Why does coffee smell so good?

Comprehensive gas chromatography (GC x GC) uses two serially coupled capillary columns with different separation mechanisms. After separation, the components are "frozen" temporarily by the so-called cryomodulator and the fractions are "injected" via a radiant heat pulse into the second dimension.

The cryomodulator takes over the function of a fraction collector with subsequent sample injection onto the second separation column. Signal detection enables classification of each component according to its retention time in the first and second dimension. This technique was used for the identification of coffee flavor components after extraction. A quadrupole mass spectrometer was used as detector.

Sample preparation and instrumentation

The coffee analyzed was a Colombian Roast coffee and the samples were prepared via simultaneous distillation and solvent extraction in a Likens-Nickerson apparatus using pentane : ether (1:1) as solvent. The flavor components were separated and detected using a Shimadzu GCMS-QP2010 Plus coupled with a Zoex loop modulator. A 30 m Rtx-wax column with an internal diameter of 0.25 mm and a film thickness of 0.25 µm was used for separation in the first dimension. A deactivated Press-Tight connector was used to connect a 2.6 m Rxi-5ms column (effective separation distance: 1 m) with an internal diameter of 0.15 mm and a film thickness of 0.1 µm to the first column. A sample volume of 0.2 µL was injected at a split ratio of 1:50. Data acquisition was carried out in full scan mode. The scan range was 40 to 285 m/z at an acquisition rate of 33 Hz.

Results

Approximately 1000 different coffee flavor components could be separated and identified via mass spectrometry. Many of the approximately 70 known pyrazine compounds formed during the roasting process were detected. Markers that are important for the roasting aroma such as 2-furfurylthiol, guaiacol, 3-(methylthio)-propanal, furfural and 2-ethyl-3,5-dimethylpyrazine could be detected.

Evaluation of the chromatograms was carried out in one dimension using the GCMSsolution software and in two dimensions using the GCImage software (Zoex). This software plots the retention time obtained with the first separation column on the X-axis and the retention time obtained on the second dimension on the Y-axis. The resulting image represents peaks as so-called "blobs" with their intensities symbolized in different colors (Figure 1).

The proposed technique will be used in future for the evaluation of the characteristics of different coffee roasts via suitable markers.

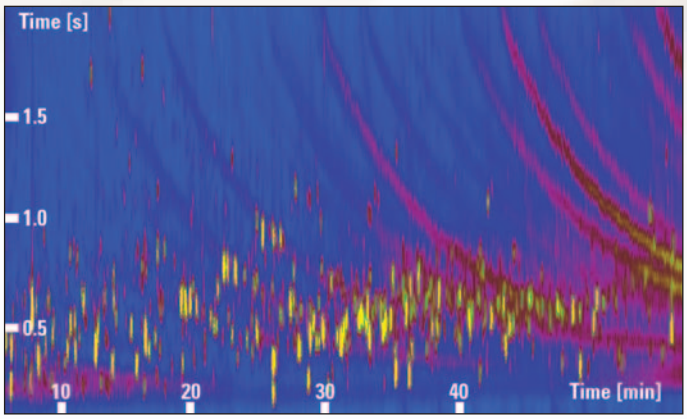

Figure 1: Colombian Roast coffee flavors analyzed using comprehensive GC-MS. The two-dimensional representation was generated using GCImage software (Zoex).

From LCGC AdS, September / October 2008