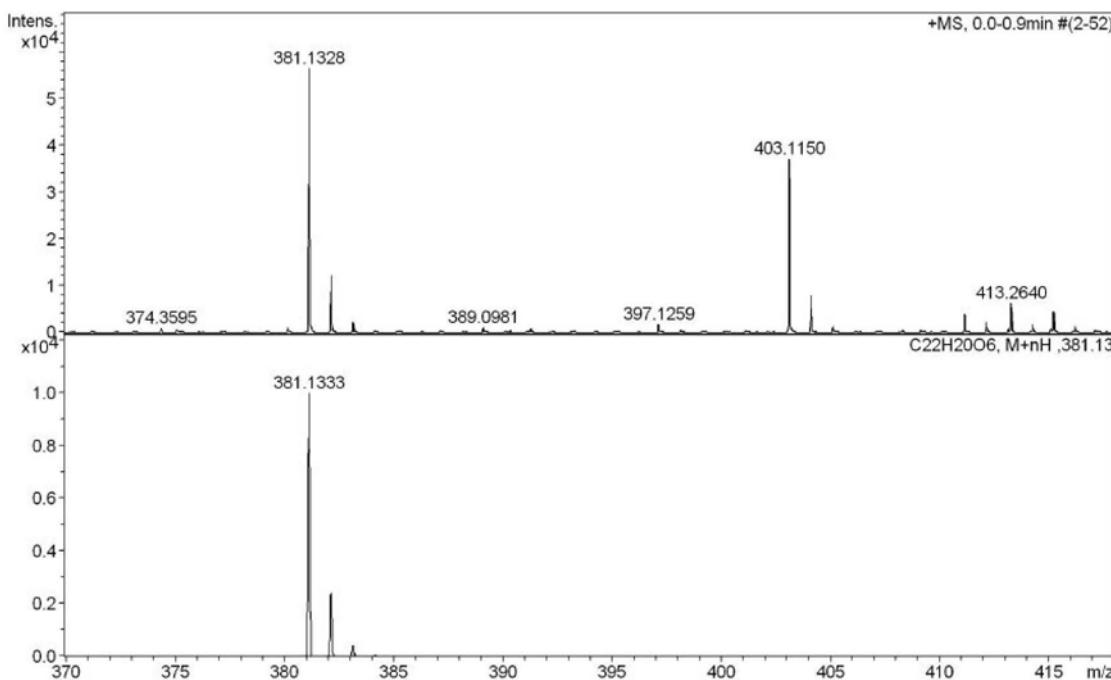
**Figure S37.** MS spectrum of isoflavone **1** (Part 1).



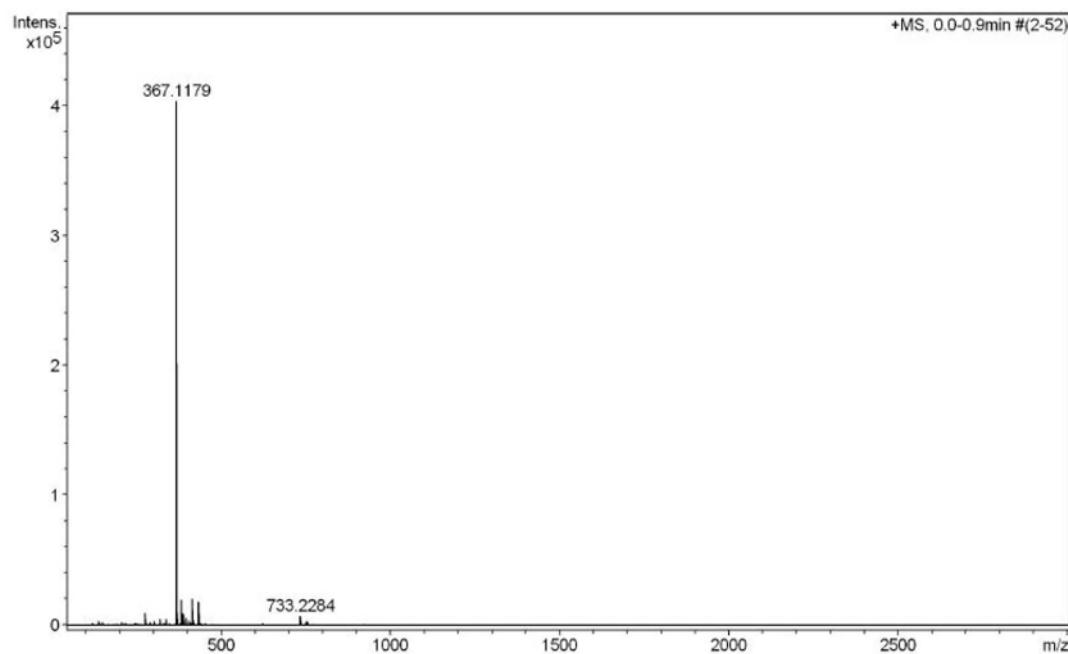
**Figure S38.** MS spectrum of isoflavone **1** (Part 2).



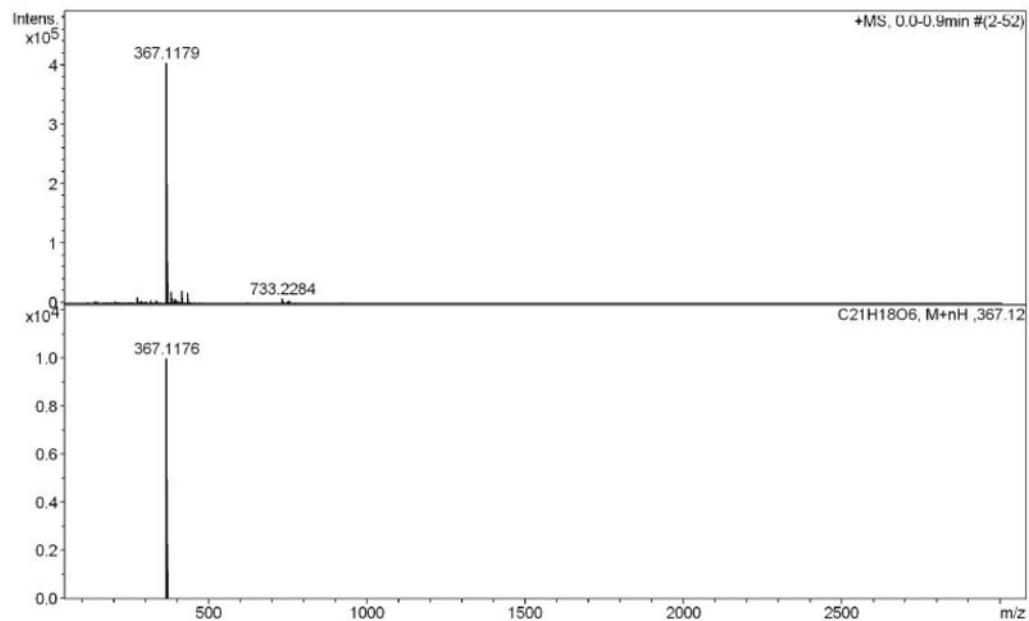
**Figure S39.** MS spectrum of isoflavone **2** (Part 1).



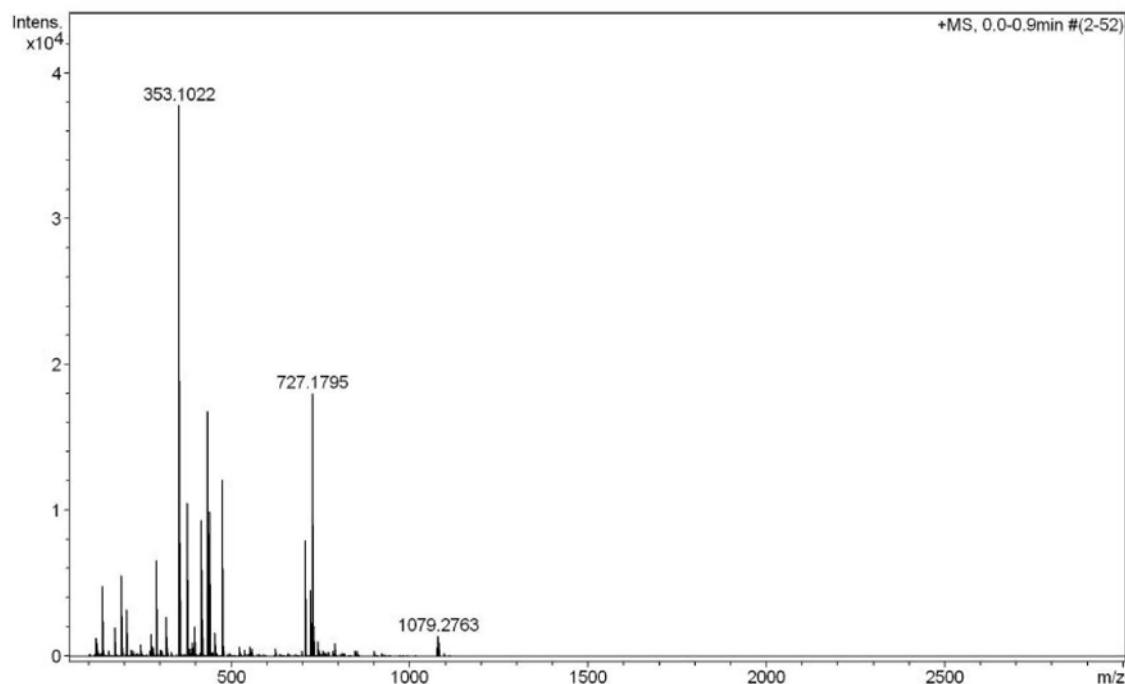
**Figure S40.** MS spectrum of isoflavone **2** (Part 2).



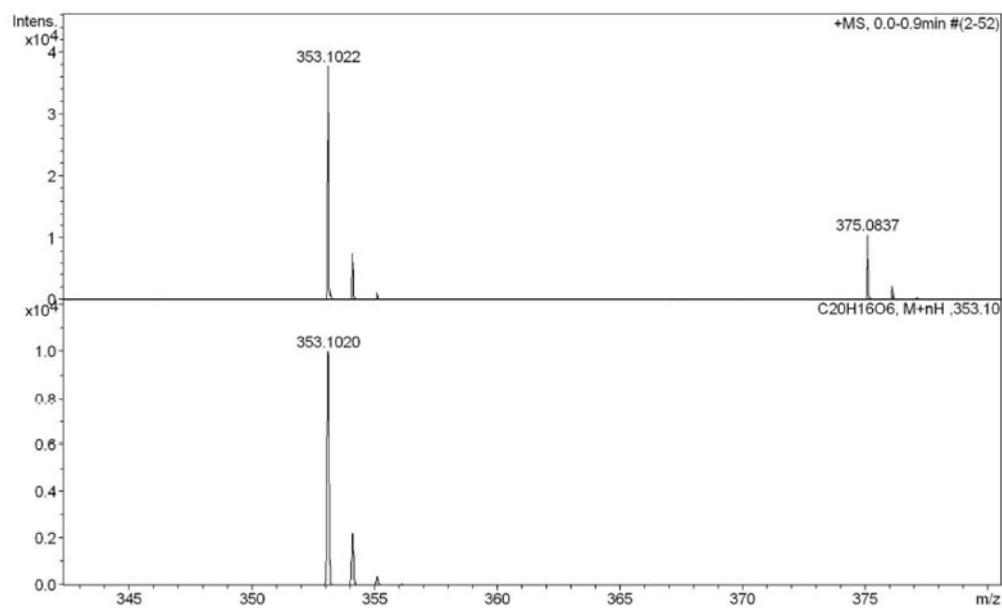
**Figure S41.** MS spectrum of isoflavone **3** (Part 1).



**Figure S42.** MS spectrum of isoflavone **3** (Part 2).



**Figure S43.** MS spectrum of isoflavone **4** (Part 1).



**Figure S44.** MS spectrum of isoflavone **4** (Part 2).

