UPLC- QTOF-MS analysis. Ultra-performance liquid chromatography (UPLC) analysis was performed using an ACQUITY UPLC™ system (Waters Corporation, Milford, MA, USA) equipped with a binary solvent delivery manager, photodiode array (PDA) and a sample manager coupled to a Micromass Q-TOF Premier™ mass spectrometer equipped with an electrospray interface (Waters Corporation). The methanol extract and the compounds isolated by column chromatography were analyzed by UPLC-QTOF-MS. The chromatographic separations were performed on a 2.1 × 100 mm, 1.7 µm ACQUITY HSS T3 C18 chromatography column. The column temperature was maintained at 35°C, and the mobile phases A and B comprised water with 0.1% formic acid and acetonitrile with 0.1% formic acid, respectively. The gradient duration program was: 0 min, 5% B; 0-1 min, 5% B; 1-8 min, 5-23% B; 8-12 min, 23-98% B; wash to 1.4 min with 98% B; and a 1.6 min recycle time. The flow rate was 0.4 ml/min. The mass spectrometer was operated in positive ion mode. N2 was used as the desolvation gas. The desolvation temperature was 350°C, the flow rate was 500 l/h, and the source temperature was 100°C. The capillary and cone voltages were 2700V and 27V, respectively. The data were collected for each test sample from 200 to 1,500 Da with 0.25-s scan time and 0.01-s interscan delay over 25-min analysis time. Leucine-enkephalin was used as the reference compound (m/z 556.2771 in the positive mode).

![Fig. S1. UPLC-QToF-MS chromatogram of isolated compounds from *Agastache rugosa* leaves.](image-url)
**Fig. S1.** MS, MS/MS, UV and HREIMS data of tilianin.
Fig. S2. MS, MS/MS, UV and HREIMS data of acacetin.
Fig. S3. $^1$H-NMR spectrum of tilianin (400 MHz, DMSO-$d_6$).

Fig. S4. $^{13}$C-NMR spectrum of tilianin (100 MHz, DMSO-$d_6$).
Fig. S5. $^1$H-NMR spectrum of acacetin (400 MHz, CD$_3$OD).

Fig. S6. $^{13}$C-NMR spectrum of acacetin (100 MHz, CD$_3$OD).