SUPPLEMENTARY MATERIAL

A new phenolic glycoside and two new monoterpenoid furocoumarins from *Aurantii Fructus Immaturus*

Ying Xiong, Meiyan Chang, Kezhong Deng*, Yongming Luo

College of Pharmacy, Jiangxi University of Traditional Chinese Medicine, Nanchang, China

Abstract

A new phenolic glycoside, citrauranoside A (**1**), and two new monoterpenoid furocoumarins, citraurancoumarin A (**2**) and citraurancoumarin B (**3**), along with four known compounds (**4-7**) were isolated from the young fruit of *Citrus aurantium* L. The structures were elucidated by their comprehensive analysis including 1D, 2DNMR, IR and mass spectra.

Keywords: Aurantii Fructus Immaturus; Coumarin; Phenolic glycoside

Supplemental file (Figure) Legend

Figure S1. HR-MS spectrum of Compound 1

Figure S2. IR spectrum of Compound 1

Figure S3. ^1H -NMR spectrum of Compound 1

Figure S4. ^1H - ^1H COSY spectrum of Compound 1

Figure S5. ^{13}C -NMR spectrum of Compound 1

Figure S6. DEPT spectrum of Compound 1

Figure S7. HSQC spectrum of Compound 1

Figure S8. The HMBC spectrum and its key correlations ($\text{H}\rightarrow\text{C}$) of Compound 1

Figure S9. HR-MS spectrum of Compound 2

Figure S10. IR spectrum of Compound 2

Figure S11. ^1H -NMR spectrum of Compound 2

Figure S12. ^1H - ^1H COSY spectrum of Compound 2

Figure S13. ^{13}C -NMR spectrum of Compound 2

Figure S14. HSQC spectrum of Compound 2

Figure S15. The HMBC spectrum and its key correlations ($\text{H}\rightarrow\text{C}$) of Compound 2

Figure S16. HR-MS spectrum of Compound 3

Figure S17. IR spectrum of Compound 3

Figure S18. ^1H -NMR spectrum of Compound 3

Figure S19. ^1H - ^1H COSY spectrum of Compound 3

Figure S20. ^{13}C -NMR spectrum of Compound 3

Figure S21. HSQC spectrum of Compound 3

Figure S22. The HMBC spectrum and its key correlations ($\text{H}\rightarrow\text{C}$) of Compound 3

Figure S1.

LXB20150325WH_C402 343 (3.352) Cm (339:344)

1: TOF MS ES+
1.81e5

Figure S2.

Figure S3.

Figure S4.

Figure S5.

Figure S6.

Figure S7.

Figure S8.

Figure S9.

Figure 10.

Figure S11.

Figure S12.

Figure S13.

Figure S14.

Figure S15.

Figure S16.

Figure S17.

Figure S18.

Figure S19.

Figure S20.

Figure S21.

Figure S22.