

Additional Information

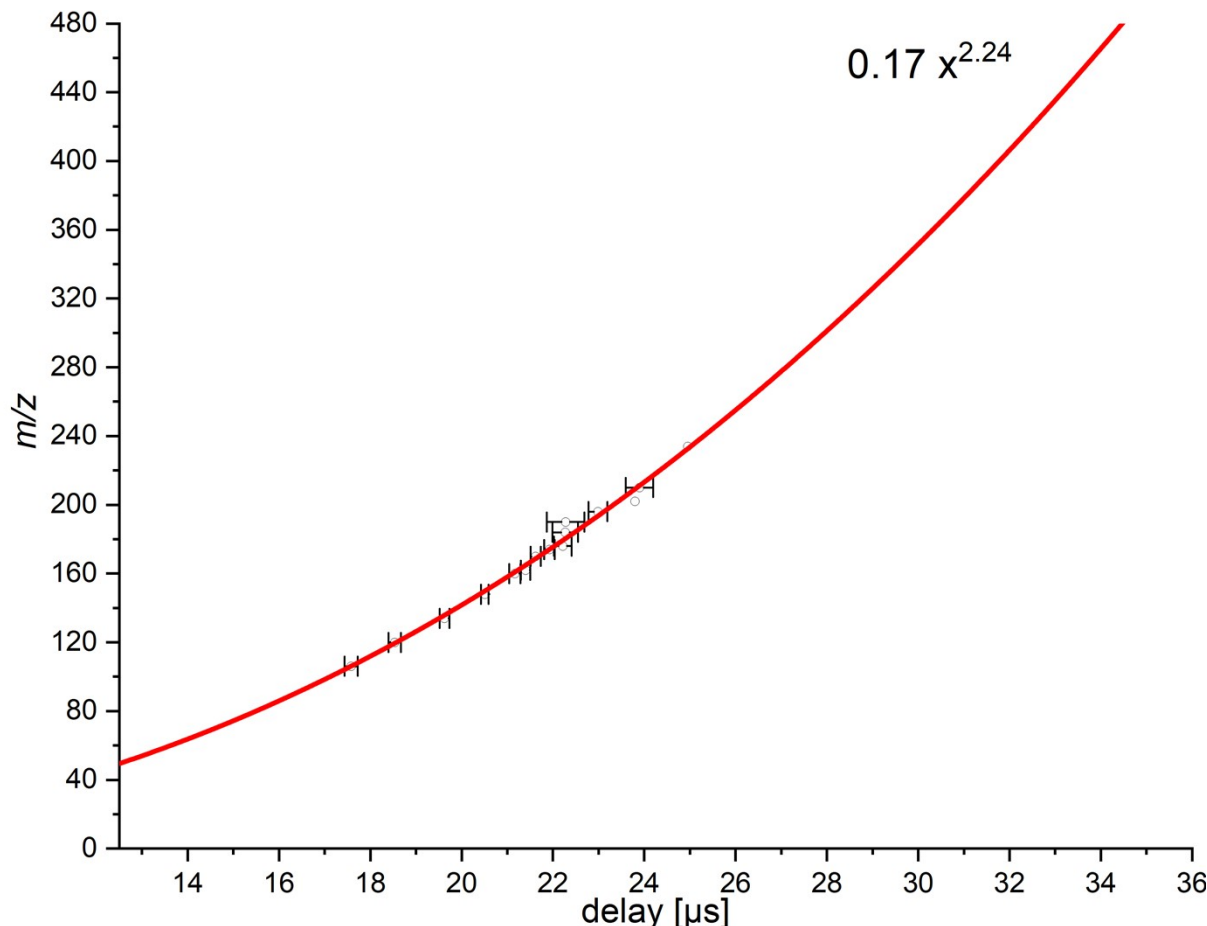


Fig. S 1 Dependency of delay time (between laser pulse and extraction into the mass separator) and corresponding extracted m/z -ratio at highest intensity (transmission). Diesel (DIN EN 590) was used for providing a broader higher mass range. The red curve indicates a wide extrapolation for the shown dependency.

Fig. S 1 shows the dependency of delay time and corresponding extracted mass. The data points were obtained by a slow delay scan and usage of a diesel sample for covering a broad m/z range. For each mass, the respective delay time at the highest signal intensity is given. The measurement was repeated three times. As expected, this dependency is not linear. The first drift stage separates ions according to their mass-to-charge ratio. This separation is, of course, less efficient than in the second drift path since both the transfer potential as well as the drift path are not designed for complete, temporal mass separation. The equation in Fig. S 1 is not based on any calculations but represents the best fit function to the available data. This curve has been extrapolated for the working range relevant to this publication. The dependency in Fig. S 1 is only suitable for the given set of applied voltages to the electronic parts of the mass spectrometer and has to be remeasured by supply voltage changes of the parts in the first drift stage. These changes alter the slope of the curve and can thus change the sensitivity of the system towards higher or lower masses.

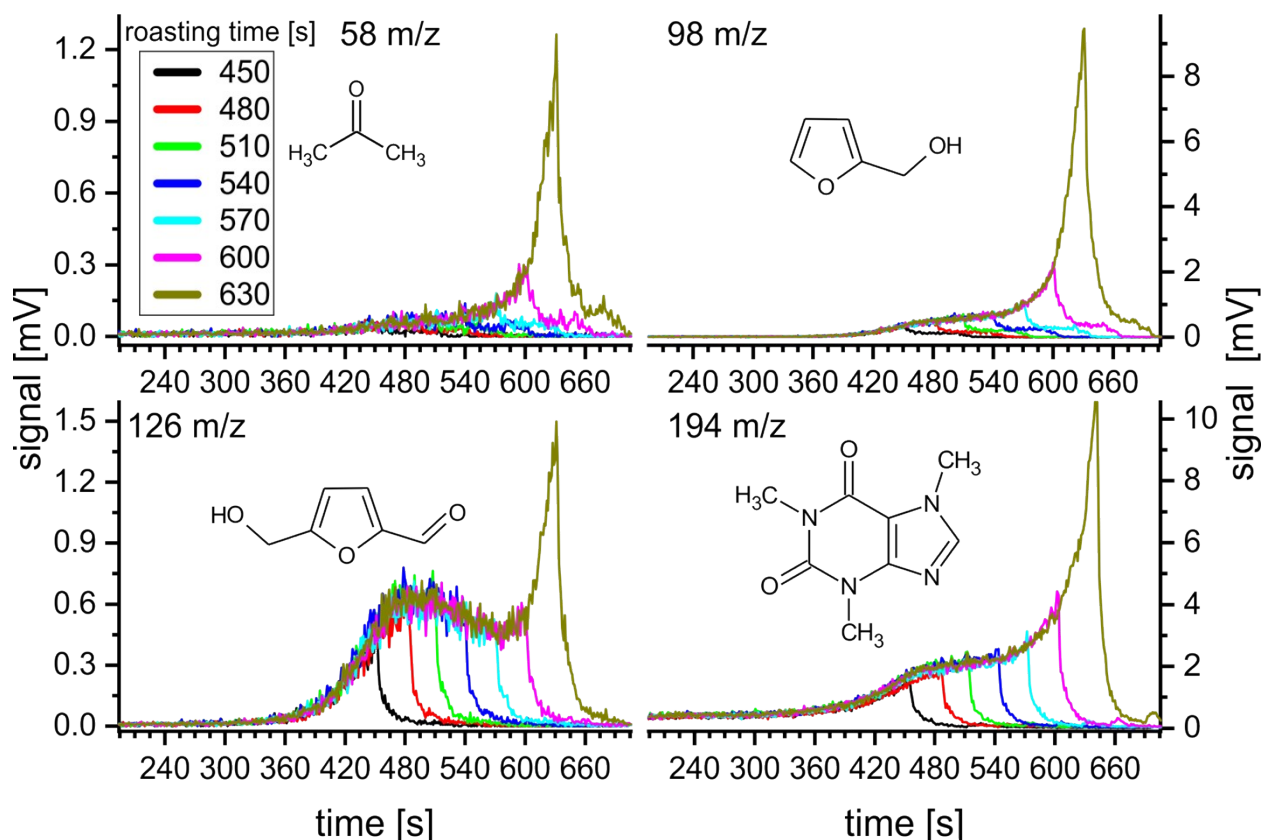


Fig. S 2 Time profiles for four different m/z -ratios and roasting times assigned to the most properly substances (58 m/z acetone, 98 m/z furfuryl alcohol, 126 m/z hydroxymethylfurfural, and 194 m/z caffeine). At each roasting time ending, the coffee in the roaster was emptied. The data shows the reproducibility of the system as each time profile shows an elongation of the previous. The data was collected with 2 Hz and is not additionally smoothed or normalized, only time-shifted for matching the same starting point. The corresponding roasting degrees (Colorette 4) for the depicted roasting times at 58 m/z are 167, 141, 124, 105, 92, 77, and 63, respectively (measured with Colorette 3b).

Fig. S 2 shows data from the monitoring of coffee roasting in an industrial coffee roaster (Jupiter 500, Probat). The coffee was roasted with the same profile and roasting time (emptying of the roaster) was varied. Four different mass traces are shown, which are tentatively assigned to acetone (58 m/z), furfuryl alcohol (98 m/z), hydroxymethylfurfural (126 m/z), and caffeine (194 m/z). Each subplot shows the mass traces for different roasting times, which are indicated in the legend of the acetone mass traces in Fig. S 2. All data are only time-shifted and are apart from this raw data. The figure shows the high reproducibility of the utilized tof-MS system. Besides, the variability of the roast gas phase is perceptible. Especially, the last part of the roast between 600 and 630 seconds shows an exponential rise in released compounds. This high dynamic behavior occurs after the second crack at elevated temperatures and marks the beginning of dark and very dark roasts. High variability of signals as indicated for the mass traces of hydroxymethylfurfural in Fig. S 2 can be exploited (among others) for gaining information on the roast process. By correlation with off-line data, real-time prediction models can be built. Low variations of the measurement results are of extraordinary importance in this regard. Furthermore, using the technique presented in this work, the robustness of the system is another highly important characteristic. If the system would only work reliable in a short period of time, e.g., for several dozen roasts in a lab, use in the industry would become impractical. In this regard, the system was tested in a real industry environment at a production site at Azul Café in Bremen, Germany.

The System was coupled to a Neptune 3000 (Probat, Germany) industrial rotating drum roaster. Over the course of three days, over 130 roasts were monitored.

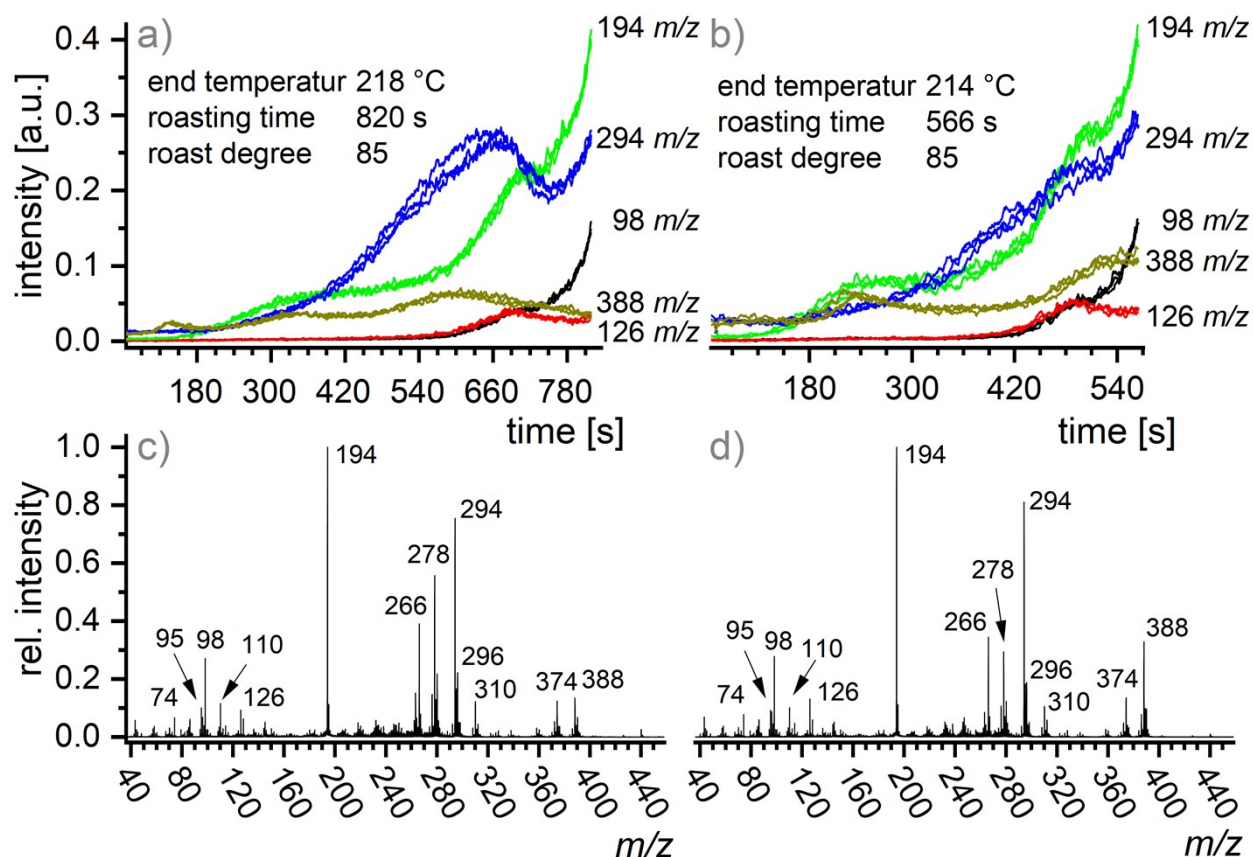


Fig. S 3: Monitoring of coffee roast gas in an industrial plant. The SPI/REMPI-tof-MS system was coupled to a rotating drum roaster with a batch capacity of roughly 500 to 600 kg of coffee. The subplots a)- c) and b)- d) are related to each other. The subplots a) and b) show the mass traces for some major signals, whereas each line is the representation of three consecutive roasts. The measurements in a) and b) differ in roast condition and coffee composition. Additionally, the roasts of b) are one hundred measurements apart from a). The subplots in c) and d) show corresponding mean mass spectra normalized to their highest signal.

The robustness of the system can be seen in Fig. S 3. The subplots a) and c) are one hundred monitored roasts apart from the ones in b) and d). Shown are some main signals for three successive roasts for each of the top plots in Fig. S 3 and their corresponding mean mass spectra in the subplot below. During the course of these one hundred roasts, one maintenance was required as the inlet of the sampling line was blocked by particles to a great extent. Air back flushing with short high-pressure pulses will solve this problem in the future. The rest of the sampling and the MS system worked reliably. The main bottleneck was the sampling setup before the MS capillary than the MS system itself. In all plots it can be seen that only very small differences occur between different roast conditions. Therefore, expanding the measuring range by exploding a second ionization method leads to advantages in finding these small differences. The REMPI-signals of 294 m/z (from Kahweol) and 388 m/z (unknown compound) show very distinct variations in their time profiles in Fig. S 3. This variation will be further exploited in future works for real-time predictions of the coffee status.