Supporting Information

Improvement of water solubility of mercaptoundecahydrododecaborate (BSH)-peptides by conjugating with ethylene glycol linker and inclusion in cyclodextrin

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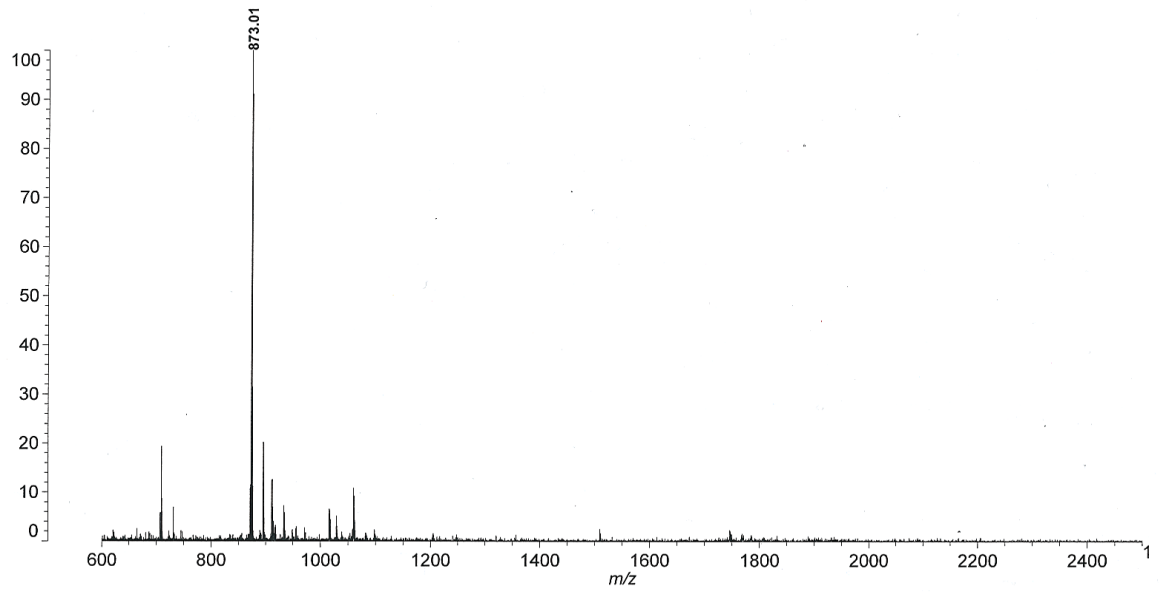

Figure S1. MALDI-Tof Mass spectrum of **BSH-3R**. An α-CHCA was used as a matrix. calcd. $[M+H]^+$ = 872.49 and obsd. $[M+H]^+$ = 873.01.

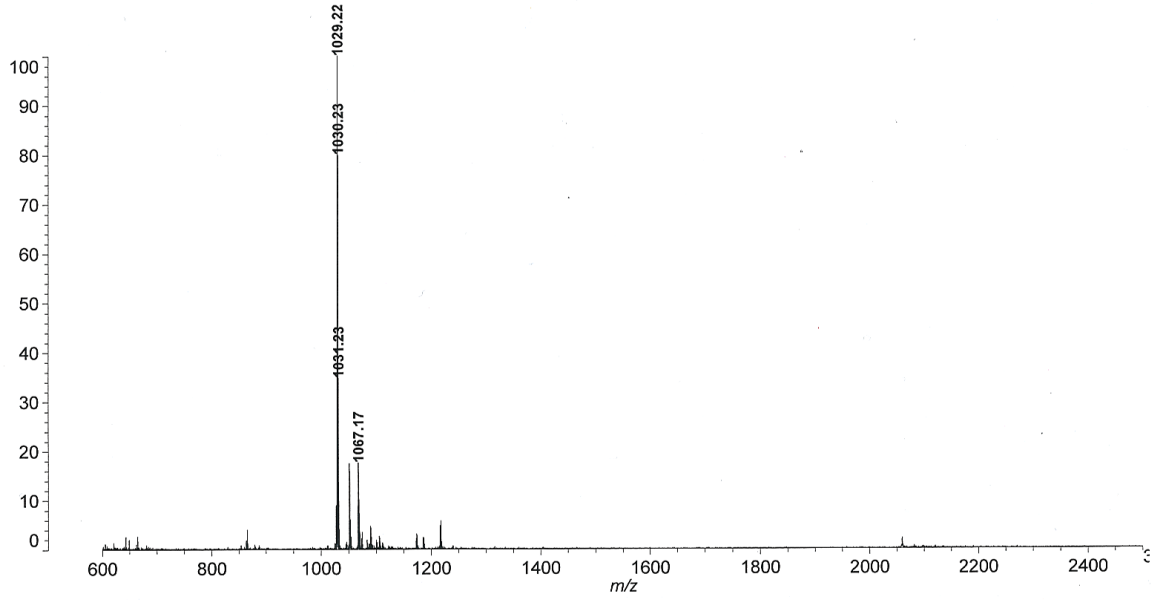

Figure S2. MALDI-Tof Mass spectrum of **BSH-4R**. An α-CHCA was used as a matrix. calcd. $[M+H]^+$ = 1028.59 and obsd. $[M+H]^+$ = 1029.22.

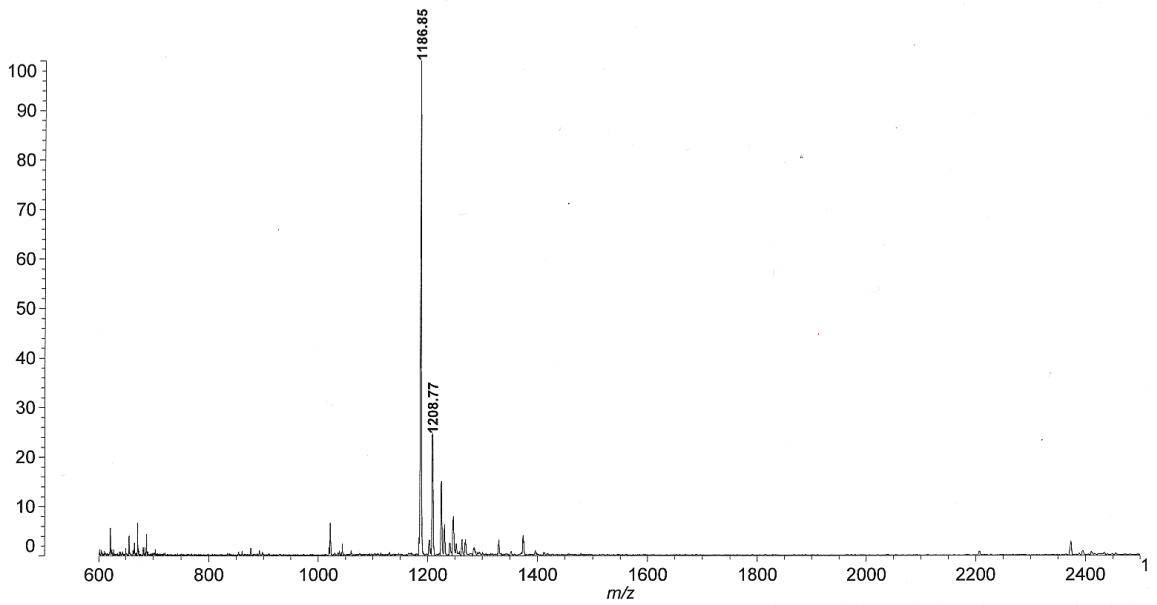

Figure S3. MALDI-Tof Mass spectrum of **BSH-5R**. An α-CHCA was used as a matrix. calcd. $[M+H]^+$ = 1184.69 and obsd. $[M+H]^+$ = 1186.85.

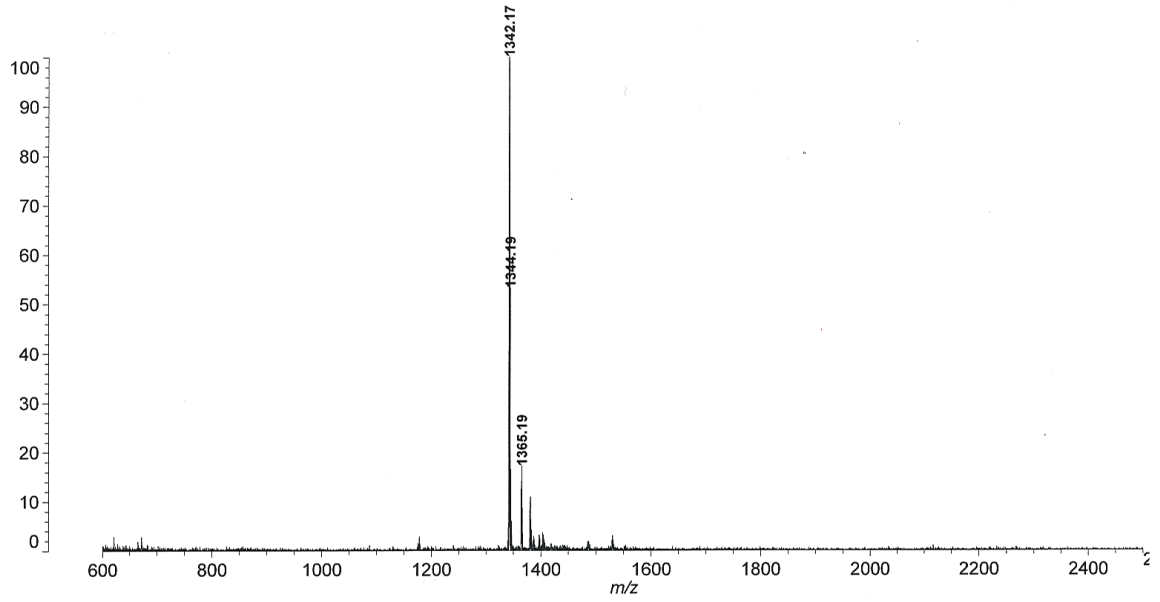

Figure S4. MALDI-Tof Mass spectrum of **BSH-6R**. An α-CHCA was used as a matrix. calcd. $[M+H]^+$ = 1340.79 and obsd. $[M+H]^+$ = 1342.17.

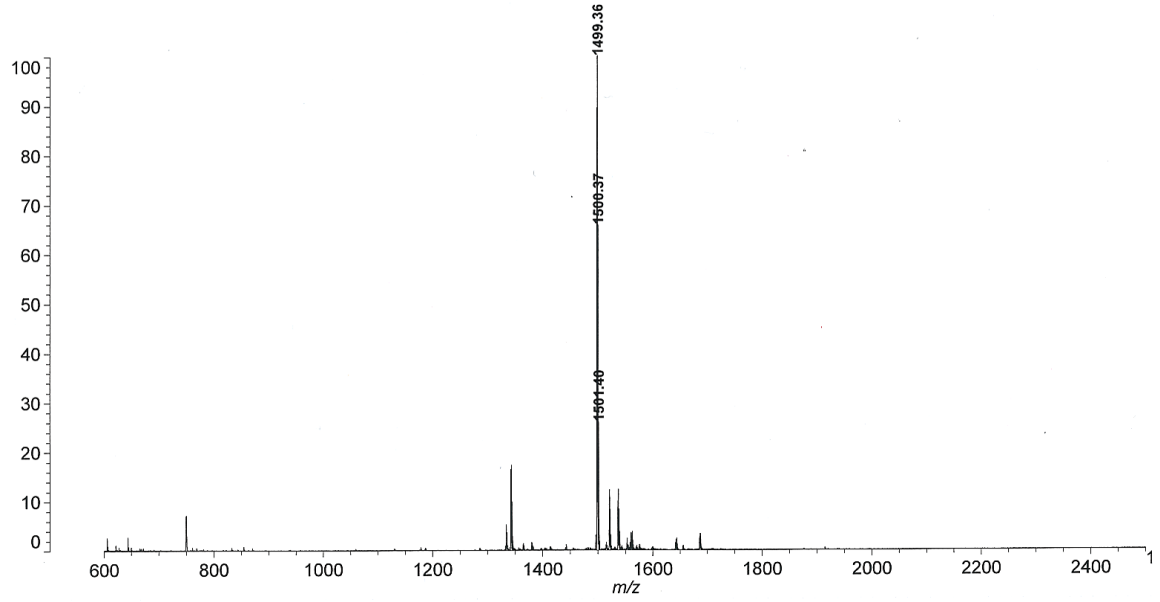

Figure S5. MALDI-Tof Mass spectrum of **BSH-7R**. An α-CHCA was used as a matrix. calcd. $[M+H]^+$ = 1496.89 and obsd. $[M+H]^+$ = 1499.36.

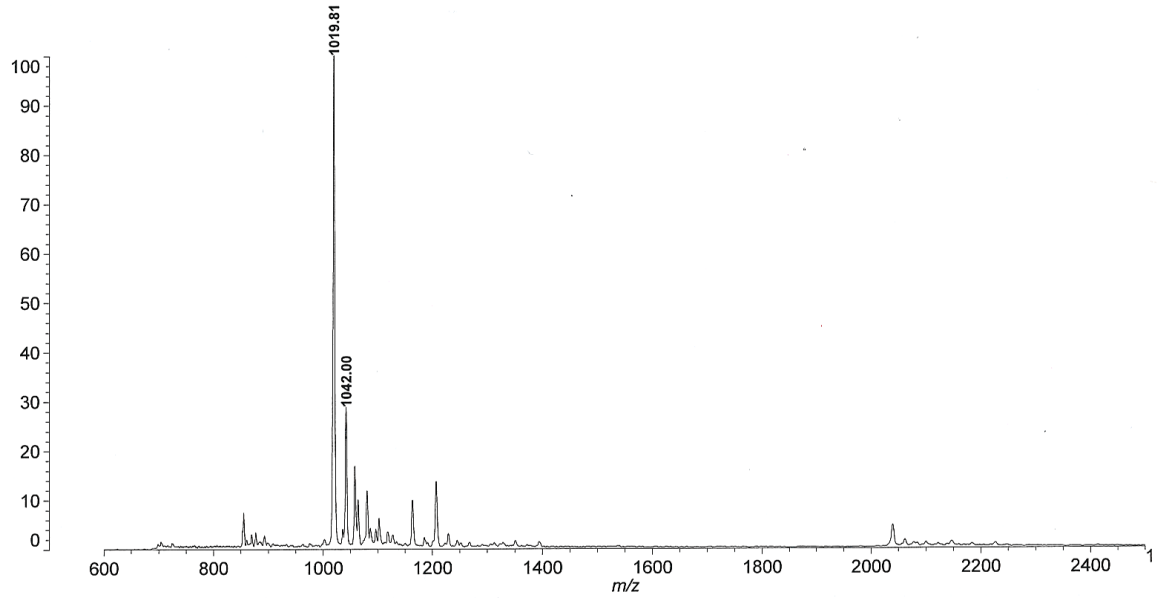

Figure S6. MALDI-Tof Mass spectrum of **BSH-2Eg-3R**. An α-CHCA was used as a matrix. calcd. $[M+H]^+$ = 1017.56 and obsd. $[M+H]^+$ = 1019.81.

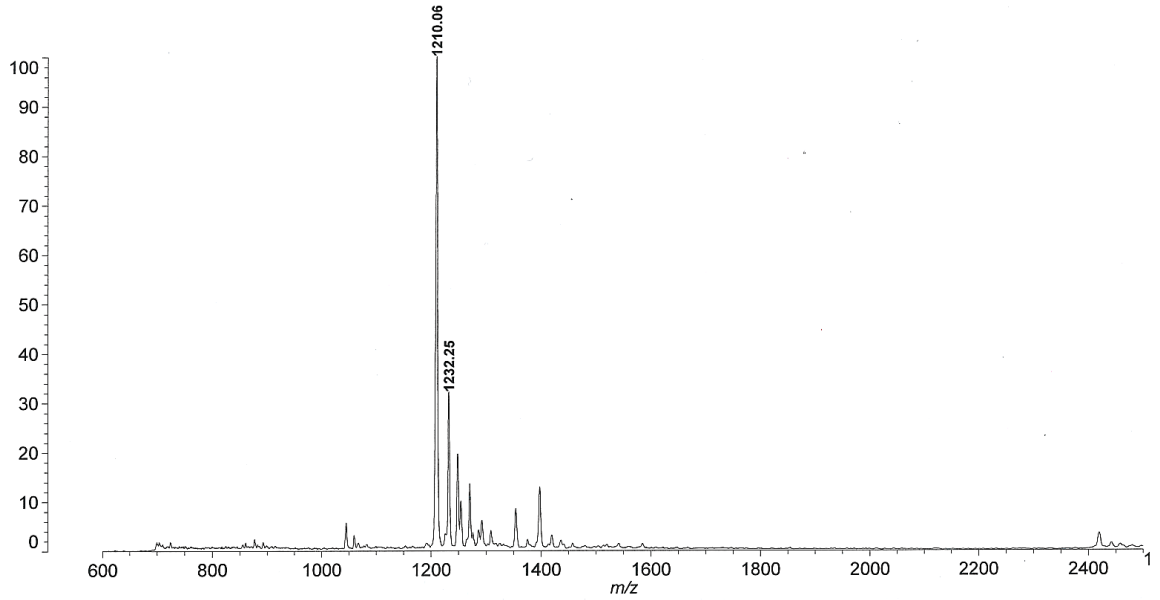

Figure S7. MALDI-Tof Mass spectrum of **BSH-6Eg-3R**. An α-CHCA was used as a matrix. calcd. $[M+H]^+$ = 1207.68 and obsd. $[M+H]^+$ = 1210.06.

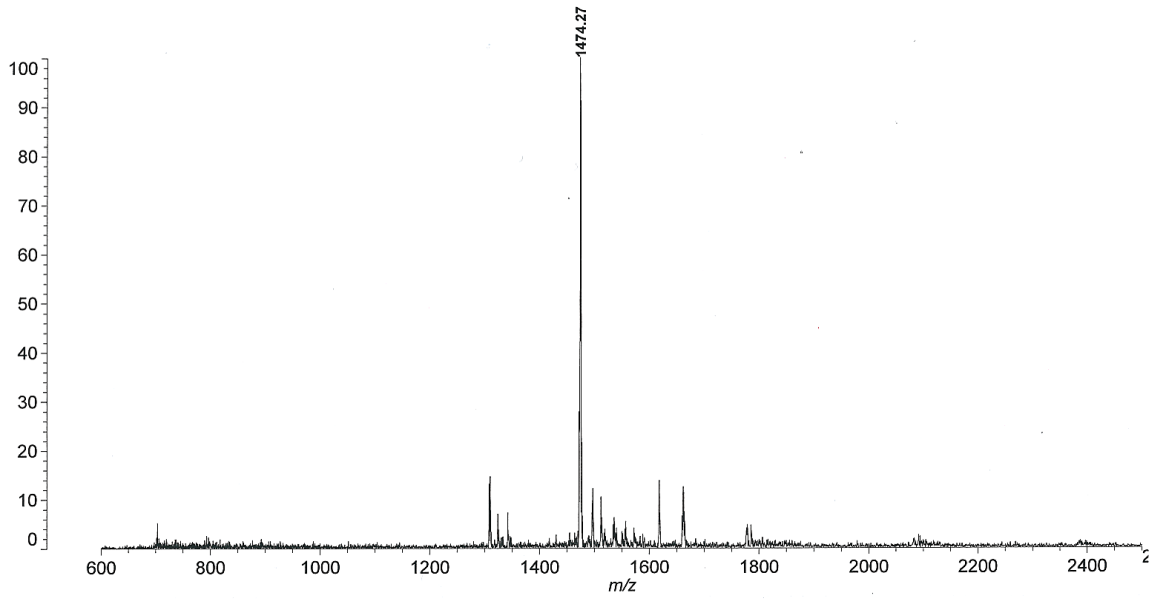

Figure S8. MALDI-Tof Mass spectrum of **BSH-12Eg-3R**. An α-CHCA was used as a matrix. calcd. $[M+H]^+$ = 1471.84 and obsd. $[M+H]^+$ = 1474.27.

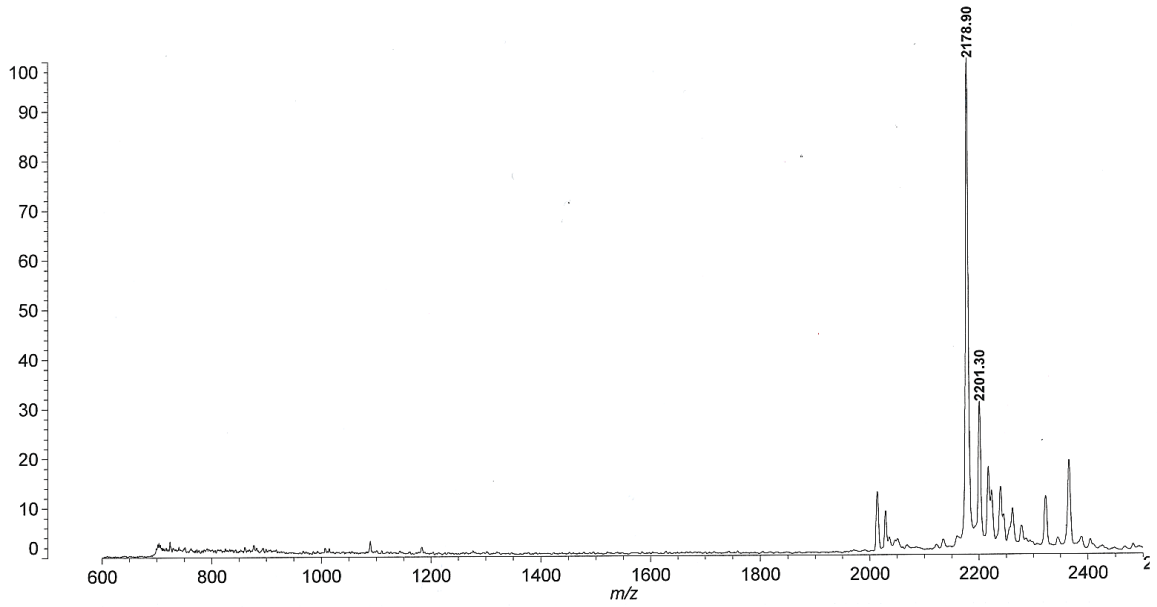

Figure S9. MALDI-Tof Mass spectrum of **BSH-28Eg-3R**. An α-CHCA was used as a matrix. calcd. $[M+H]^+$ = 2176.26 and obsd. $[M+H]^+$ = 2178.90.

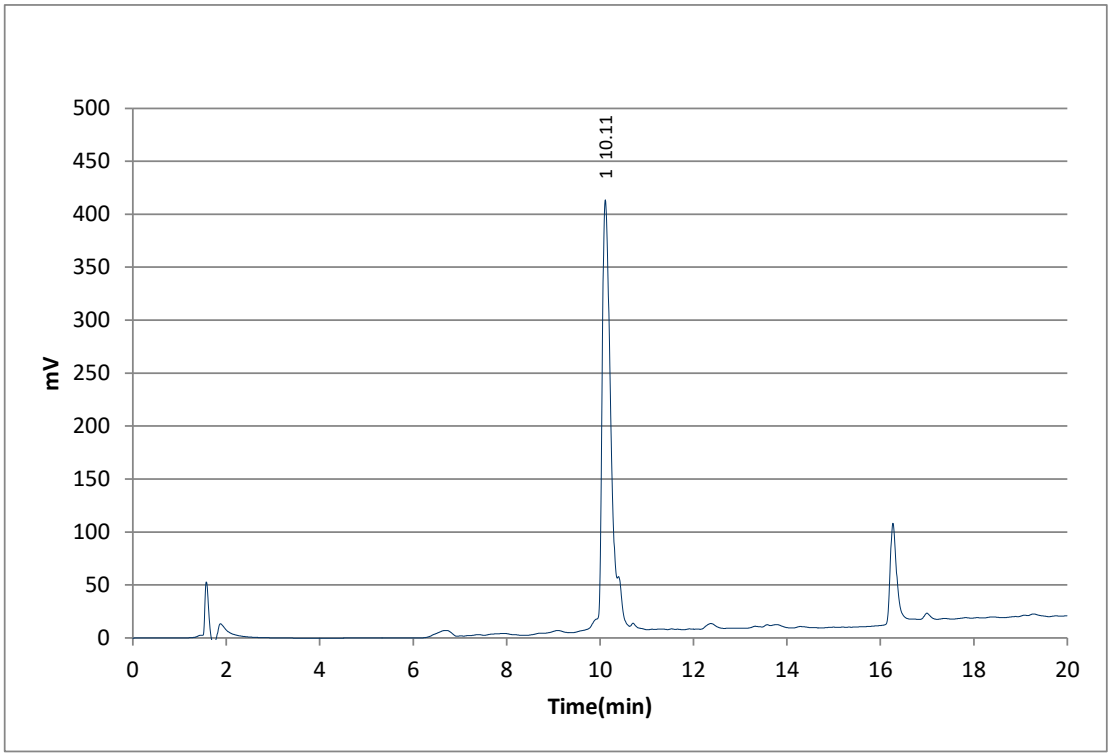

Figure S10. RP-HPLC chart of **BSH-3R** on C18 column. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 230 nm with a gradient of 0-100% for 20 min.

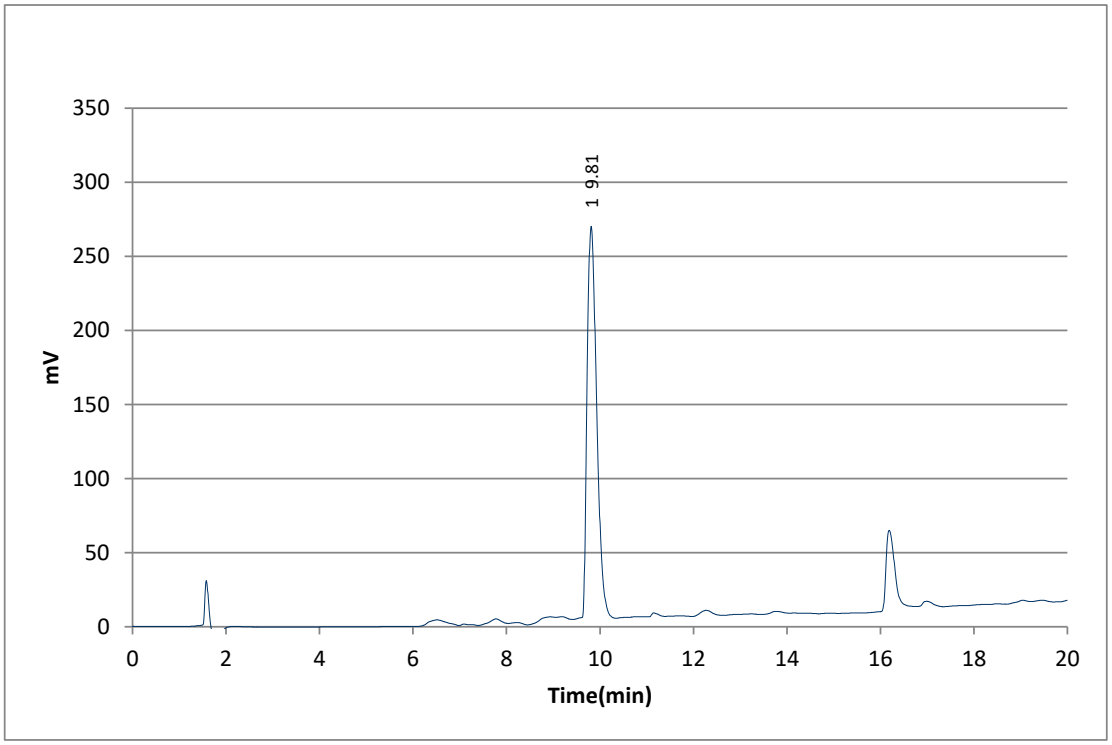

Figure S11. RP-HPLC chart of **BSH-4R** on C18 column. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 230 nm with a gradient of 0-100% for 20 min.

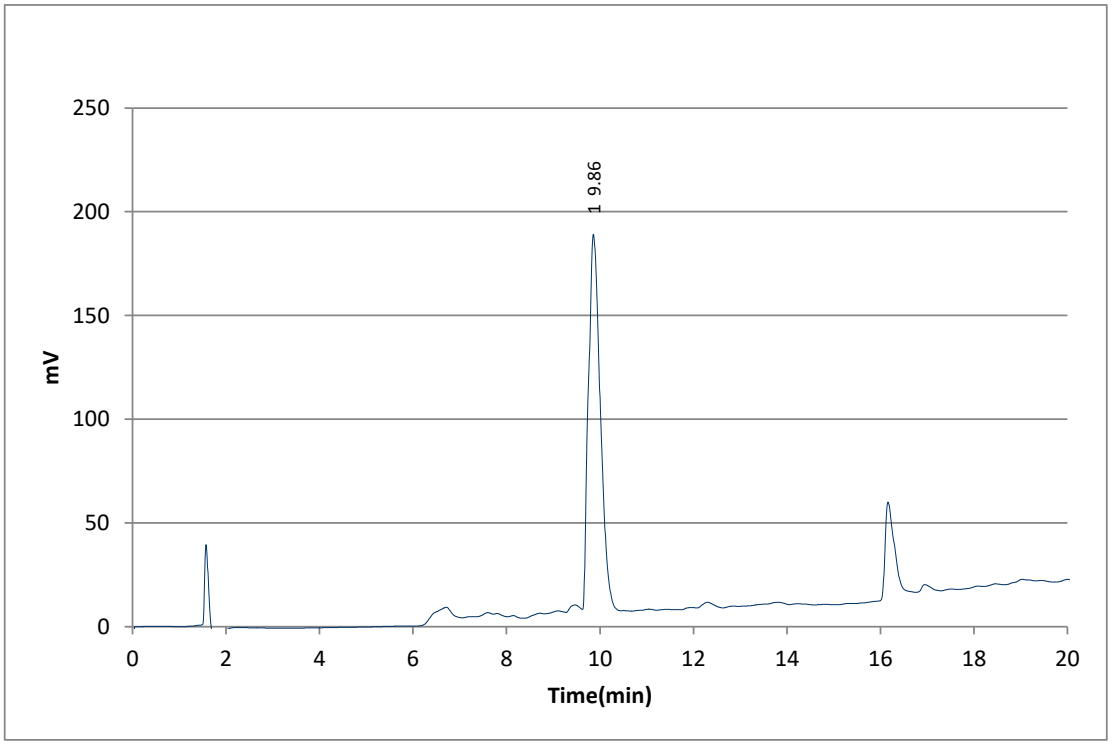

Figure S12. RP-HPLC chart of **BSH-5R** on C18 column. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 230 nm with a gradient of 0-100% for 20 min.

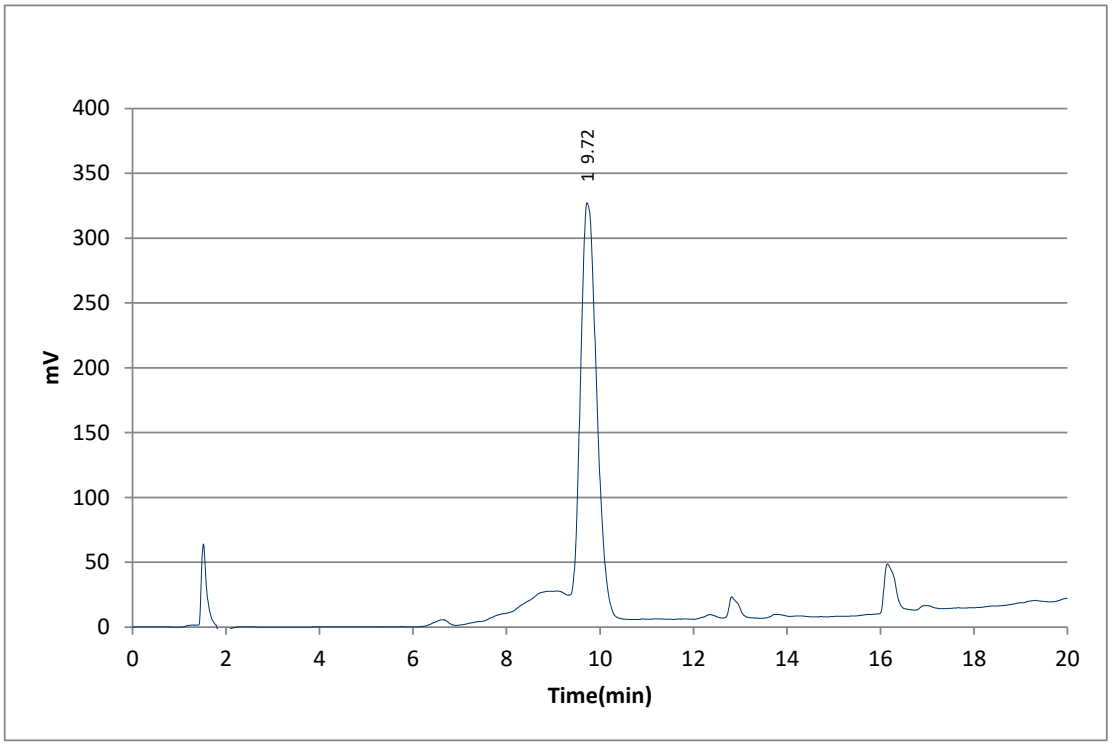

Figure S13. RP-HPLC chart of **BSH-6R** on C18 column. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 230 nm with a gradient of 0-100% for 20 min.

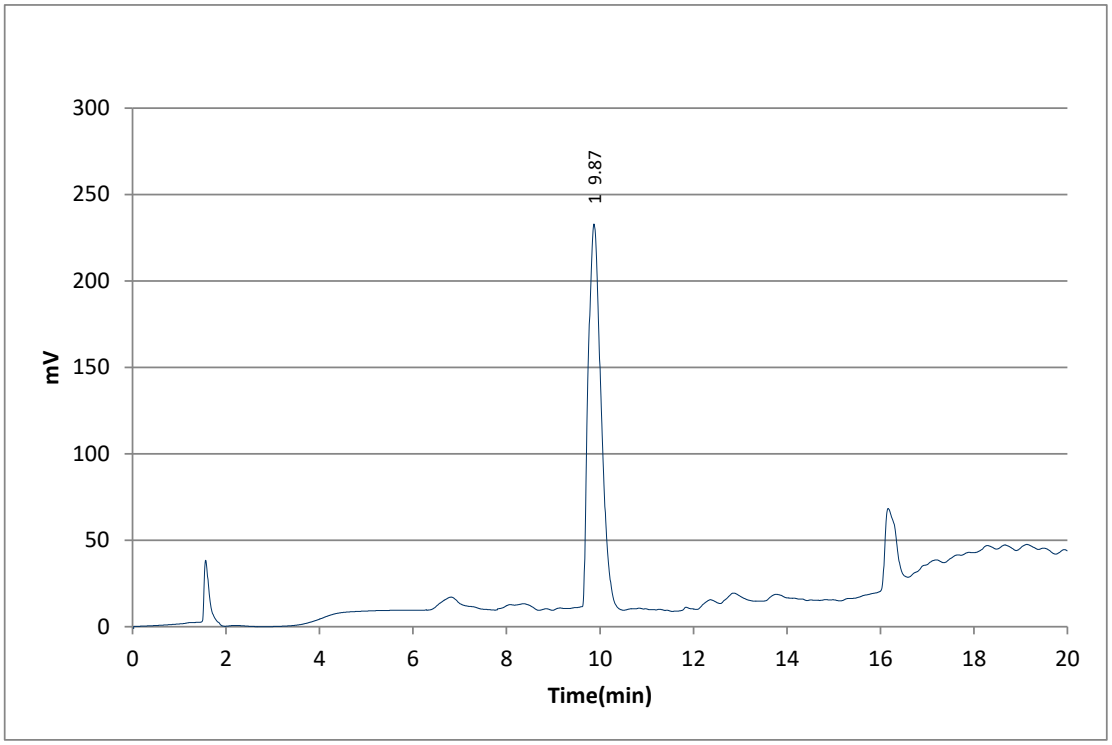

Figure S14. RP-HPLC chart of **BSH-7R** on C18 column. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 230 nm with a gradient of 0-100% for 20 min.

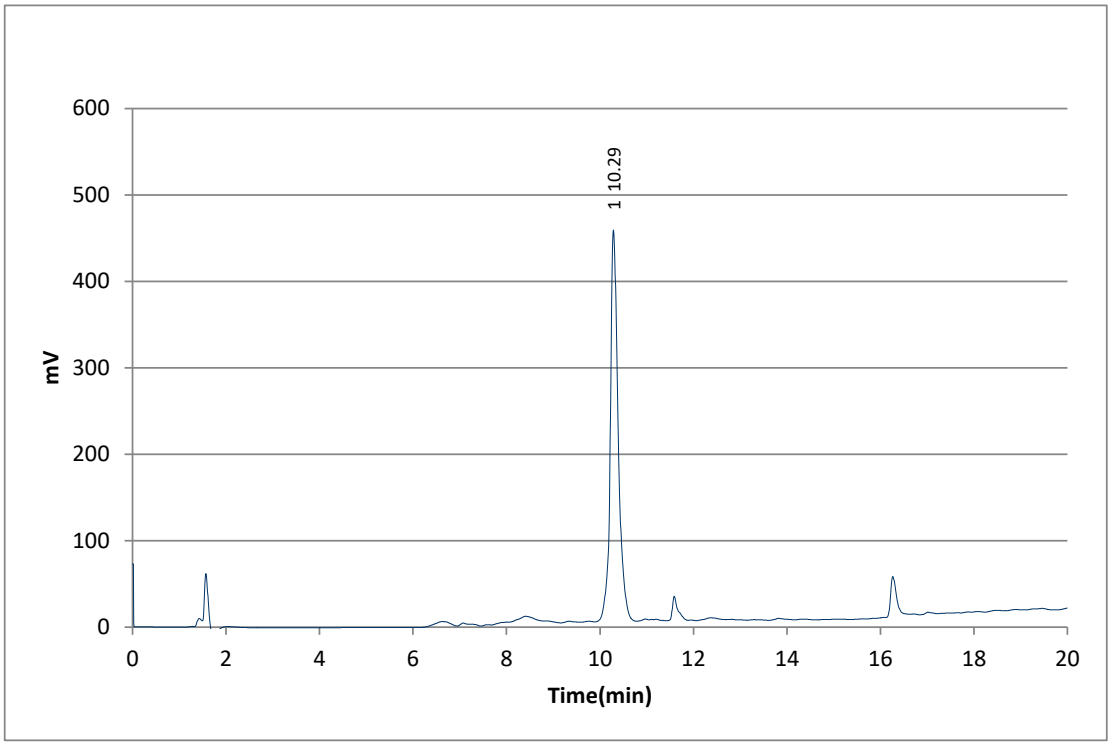

Figure S15. RP-HPLC chart of **BSH-2Eg-3R** on C18 column. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 230 nm with a gradient of 0-100% for 20 min.

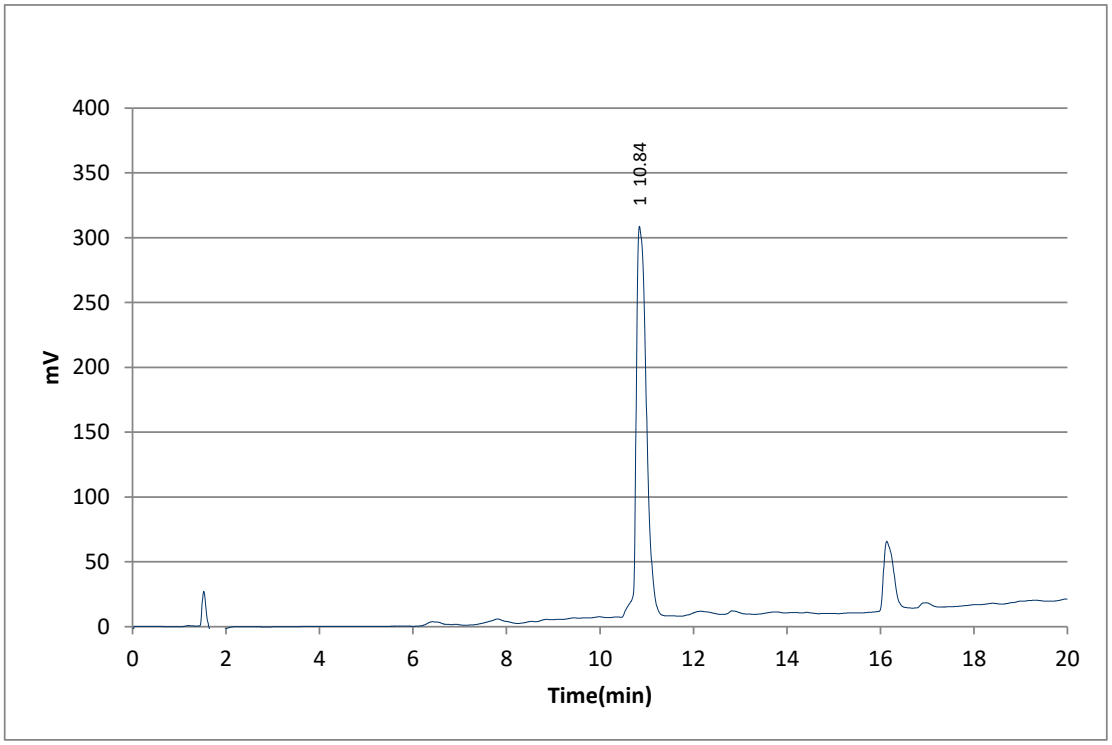

Figure S16. RP-HPLC chart of **BSH-6Eg-3R** on C18 column. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 230 nm with a gradient of 0-100% for 20 min.

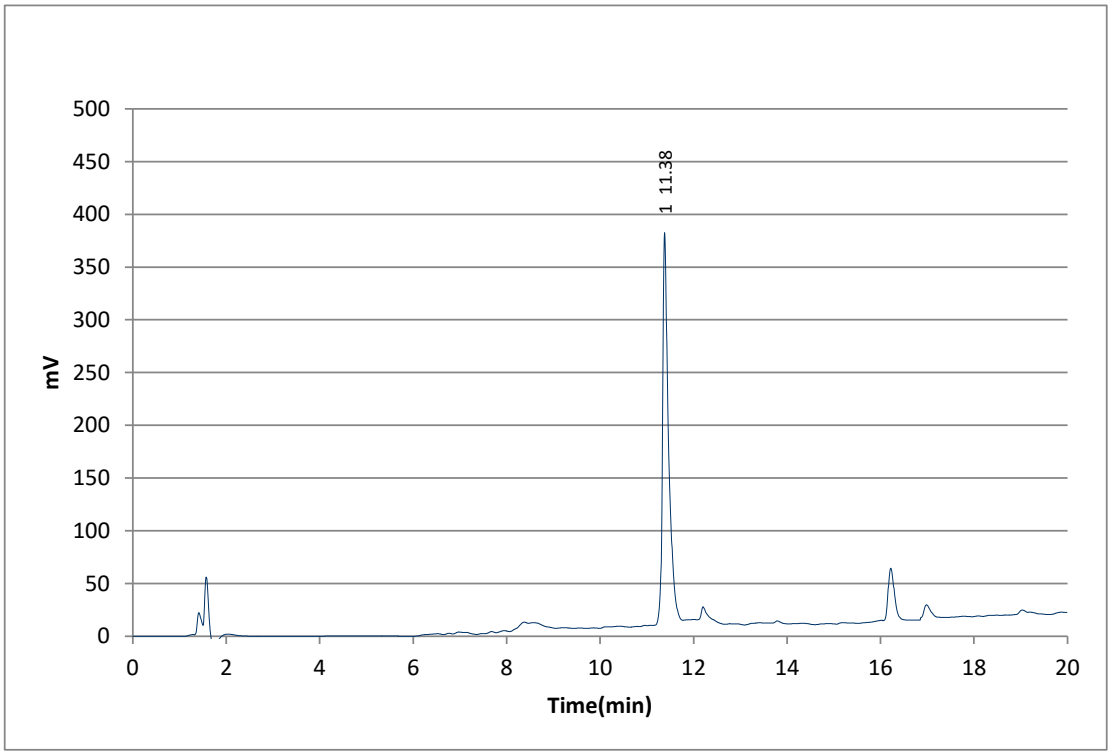

Figure S17. RP-HPLC chart of **BSH-12Eg-3R** on C18 column. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 230 nm with a gradient of 0-100% for 20 min.

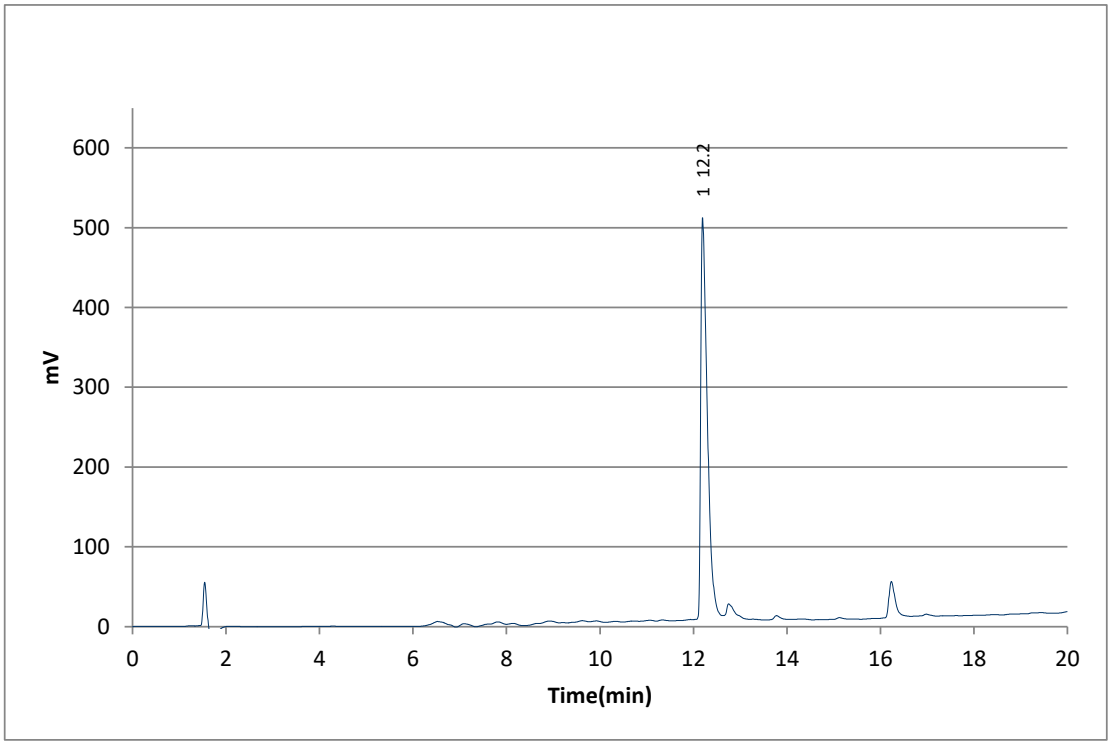

Figure S18. RP-HPLC chart of **BSH-28Eg-3R** on C18 column. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 230 nm with a gradient of 0-100% for 20 min.

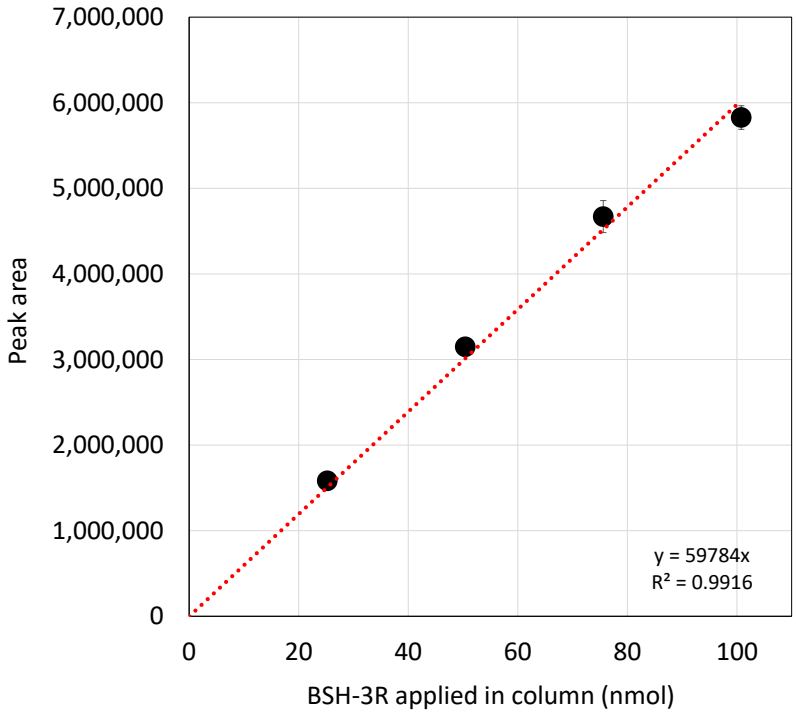

Figure S19. Calibration curve for estimation of water solubility of **BSH-3R**.

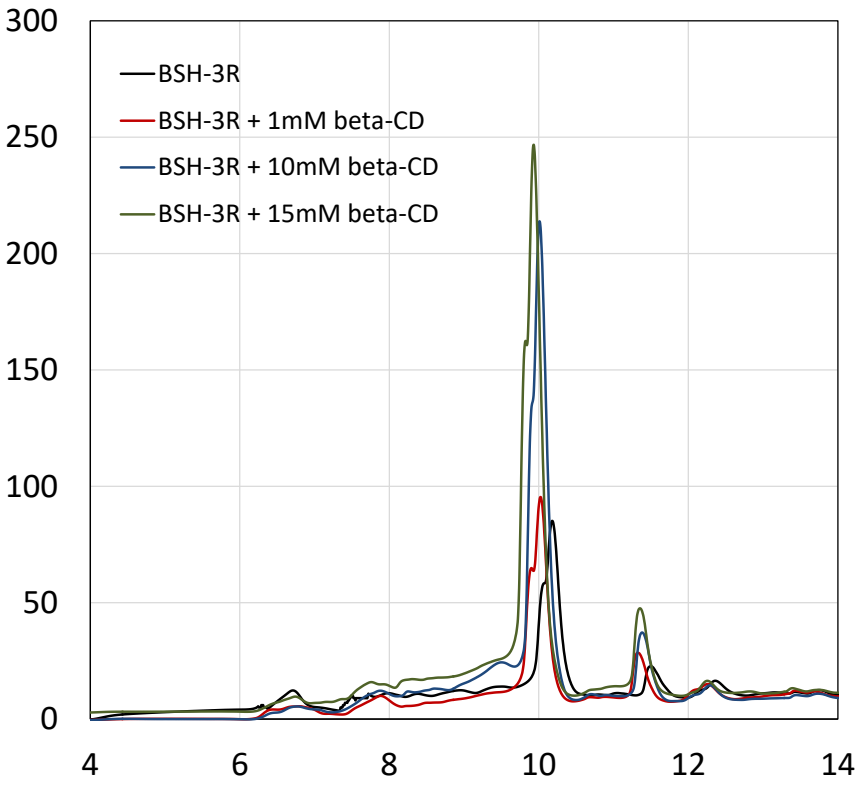

Figure S20. HPLC charts of **BSH-3R** treated with various concentration of β-CD.