

Identification of Non-Volatile Compounds Generated during Storage That Impact Flavor Stability of Ready-to-Drink Coffee

Supplemental Material

Hao Lin, Edison Tello, Christopher T. Simons and Devin G. Peterson

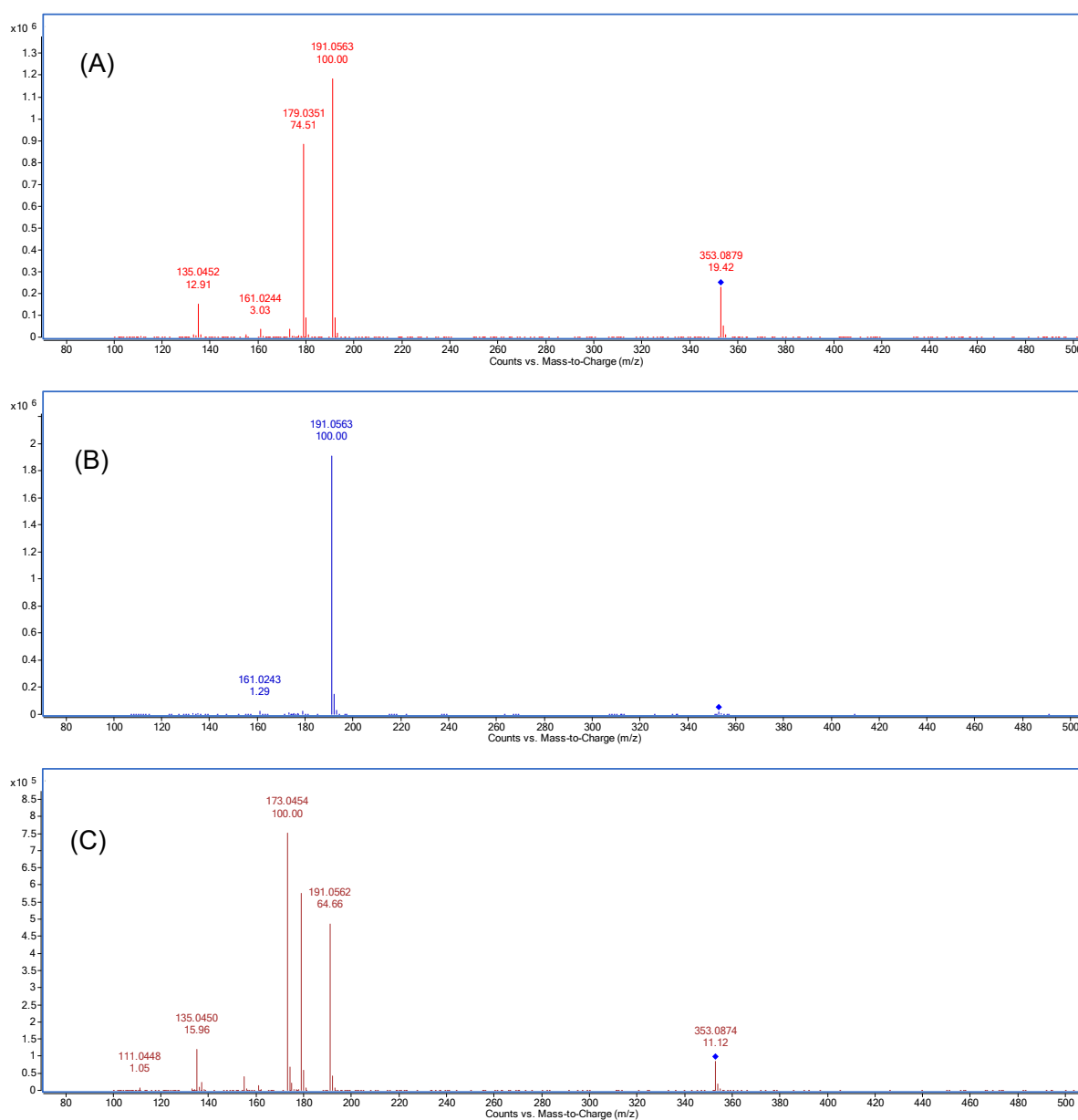


Figure S1. MS/MS fragmentation of (A) feature 2.68_353.1, 3-caffeoylquinic acid, (B) feature 3.22_353.1, 5-caffeoylquinic acid, (C) feature 3.36_353.1, 4-caffeoylquinic acid

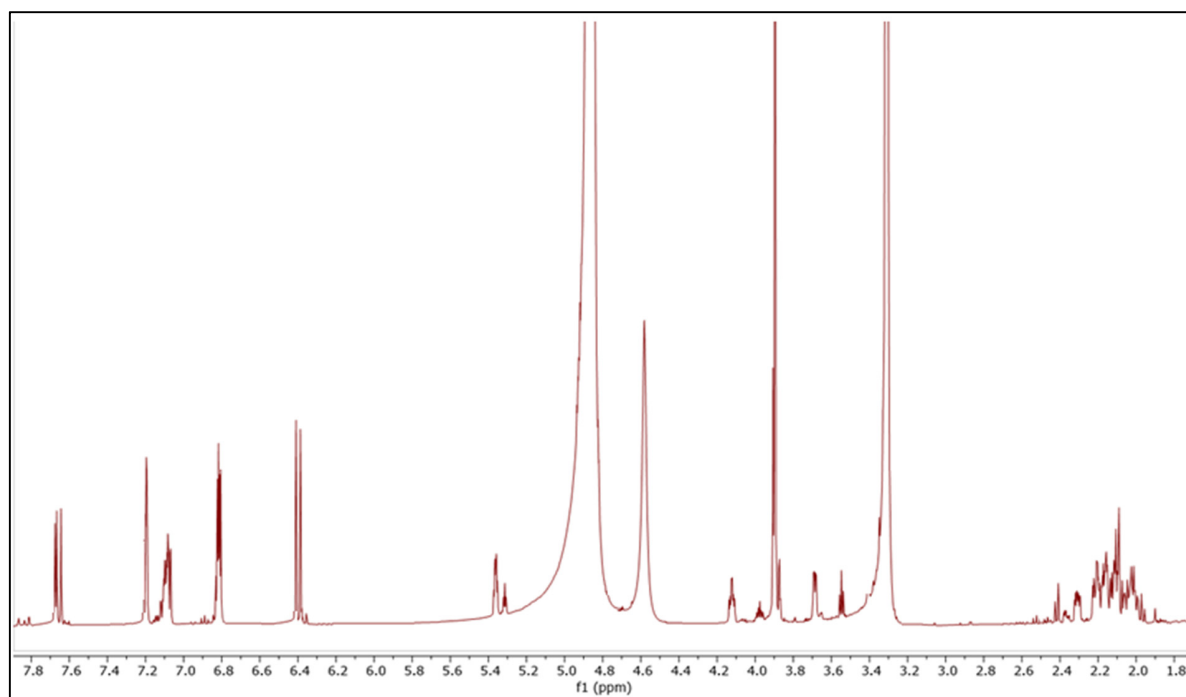


Figure S2. ^1H NMR experiments of 3-O-feruloylquinic acid.

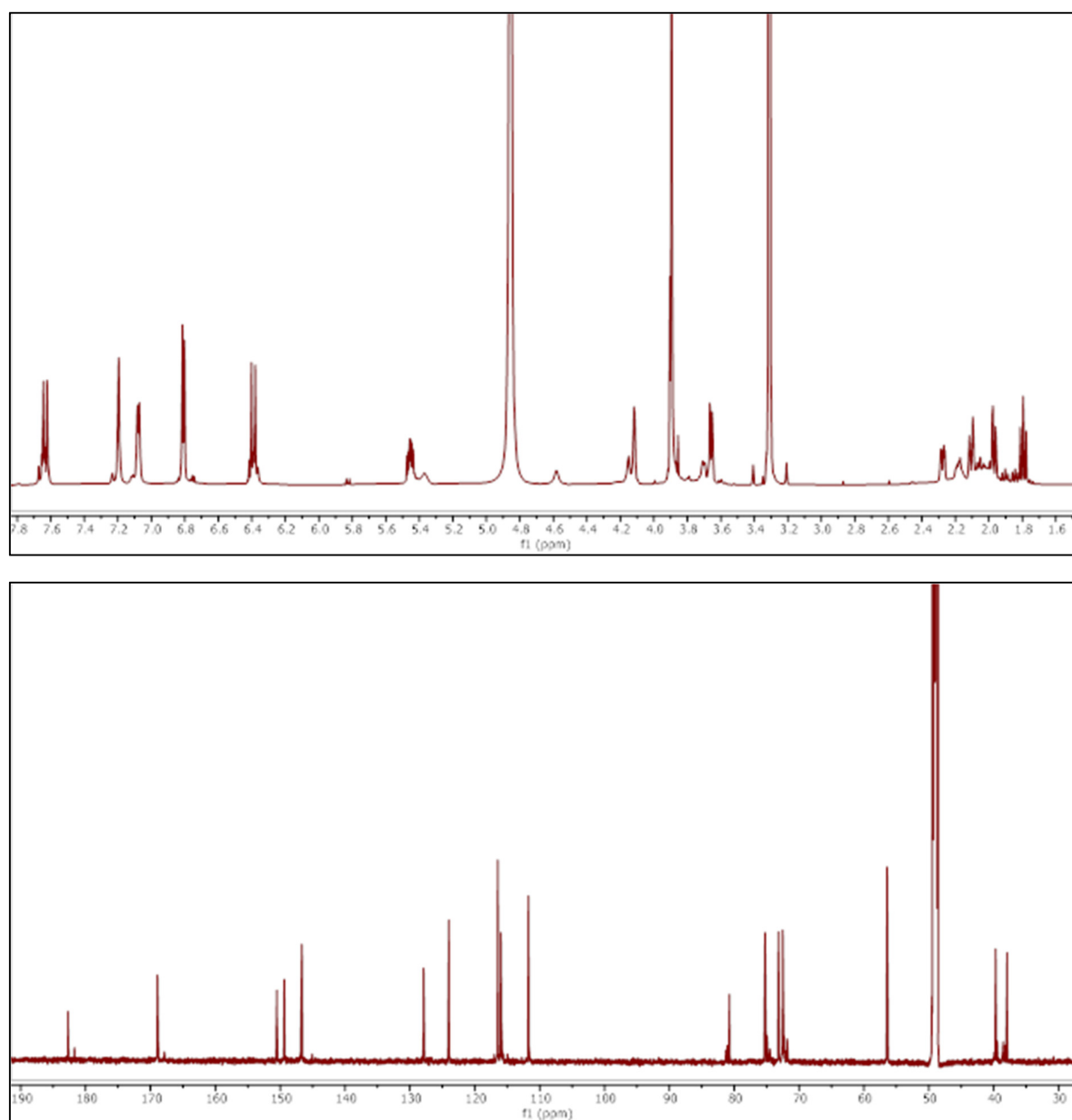


Figure S3. ^1H and ^{13}C NMR experiments of 5-O-feruloylquinic acid.

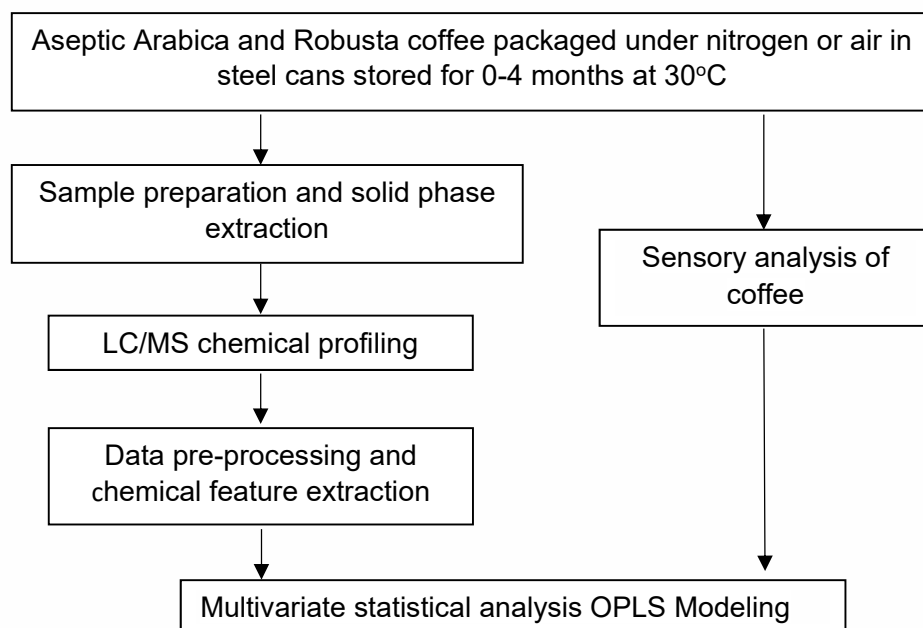


Figure S4. Scheme of chemical profiling and data analysis

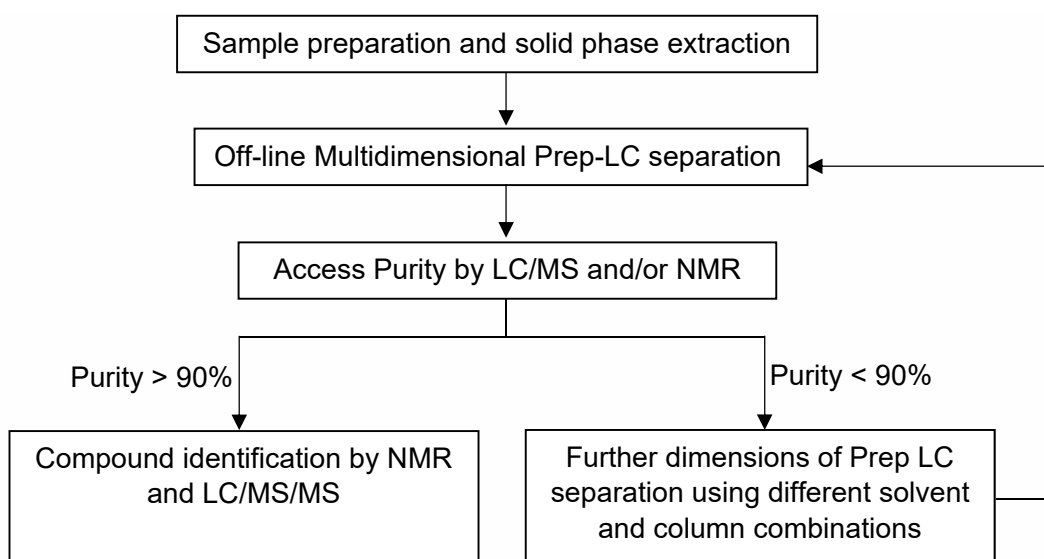


Figure S5. Scheme of fractionation of highly predictive features