Flavor release measurement by atmospheric pressure chemical ionization ion trap mass spectrometry, construction of interface and mathematical modeling of release profiles

An instrumental on-line retronasal flavor analysis was developed to obtain information about the release of flavor compounds in expired air from humans during eating. The volatile flavor compounds were measured by ion trap mass spectrometry with an atmospheric pressure chemical ionization source (APCI). An interface was designed to sample the breath directly from the nose. The repeatability in vitro for seven different flavor compounds came out with relative standard deviation less than 10% in most cases, which is acceptable. In vitro quantification was carried out by a determination of the concentration in the gas phase over a flavor solution by GC/MS, followed by measurements of intensities by the APCI ion trap. Ion suppression by acetone in the breath was negligible at concentration levels relevant in these experiments. The instrumental limits of detection for menthone and menthol coincide with that of the flavor detection threshold. An application study on the release of menthone and menthol from chewing gum by a group of six test persons was performed. Flavored chewing gum was used as a model matrix because of the long chewing periods and the simplicity of the system. It is concluded that the interface and the method can be used to measure breath from the nose. A mathematical model of the data was developed to give a quantitative method for description and characterization of the release of flavor compounds. The release profiles consisted of two sequences, one for a chewing period, and one for a phasing out process. The proposed method for modeling provided a reasonable description of the release process. In addition to flavor compounds, this new interface and mathematical application could provide information on chemicals in the human breath which could be interesting, for example, within medical diagnosis.

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