

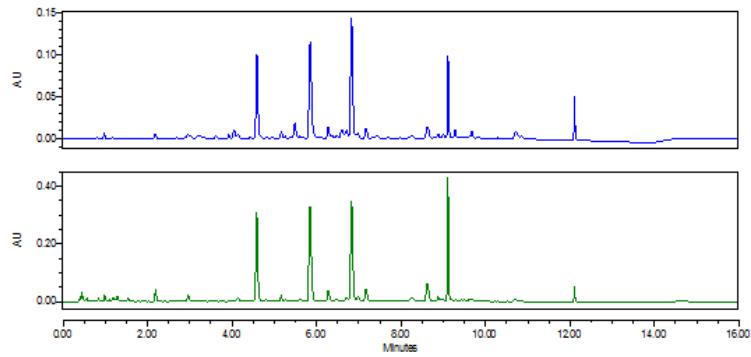
## **Electronic Supplementary Information**

### **Detailed Phytochemical Characterization of Bergamot Polyphenolic Fraction (BPF) by UPLC-DAD-MS and LC-NMR**

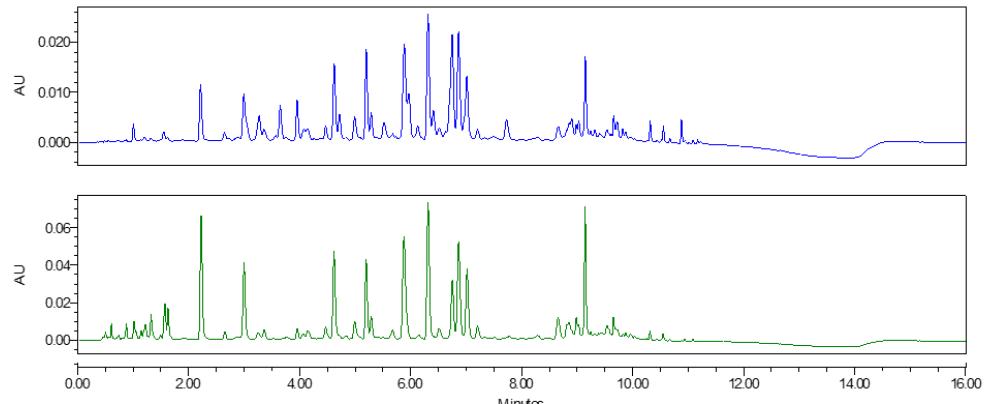
Carmen Formisano,<sup>†</sup> Daniela Rigano,<sup>†</sup> Annalisa Lopatriello,<sup>†</sup> Carmina Sirignano,<sup>†</sup> Giuseppe Ramaschi,<sup>‡</sup> Lolita Arnoldi,<sup>‡</sup> Antonella Riva,<sup>‡</sup> Nicola Sardone<sup>‡,\*</sup> and Orazio Taglialatela-Scafatit,<sup>\*</sup>

<sup>†</sup> Department of Pharmacy, School of Medicine and Surgery, University of Naples Federico II, Via D. Montesano 49, 80131 Naples, Italy;

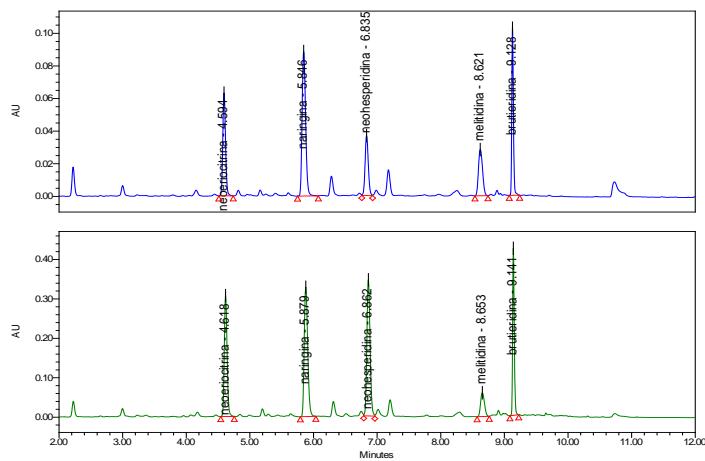
<sup>‡</sup> INDENA SpA, Via Don Minzoni 6, 20090 Settala (Mi), Italy



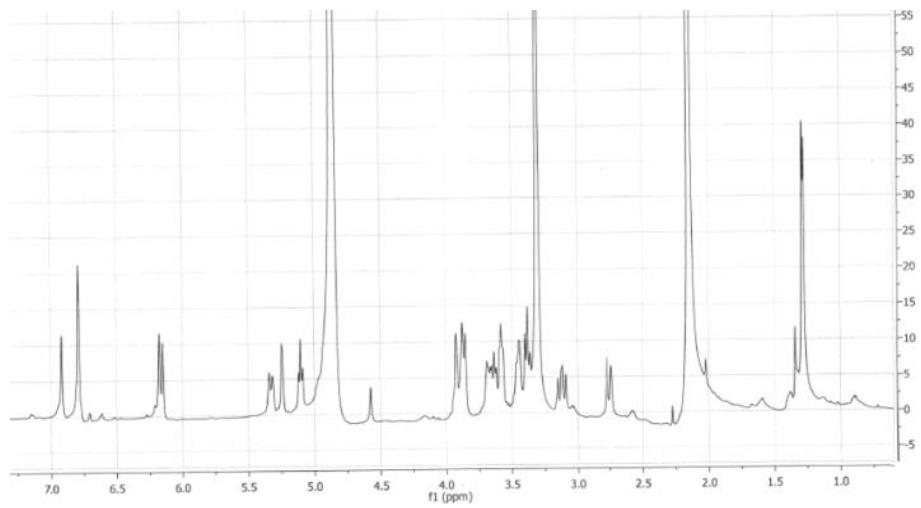
**Figure S1.** HPLC profile at 285 nm of BPF (top) and bergamot juice (bottom)



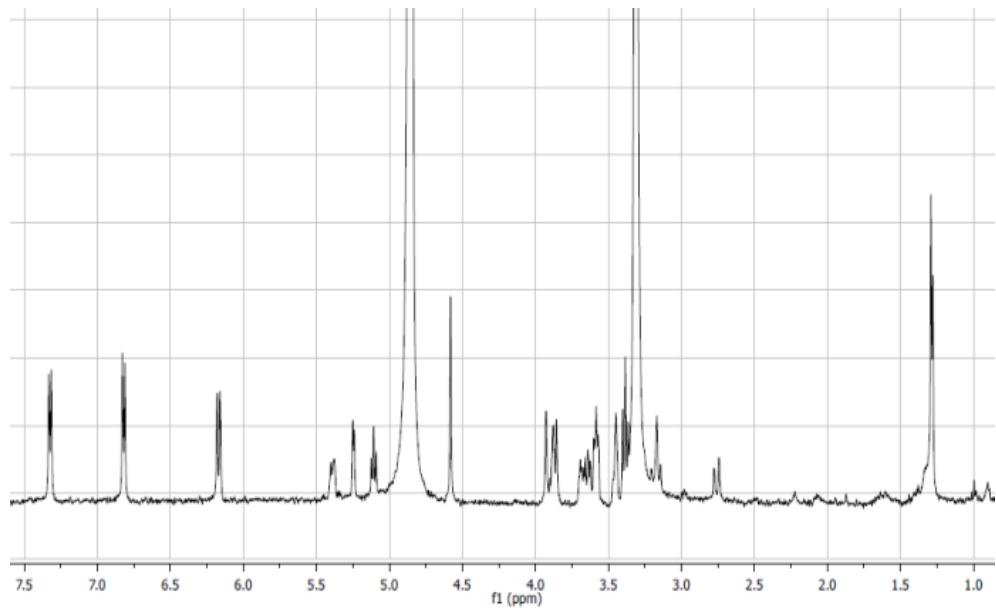
**Figure S2.** HPLC profile at 340 nm of BPF (top) and bergamot juice (bottom)



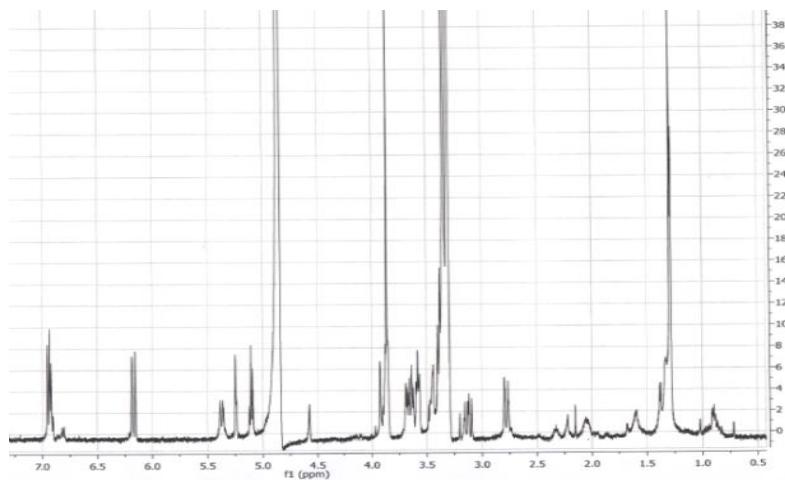
**Figure S3.** HPLC profile at 285 nm of hand-squeezed bergamot juice (top) and industrial bergamot juice used for BPF preparation (bottom)



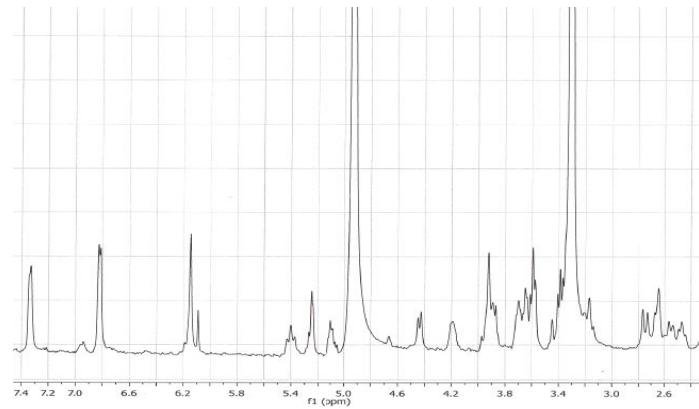
**Figure S4.** <sup>1</sup>H NMR spectrum of neoeriocitrin (**1**)



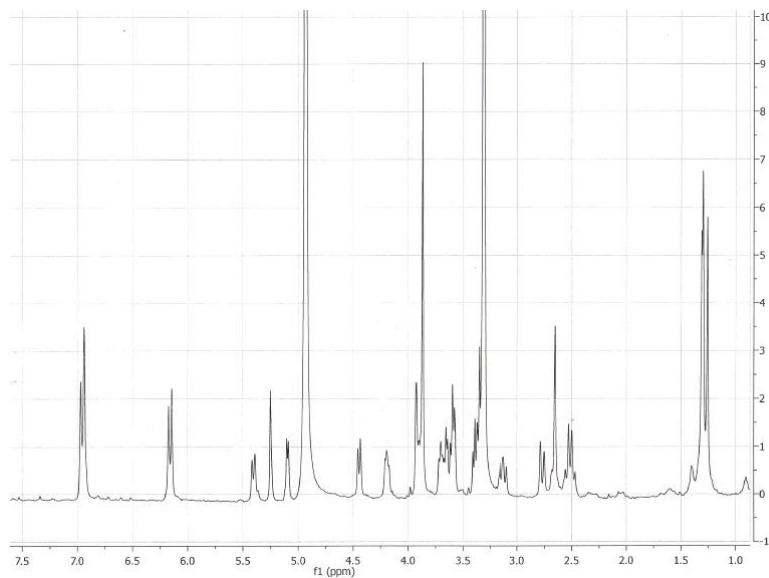
**Figure S5.** <sup>1</sup>H NMR spectrum of naringin (**2**)



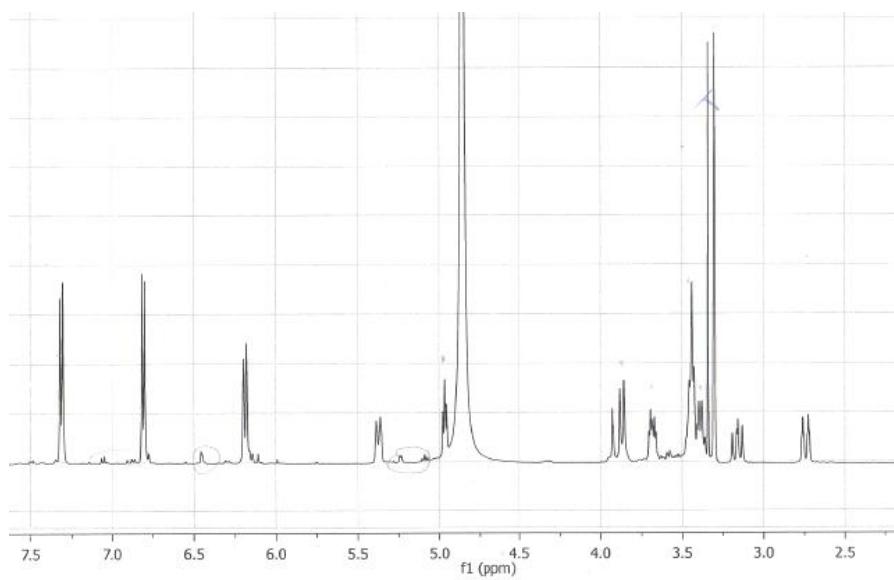
**Figure S6.** <sup>1</sup>H NMR spectrum of neohesperidin (3)



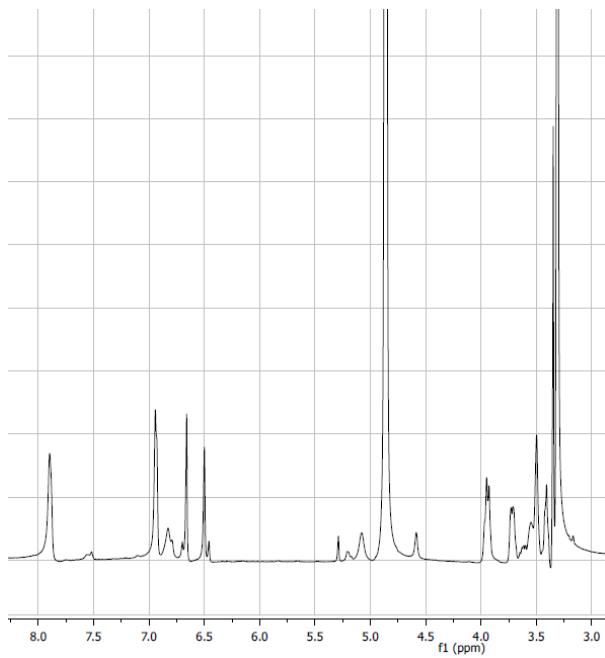
**Figure S7.** <sup>1</sup>H NMR spectrum of melitidin (4)



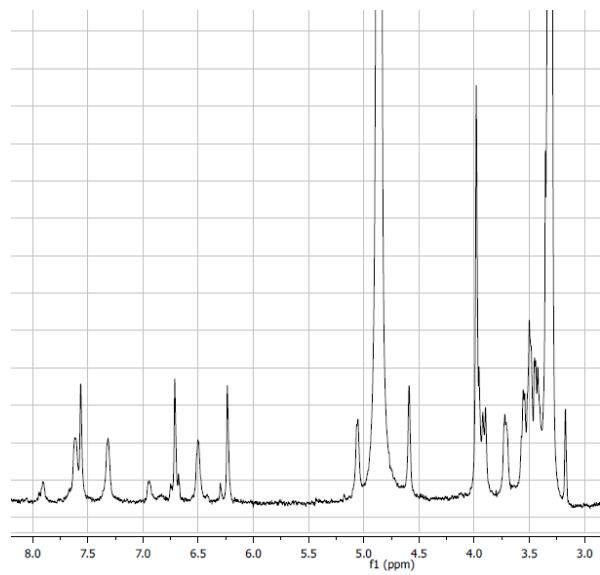
**Figure S8.** <sup>1</sup>H NMR spectrum of brutieridin (5)



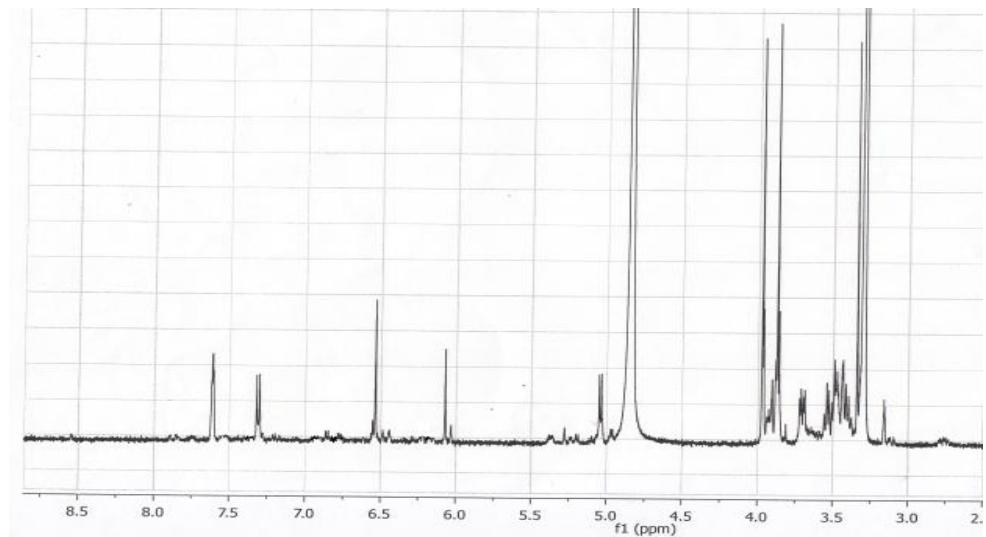
**Figure S9.** <sup>1</sup>H NMR spectrum of naringenin-7- $\beta$ -glucoside (prunasin) (**9**)



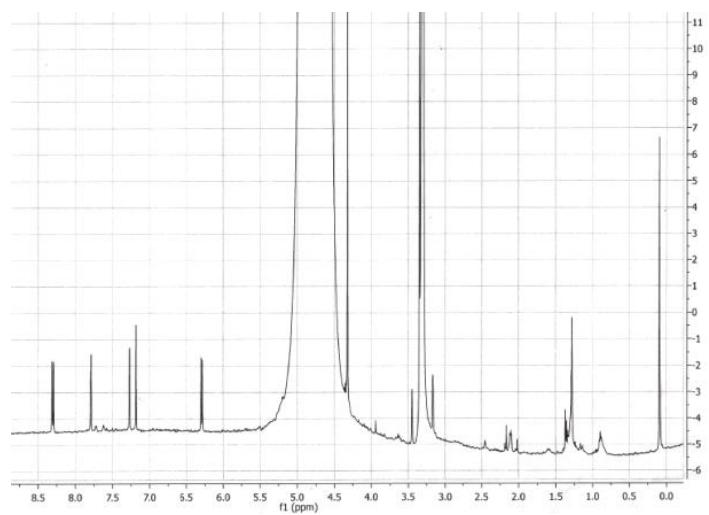
**Figure S10.** <sup>1</sup>H NMR spectrum of apigenin-6- $\beta$ -glucoside (isovitexin) (**16**)



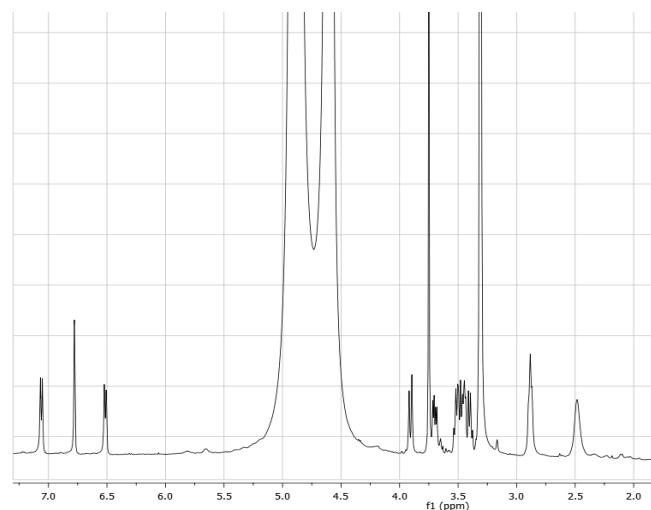
**Figure S11.** <sup>1</sup>H NMR spectrum of diosmetin-7-O- $\beta$ -glucoside (**21**)



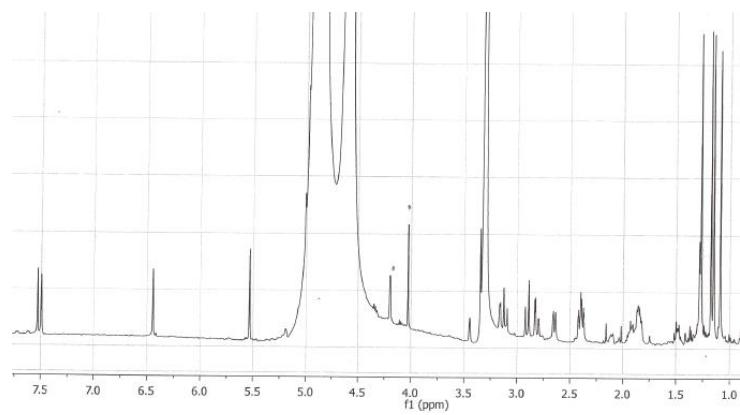
**Figure S12.** <sup>1</sup>H NMR spectrum of demethoxycentaureidin-7-O- $\beta$ -glucoside (**22**)



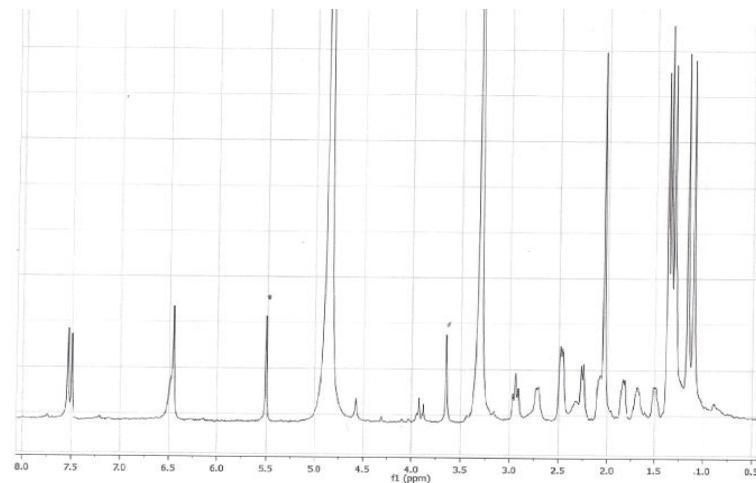
**Figure S13.** <sup>1</sup>H NMR spectrum of bergaptene (28)



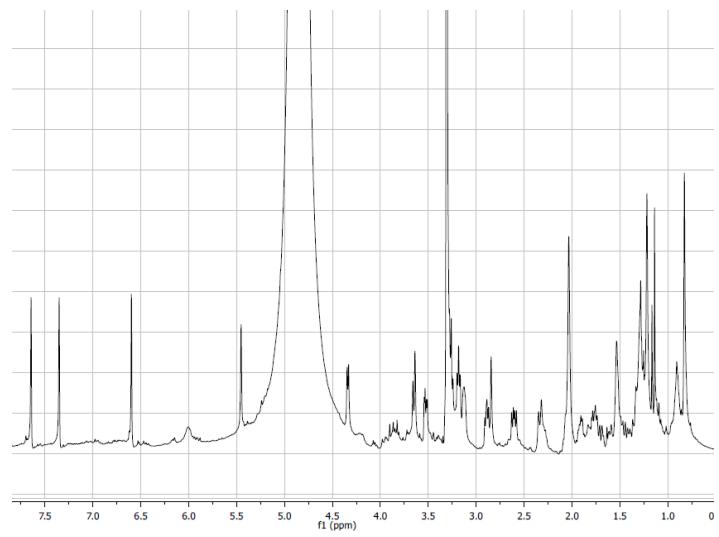
**Figure S14.** <sup>1</sup>H NMR spectrum of 2-O- $\beta$ -glucopyranose-2-hydroxy-4-methoxyhydrocinnamic acid (36)



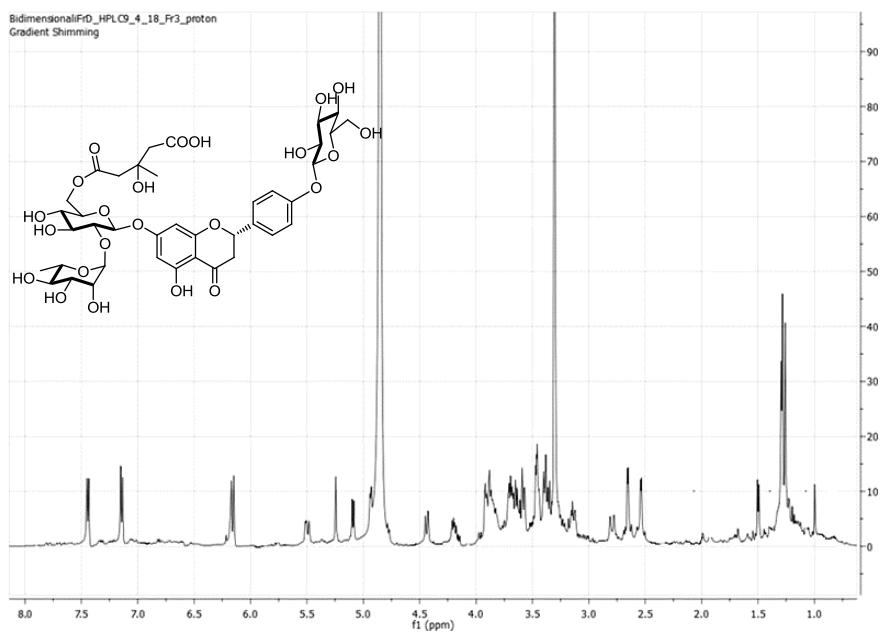
**Figure S15.** <sup>1</sup>H NMR spectrum of limonin (37)



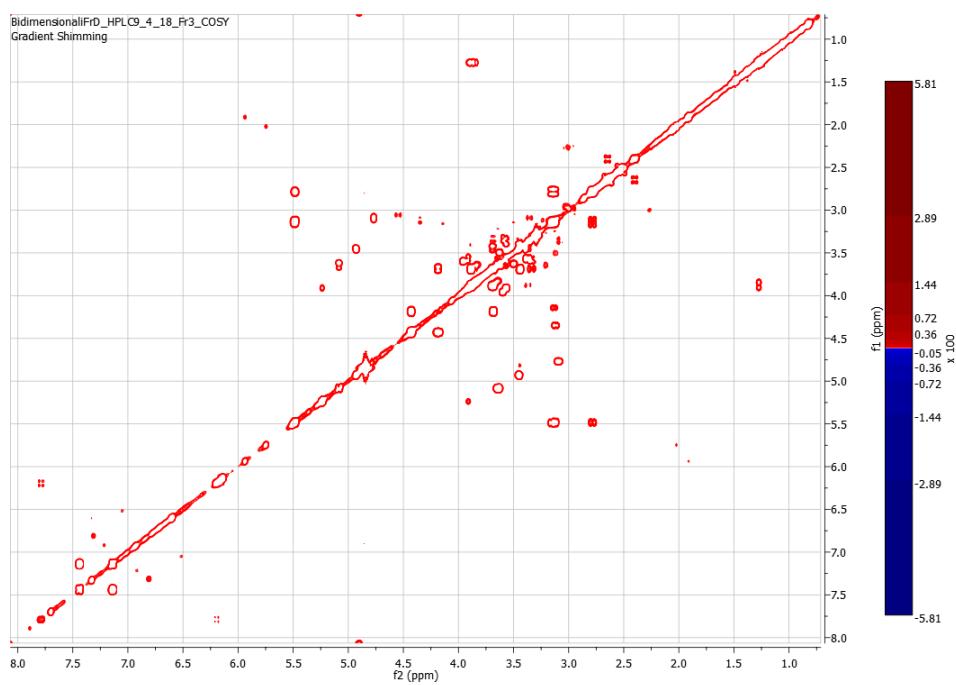
**Figure S16.** <sup>1</sup>H NMR spectrum of nomilinic acid (38)



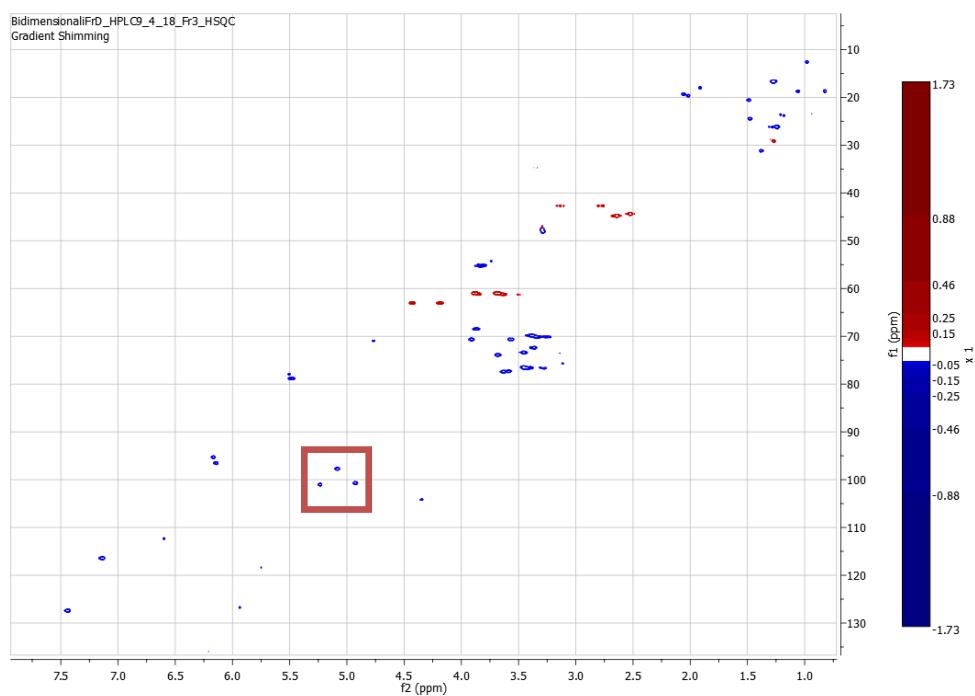
**Figure S17.** <sup>1</sup>H NMR spectrum of nomilinic acid glucoside (39)



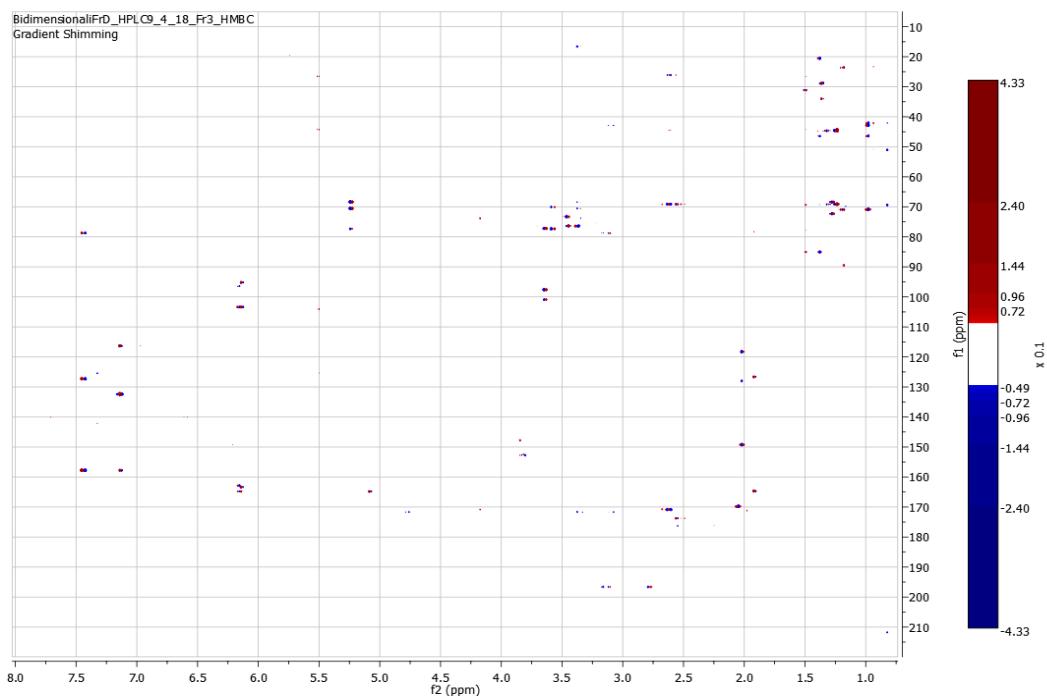
**Figure S18.**  $^1\text{H}$  NMR spectrum of bergamjuicin (35)



**Figure S19.** 2D COSY spectrum of bergamjuicin (35)



**Figure S20.** 2D HSQC spectrum of bergamjuicin (**35**)  
(correlations for anomeric positions are highlighted in the square)



**Figure S21.** 2D HMBC spectrum of bergamjuicin (**35**)