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Direct analysis of volatile compounds during coffee and tea brewing with Proton Transfer Reaction Time of Flight Mass Spectrometry

Coffee and tea are the two most consumed beverages in the world. Reasons for consuming them are varied and include the energy boost from their caffeine content, multiple health benefits and, above all, a pleasant sensory experience while drinking a cup of tea or coffee. Aroma is one of the main contributors to the sensory perception, and therefore of utmost importance for both coffee and tea. This thesis work focuses on the development of simple, fast, sensitive and reliable methods based on PTR-TOF-MS for the analysis of volatile organic compounds and how they are extracted into the liquid phase during the brewing of both coffee and tea.

In a first study, an on-line method to analyze extracted volatiles directly from the coffee flow was developed and applied to the study of single dose coffee capsules. Volatile concentration could be followed at 1 Hz resolution during the 42 seconds that the coffee extraction last. Differences in extraction between compounds were revealed, implying an aroma profile that changed with extraction time. Coffee capsules could be differentiated according to their extraction profiles by unsupervised statistical methods (Principal component analysis, PCA; and Hierarchical Cluster Analysis, HCA). A follow up study was performed using a semi-automatic coffee machine and varying the brewing parameters (temperature and pressure). The different brewing conditions resulted in different time-intensity profiles that could be differentiated by PCA. Furthermore, all the compounds extracted were grouped according to their extraction profiles into 5 families by HCA and Self Organizing Three Algorithm (SOTA), with compounds in the same family sharing their physicochemical characteristics (mainly water solubility and volatility). An increase in either brewing pressure or temperature resulted in an increase in compound extraction. However, differences were only significant in the second part of the extraction (after 10-15 seconds) and more pronounced in the less polar compounds.

In the case of tea, a preliminary study was performed in order to obtain the volatile profiles of a large number of commercial teas. In that study, an automated headspace sampling method was used in combination with PTR-TOF-MS to allow the screening of a large amount of samples in a short time. The aroma profiles of 63 black teas and 38 green teas were analyzed for both full leaves and the infusion obtained after brewing the leaves. Differences between leaves and infusions were found, indicating incomplete extraction of some compounds (e.g. terpenes) and formation of others (e.g. alcohols) during hot water extraction. Using multivariate analysis, black and green teas were successfully discriminated. Also the origin of the samples could be partially discriminated although with some miss-assignments, mainly between neighboring countries. The extraction of volatiles from tea leaves and how it is affected by several parameters (leaf size, temperature, brewing time and water composition) was further studied. Tea aliquots were taken every 30 seconds during five minutes and the headspace was analyzed with PTR-TOF-MS coupled to an autosampler. An increase in brewing temperature resulted in increased volatile extraction, with differences more pronounced at longer brewing times. Reduced leaf size resulted in faster extraction, a difference that was more significant during the first minute of brewing. On the other hand, water mineralization had low impact on the extraction kinetics and the volatile aroma content in the cup. Using PCA and HCA, not only the

impact of brewing parameters was assessed but also different sets of brewing conditions resulting in analogous volatile profiles (i.e. same aroma profile) were identified.

The positive outcomes of this thesis support the use of PTR-TOF-MS to follow the extraction of volatile aroma compounds during preparation of hot beverages, both on-line and off-line. The use of multivariate methods on the dynamic data increased the applicability of the methods allowing differentiation of samples according to its composition (e.g. coffee capsules), country of origin (e.g. tea origins) or parameters used for preparation (e.g. temperature-pressure combinations).