SUPPLEMENTARY MATERIAL

Determination of a New Chromone from *Aurantii Fructus Immaturus* by DFT/GIAO Method

Zhe Jiang^{1,2}, Fang Liu^{1,2}, Aijiao Zhong¹, Jiaxiu Dugu¹ and Xuezheng Li^{1,2}

¹ *Department of Pharmacy, Yanbian University Hospital, Yanji, Jilin Province, 133000, PR China.*

² *Yanbian University College of Pharmacy, Yanji, Jilin Province, 133000, PR China.*

Investigation of EtOAc fraction from the 95% ethanol extract of *Aurantii Fructus Immaturus* led to the isolation of one new chromone (**1**) and seven known flavonoids (**2-8**). Their structures were elucidated mainly by NMR and HR-ESI-MS, as well as on comparison with the reported NMR data. The final substituent pattern of **1** was defined by comparison of ¹³C NMR data calculated by DFT/GIAO with those of experimental NMR data.

Key words: *Aurantii Fructus Immaturus*; chromone; GIAO

Figure S1. ¹H spectrum of compound **1**

Figure S2. ¹³C spectrum of compound **1**

Figure S3. HSQC spectrum of compound **1**

Figure S4. HMBC spectrum of compound **1**