Supplementary Data for

Rhamnellosides A and B, ω -Phenylpentaene Fatty Acid Amide Diglycosides from the Fruits of *Rhamnella franguloides*

Kyo Bin Kang,^{1,†} Ming Gao,^{2,†} Geum Jin Kim,² Hyukjae Choi,^{2,*} and Sang Hyun Sung^{1,*}

¹College of Pharmacy and Research Institute of Pharmaceutical Sciences, Seoul National University, Seoul 08826, Republic of Korea

² College of Pharmacy, Yeungnam University, Gyeongsan 38541, Republic of Korea

⁺ These authors equally contributed to this work.

*Correspondence to:

Sang Hyun Sung (shsung@snu.ac.kr)

Hyukjae Choi (<u>h5choi@yu.ac.kr</u>)

Table of Contents

- Figure S1. UHPLC–Q/TOF–MS base peak ion (BPI) chromatograms of methanol extracts of (a) *B. berchemiifolia* and (b) *R. franguloides* fruits. Peak numbers designate the isolated compounds 1–8.
- Figure S2. The MS spectrum of 1
- Figure S3. The MS/MS spectrum of 1
- **Figure S4.** The ¹H NMR (850 MHz, DMSO- d_6) spectrum of **1**
- Figure S5. The ${}^{1}\text{H}{}^{-1}\text{H}$ COSY (850 MHz, DMSO- d_{6}) spectrum of 1
- Figure S6. The HSQC (850 MHz, DMSO-d₆) spectrum of 1
- Figure S7. The HMBC (850 MHz, DMSO- d_6) spectrum of 1
- **Figure S8.** The *J*-resolved (850 MHz, DMSO- d_6) spectrum of **1**, expanded for the polyene region.
- Figure S9. UV and CD spectra of 1
- Figure S10. The MS spectrum of 2
- Figure S11. The MS/MS spectrum of 2
- **Figure S12.** The ¹H NMR (850 MHz, DMSO- d_6) spectrum of **2**
- Figure S13. The 1 H- 1 H COSY (850 MHz, DMSO- d_{6}) spectrum of 2
- Figure S14. The HSQC (850 MHz, DMSO-*d*₆) spectrum of 2
- Figure S15. The HMBC (850 MHz, DMSO-*d*₆) spectrum of 2
- **Figure S16.** The *J*-resolved (850 MHz, DMSO-*d*₆) spectrum of **2**, expanded for the polyene region.
- Figure S17. UV and CD spectra of 2
- Figure S18. TLC for determining sugar moieties in hydrolysates of 1 (a) and 2 (b). Standards of glucose, arabinose, and xylose were spotted together.
- Figure S19. HPLC chromatograms for analyzing sugar derivatives in hydrolysates of 1 and 2.
 (a) D-glucose standard derivative (b) (c) D-xylose standard derivative (d) L-xylose standard derivative (e) derivatized hydrolysate of compound 1 (f) derivatized hydrolysate of compound 2.
- Figure S20. HPLC-DAD/MS chromatograms in C3 Marfey's analyses on the Leu unit of the hydrolysate of 1. (a) L-FDAA derivatized L/D mixture of Leu, (b) L-FDAA

derivatized hydrolysate of **1**.

Figure S21. HPLC-UV (340 nm) chromatograms in C3 Marfey's analyses on the Leu and Ile units of the hydrolysate of 2. (a) L-FDAA derivatized L/D standard mixtures of Leu/Ile/*allo*-Ile, (b) L-FDAA derivatized hydrolysate of 2, (c) co-injected L-FDAA derivatized the standard mixture and hydrolysate of 2.



Figure S1. UHPLC–Q/TOF–MS base peak ion (BPI) chromatograms of methanol extracts of (a) *B. berchemiifolia* and (b) *R. franguloides* fruits. Peak numbers designate compounds **1–8**.



Figure S2. The MS spectrum of 1



Figure S3. The MS/MS spectrum of 1





Figure S5. The ${}^{1}\text{H}{}^{-1}\text{H}$ COSY (850 MHz, DMSO- d_{6}) spectrum of **1**



Figure S6. The HSQC (850 MHz, DMSO-*d*₆) spectrum of 1



Figure S7. The HMBC (850 MHz, DMSO-*d*₆) spectrum of 1



Figure S8. The *J*-resolved (850 MHz, DMSO-*d*₆) spectrum of **1**, expanded for the polyene region.



Figure S9. UV and CD spectra of 1



Figure S10. The MS spectrum of 2



Figure S11. The MS/MS spectrum of 2



Figure S12. The ¹H NMR (850 MHz, DMSO-*d*₆) spectrum of 2



Figure S13. The 1 H- 1 H COSY (850 MHz, DMSO- d_{6}) spectrum of **2**



Figure S14. The HSQC (850 MHz, DMSO-*d*₆) spectrum of 2



Figure S15. The HMBC (850 MHz, DMSO-*d*₆) spectrum of 2



Figure S16. The *J*-resolved (850 MHz, DMSO-*d*₆) spectrum of **2**, expanded for the polyene region.



Figure S17. UV and CD spectra of 2



Figure S18. TLC for determining sugar moieties in hydrolysates of **1** (a) and **2** (b). Standards of glucose, arabinose, and xylose were spotted together.



Figure S19. HPLC chromatograms for analyzing sugar derivatives in hydrolysates of 1 and 2. (a) D-glucose standard derivative (b) (c) D-xylose standard derivative (d) L-xylose standard derivative (e) derivatized hydrolysate of compound 1 (f) derivatized hydrolysate of compound 2.



Figure S20. HPLC-DAD/MS chromatograms in C3 Marfey's analyses on the Leu unit of the hydrolysate of **1**. (a) L-FDAA derivatized L/D mixture of Leu, (b) L-FDAA derivatized hydrolysate of **1**.



Figure S21. HPLC-UV (340 nm) chromatograms in C3 Marfey's analyses on the Leu and Ile units of the hydrolysate of **2**. (a) L-FDAA derivatized L/D standard mixtures of Leu/Ile/*allo*-Ile, (b) L-FDAA derivatized hydrolysate of **2**, (c) co-injected L-FDAA derivatized the standard mixture and hydrolysate of **2**.