GC×GC-TOF-MS with Tandem Ionization: advantages of adding an extra-dimensions to hazelnuts (*Corylus avellana* L.) primary metabolome profiling

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Abstract

This study focuses on hazelnuts (*Corylus avellana* L.) primary metabolome (i.e., amino acids, mono and disaccharides, low molecular weight acids and amines) and its characteristic fingerprint as a function of geographical origin, harvest year, post-harvest drying and storage time. Its information potential is of great interest to predict hazelnuts sensory quality after industrial roasting. Most of the (key)-aroma compounds and potent odorants [1] derive from non-volatile precursors that, once mapped, may objectively represent nuts potential quality.

GC×GC-TOF MS patterns of derivatized primary metabolites (oximation-sylilation) account of about 500 peak-regions, most of them identified by matching linear retention indices and MS spectra at 70 eV. Characteristic fingerprints at 70 and 12 eV ionization energy enable both sample clustering on the basis of key-variables and results cross-validation. In addition, soft ionization energy at 12 eV produces spectra with a complementary information power and higher specificity for most of the informative analytes. Spectra at 12 eV have higher relative ratio for heavier fragments and lower intensity for derivatization agents.

By combining data from primary metabolite distribution and volatiles, produced after lab-scale model roasting, several positive correlations (statistically relevant) between precursors and Maillard reaction products confirm the consistency of the proposed approach and the high flexibility of the analytical platform.

References

[1] J. Kiefl et al. J. Agric. Food Chem. 61 (2013) 5226–5235.