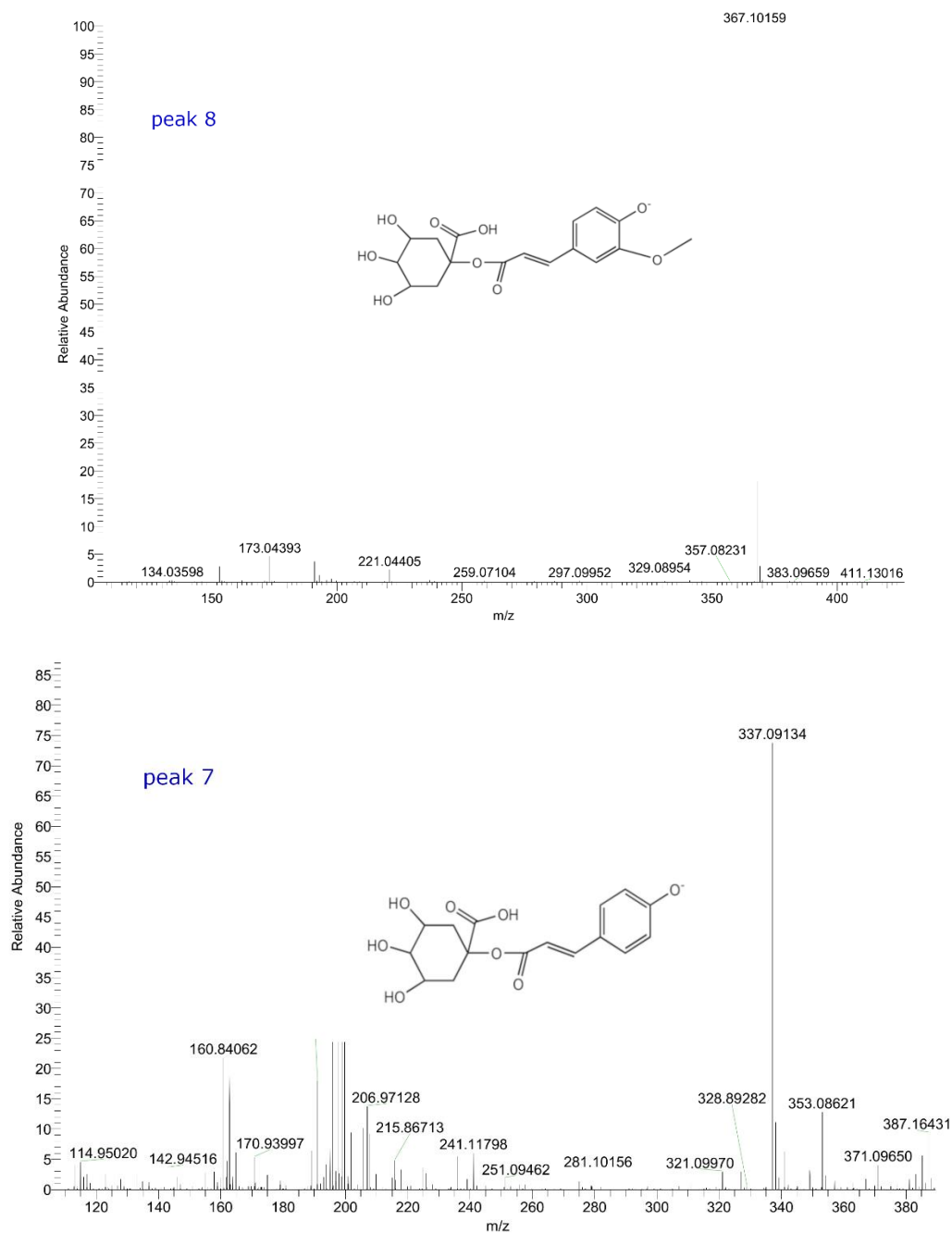
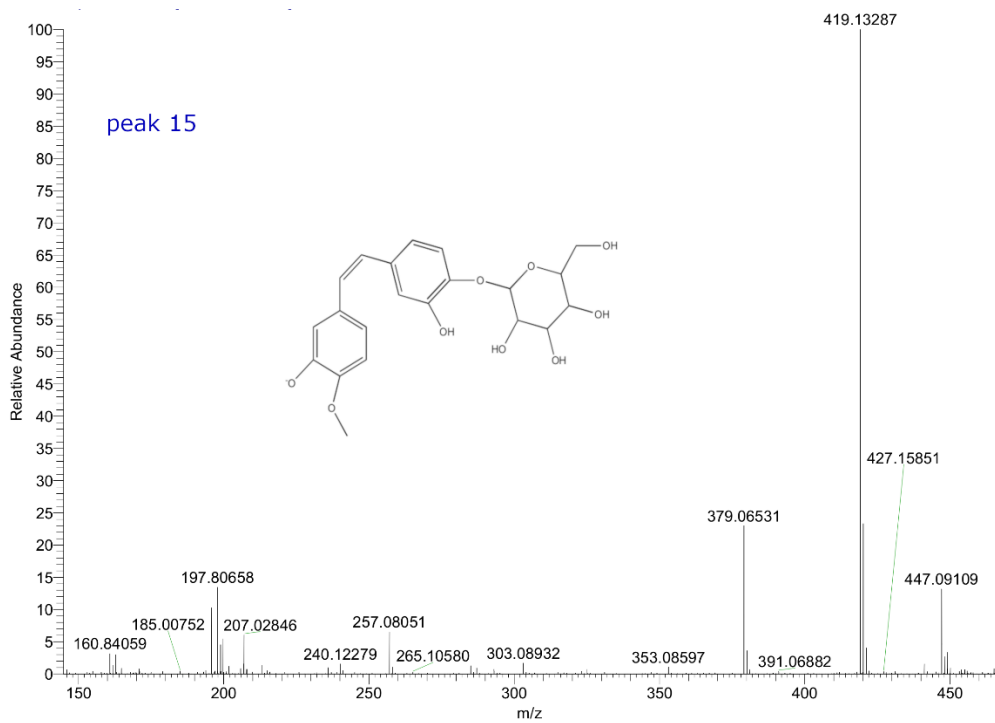
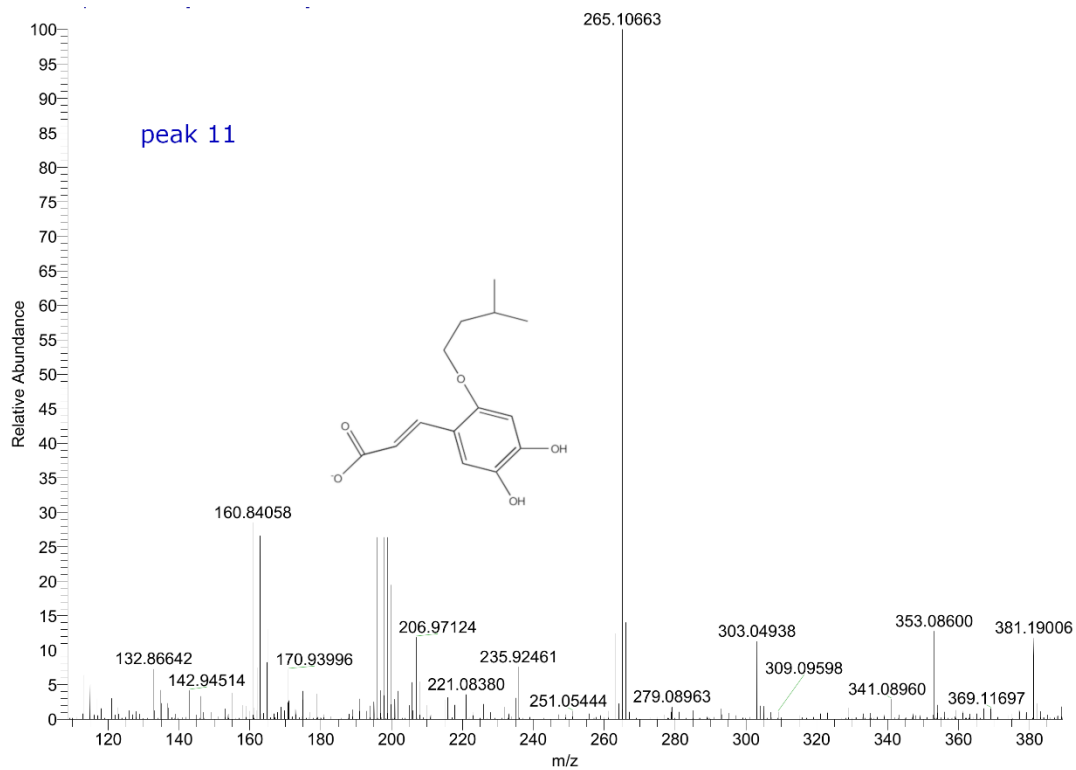
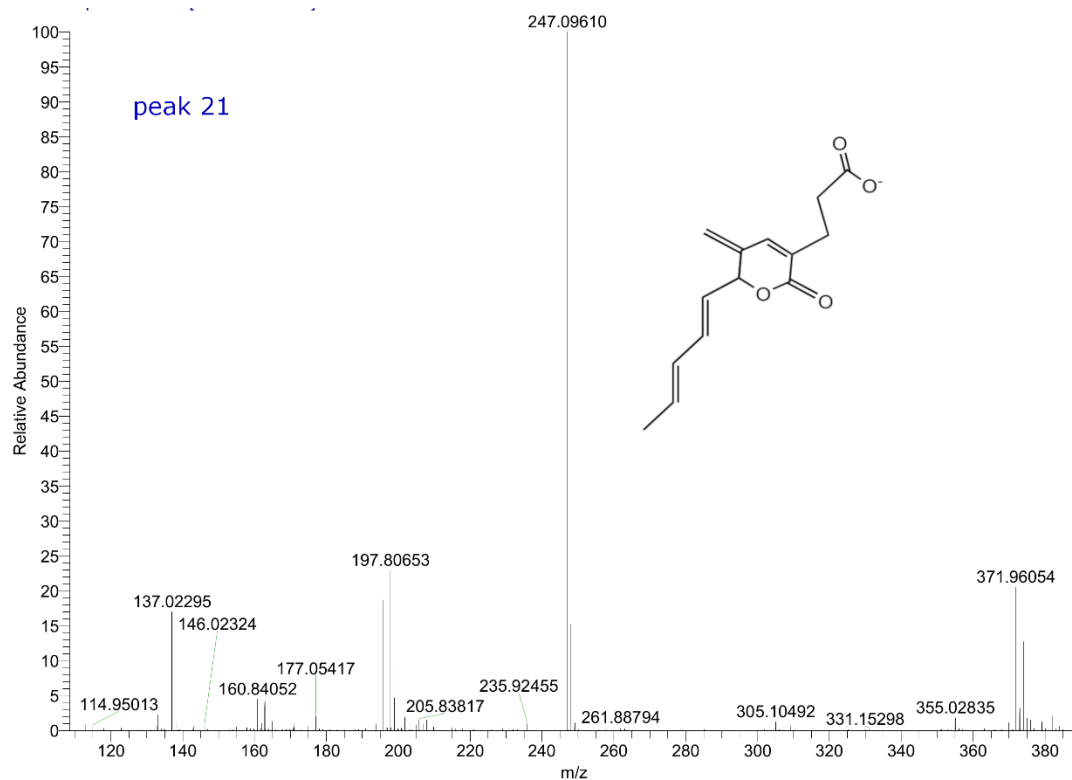
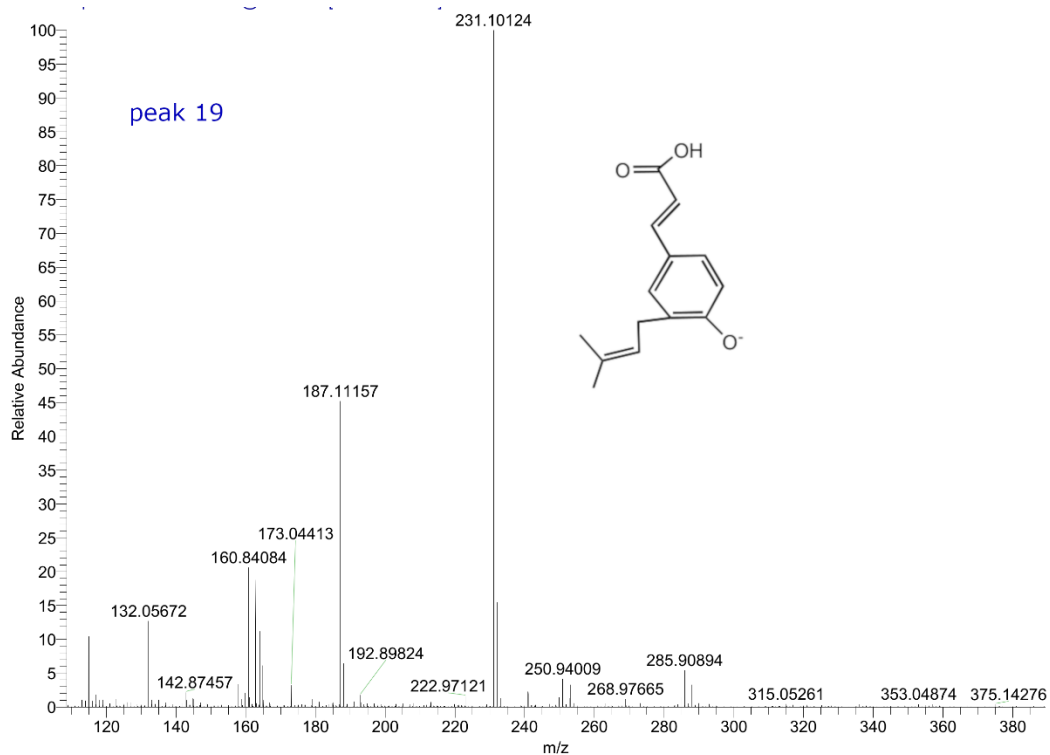


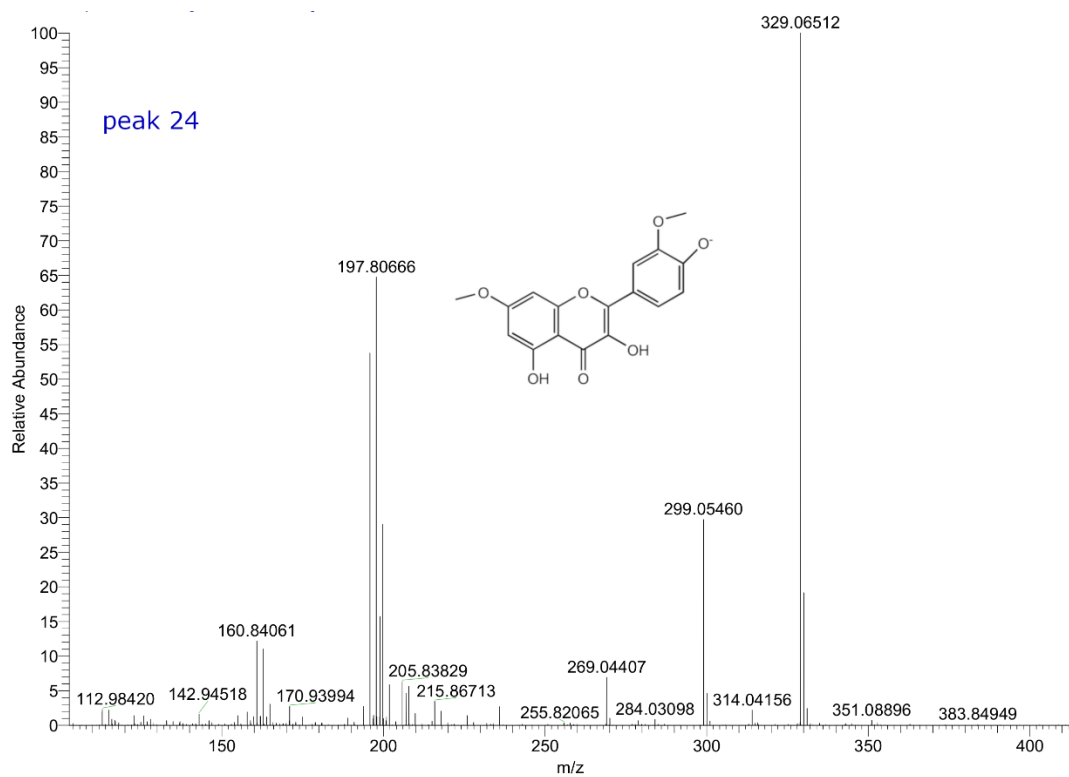
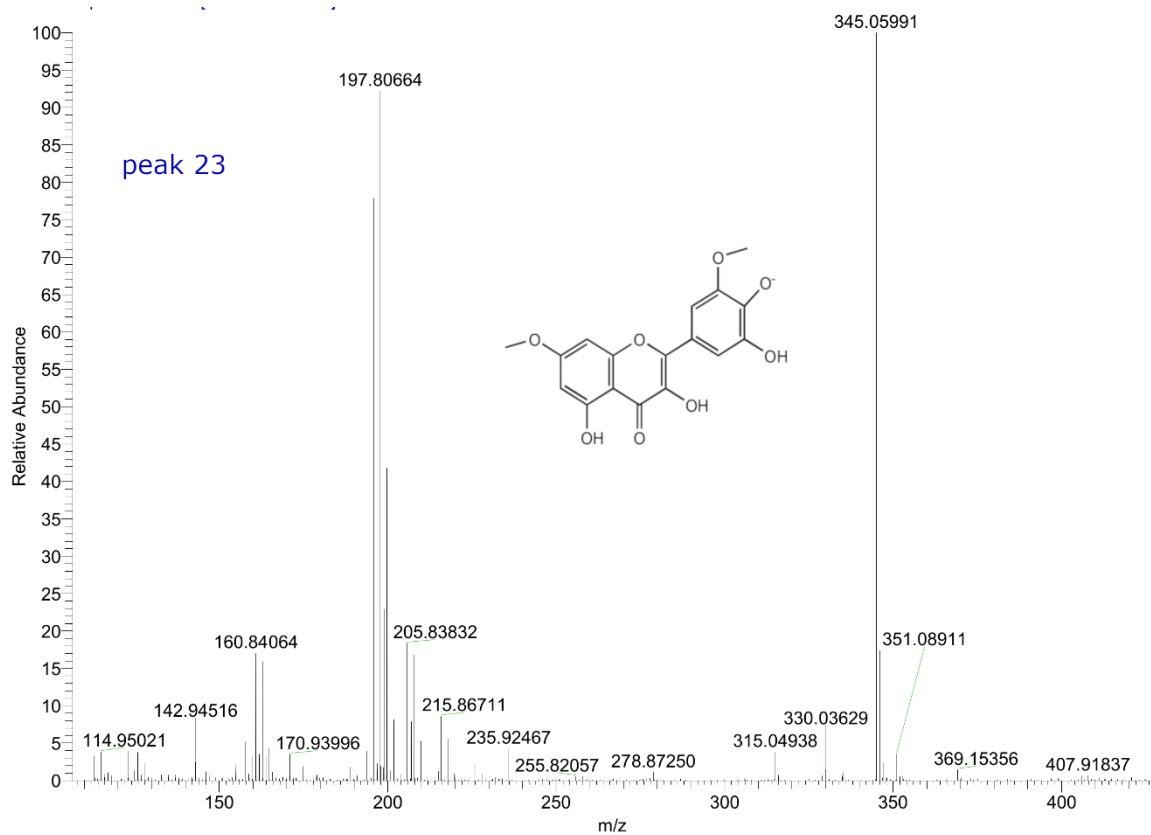
Supplementary material for the article: UHPLC-MS metabolome fingerprinting, anti-ulcer,
antioxidant and cytotoxicity activities of *Baccharis grisebachii* lyophilized decoction.

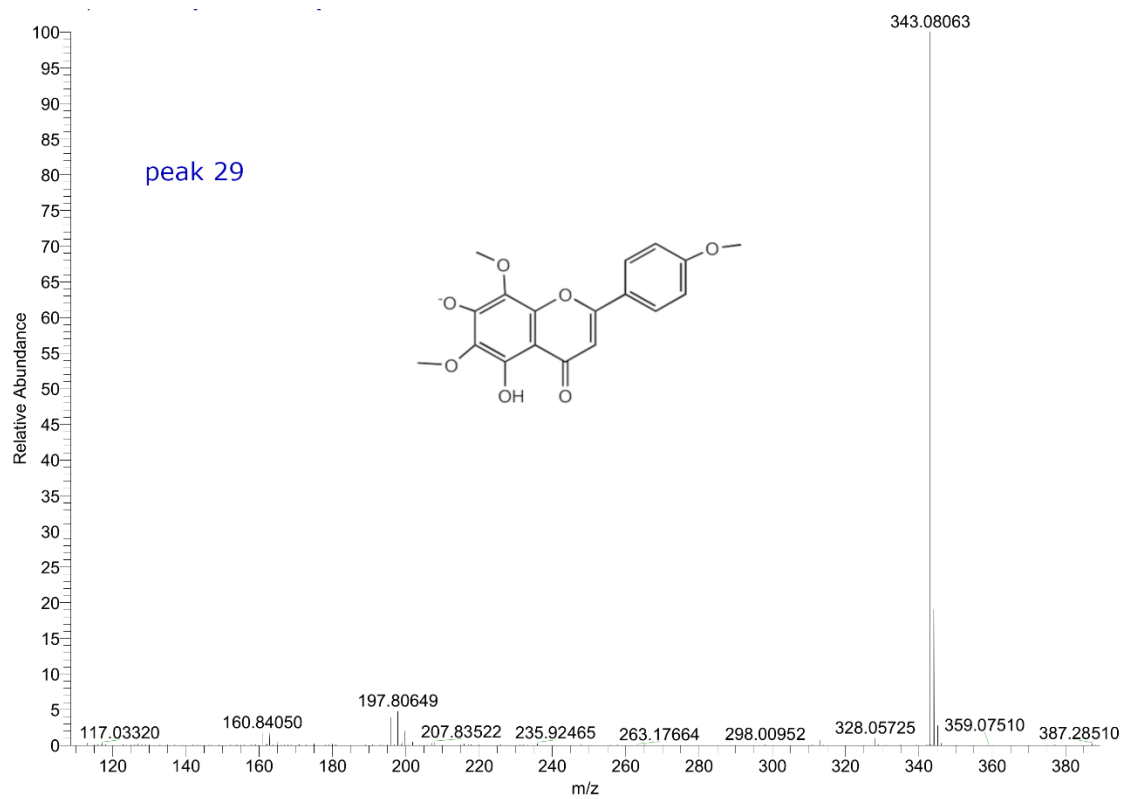
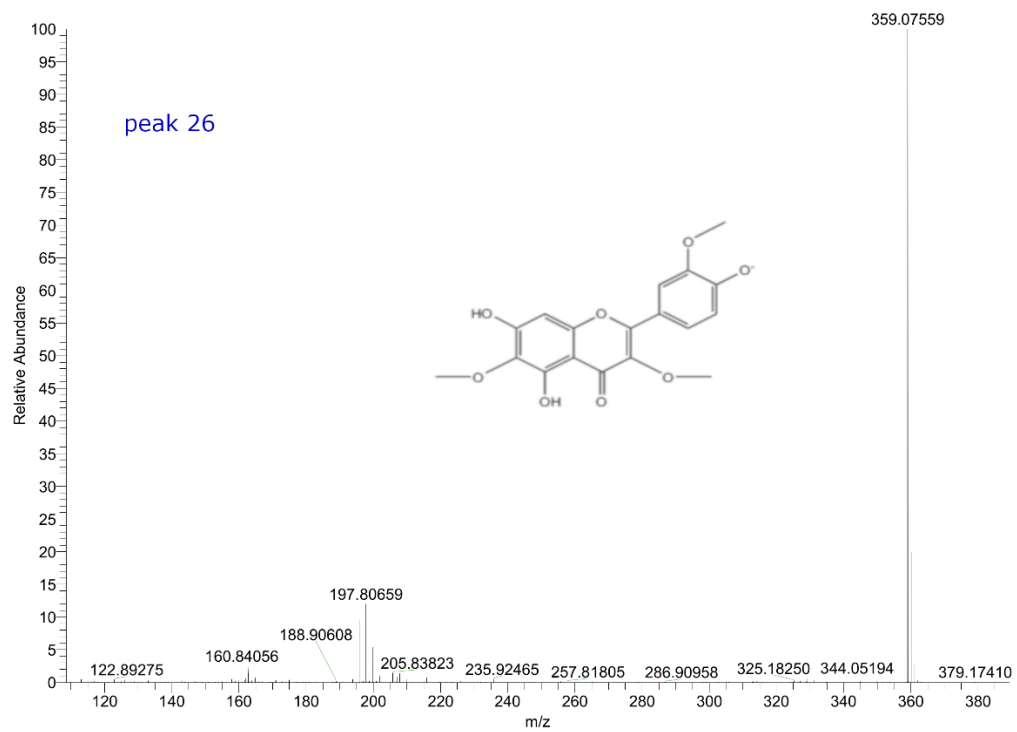
Fig. S1. Full HR orbitrap MS spectra and tentative structures of some detected peaks (peaks 7, 8, 11, 15, 19, 21, 23, 24, 26, 29, and 30), signal at 197 is an artifact of the solvent system).

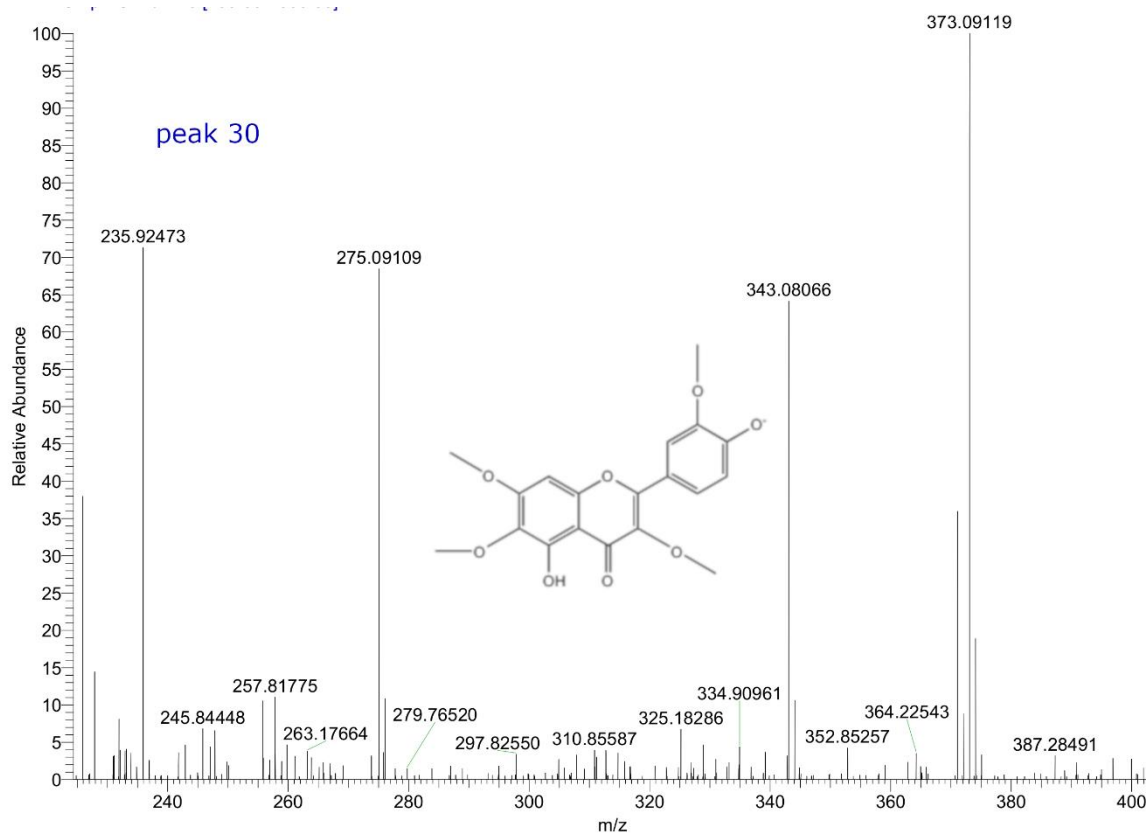












Mass spectrometry conditions: The HESI parameters were as follows: sheath gas flow rate, 75 units; auxiliary gas unit flow rate, 20; capillary temperature, 400 °C; auxiliary gas heater temperature, 500 °C; spray voltage, 2500 V (for ESI-); and S lens, RF level 30. Full scan data in positive and negative (it was chosen the negative for phenolic compounds) were acquired at a resolving power of 70,000 FWHM (full width half maximum) at m/z 200. For the compounds of interest, a scan range of m/z 100-1000 was chosen; the automatic gain control (AGC) was set at 3×10^6 and the injection time was set to 200 ms. The scan-rate was set at 2 scans s^{-1} . External calibration was performed using a calibration solution in positive and negative modes. For confirmation purposes, a targeted MS-MS analysis was performed using the mass inclusion list, with a 30 s time window, with the Orbitrap spectrometer operating both in positive and negative modes at 17,500 FWHM (m/z 200). The AGC target was set to 2×10^5 , with the maximum injection time of 20 ms. The precursor ions were filtered by the quadrupole, which operated at an isolation window of m/z 2. The fore vacuum, high vacuum and ultrahigh vacuum were maintained at approximately 2 mbar, from 105 and below 1010 mbar, respectively. Collision energy (HCD cell) was operated at 5 ev while full MS detections at energy: 0 ev for phenolic compound. Detection was based on calculated exact mass and on retention time of all compounds. The mass tolerance window was set to 5 ppm for the two modes.

