

**Supplementary Figure S2.** Full MS scan and MS/MS fragmentation spectra of ion with  $m/z$  515.1444. This figure reports a full scan spectrum (A) acquired by analysing a representative extract of a syrup sample in positive ionization mode using HILIC separation, and the corresponding HCD fragmentation spectra (B and C) obtained by applying a normalized collision energy of 23%. The isotopic distribution of the precursor ion suggested the presence of two charges (A). We observed the presence of nine precursor-to-product ion transitions deriving from this doubly charged ion (B). The absence of relevant product ions above  $m/z$  515 indicated that such doubly charged ion was probably deriving from a  $2M^{++}$  instead of an  $M^{++}$  adduct (C).

