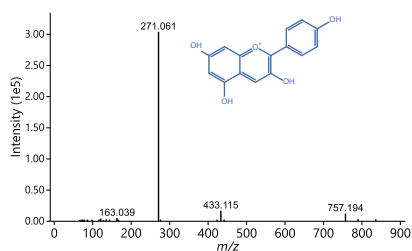
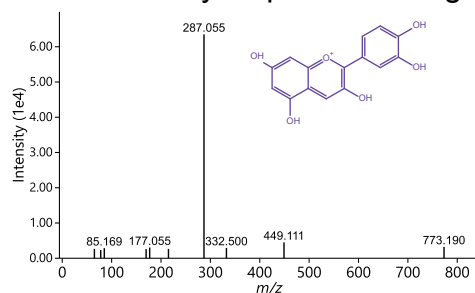


Supplementary Fig. 2

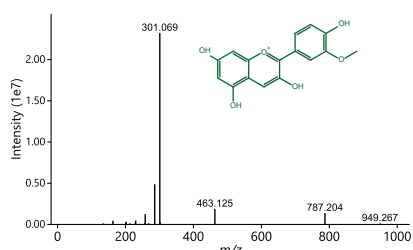
A.



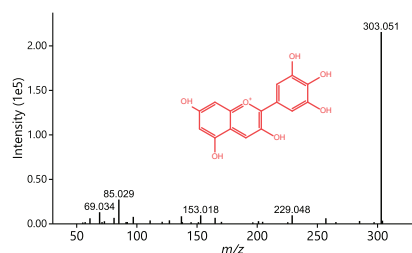
Pelargonidin 3-caffeoyl sophoroside 5-glucoside



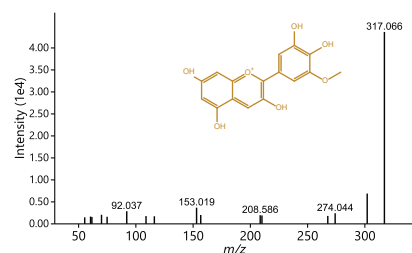
Cyanidin 3-caffeoyl sophoroside 5-glucoside



Peonidin 3-caffeoyl sophoroside 5-glucoside

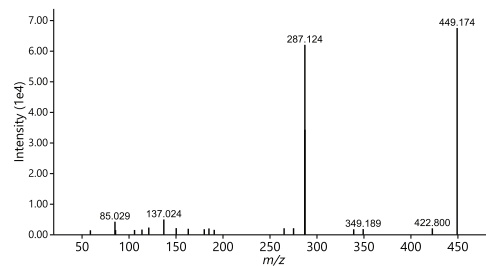


Delphinidin glucoside

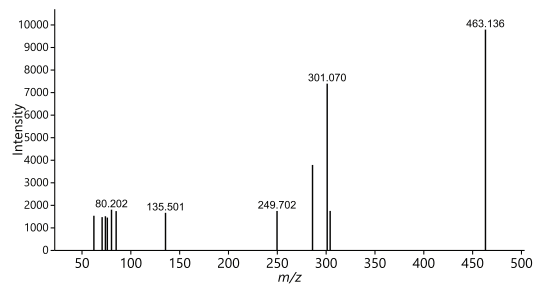


Petunidin glucoside

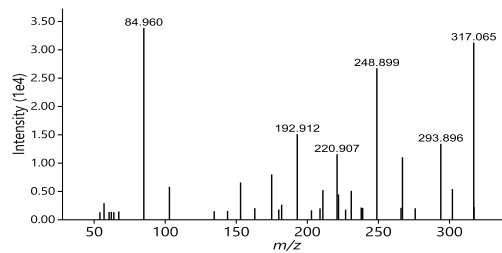
B.



Kaempferol hexoside



Chrysoeriol hexoside



Isorhamnetin

Supplementary Figure 2: Example MS/MS spectra of (A) anthocyanins and (B) flavonoids of the same parent ion mass detected in our LC-MS datasets and present in the MS/MS molecular network. (A) Spectra of 3-caffeoyl sophoroside 5-glucoside of cyanidin, peonidin, pelargonidin, petunidin, delphinidin. The aglycone originating from the flavylum core is the most intense fragment. (B) For the tentatively identified flavonoids, there are typically two intense fragments, one with the glucoside.