

Electronic Supplementary Information of

Hyper-fast gas chromatography and single-photon ionisation time-of-flight mass spectrometry with integrated electric modulator-based sampling for headspace and on-line VOC analysis

Christian Gehm,^a Kevin Schnepel,^a Hendryk Czech,^{*a,b} Toni Miersch,^a Sven Ehlert^c and Ralf Zimmermann^{a,b}

^a Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, 18059 Rostock, Germany
email: hendryk.czech@uni-rostock.de

^b Joint Mass Spectrometry Centre, Cooperation Group "Comprehensive Molecular Analytics" (CMA), Helmholtz Zentrum München, 81379 München, Germany

^c Photonion GmbH, 19061 Schwerin, Germany

Table of Contents

Figure S1...	Carbon number vs. retention time for n-alkanes
Figure S2	Headspace analysis of needles with focus on m/z 204 and m/z 196
Figure S3...	Roast profile
Figure S4...	Individual contribution to the modified Flavour Quality Index (FQI _{mod})
Figure S5	Comparison of mass spectra from direct SPI-TOFMS and fastGC-SPI-TOFMS

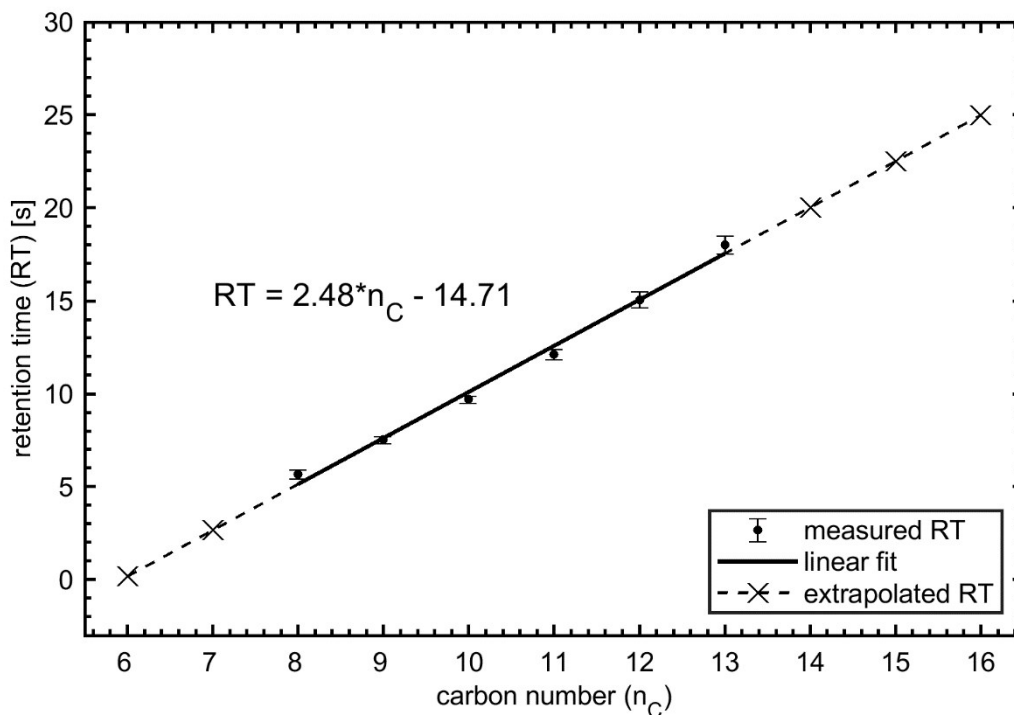


Fig. S1 Retention times for *n*-alkanes from *n*-octane (C8) to *n*-tridecane (C13) with linear fit (solid line) and one standard deviation (1σ) of 7 repeated analyses. The dashed line indicate extrapolation of the fitted retention times to shorter and longer *n*-alkanes for calculating linear retention indices (LRI).

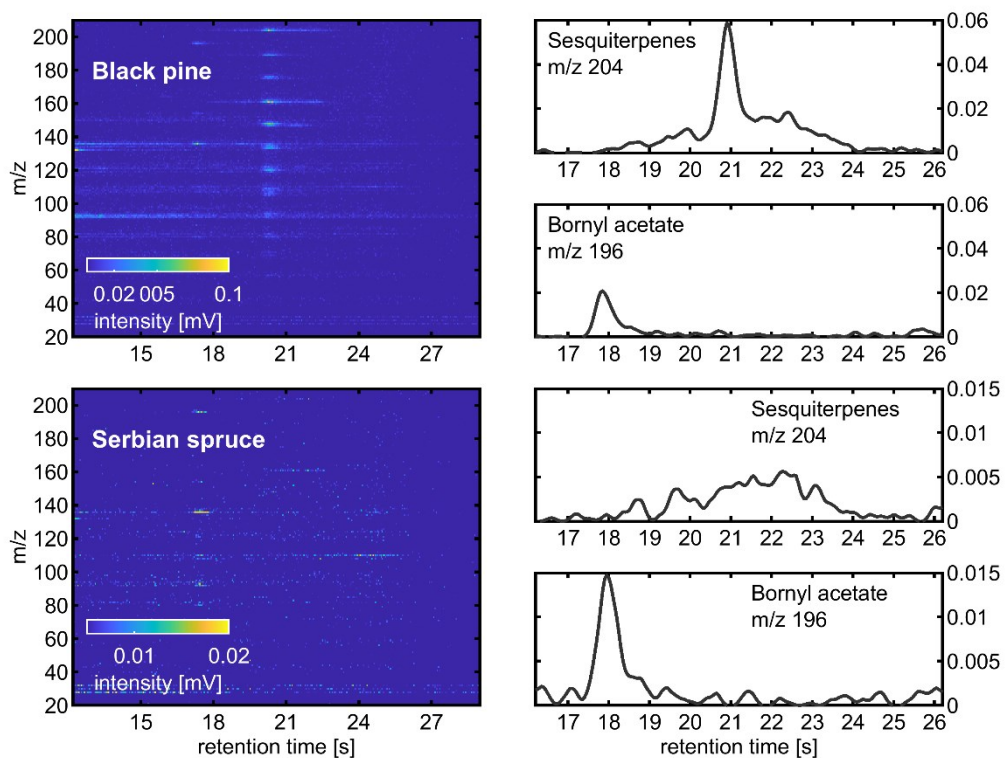


Fig. S2 Imageplots of chromatogram from headspace analysis of Black pine and Serbian spruce needles with ion traces of m/z 204 and m/z 196 belonging to sesquiterpenes and bornyl acetate.

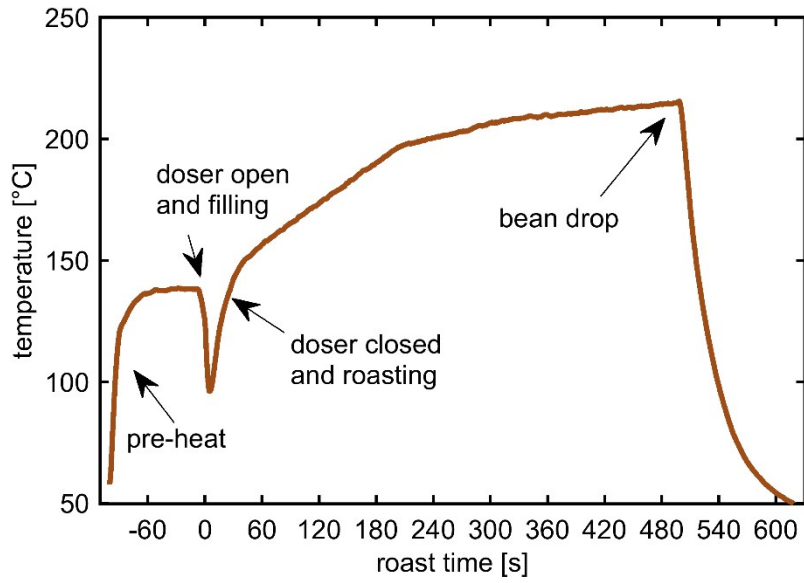


Fig. S3 Roast profile applied on drum roaster (Probatino, batch size of 1.5 kg) on Arabica beans from Brazil and Colombia as well as Robusta from Vietnam. At 0 s the roasting starts with slightly decreasing temperature over progressing roast time. The time of bean drop (approximately 500 s is equivalent with the bean drop at 615 s in Fig. 7 depicting the measurement time).

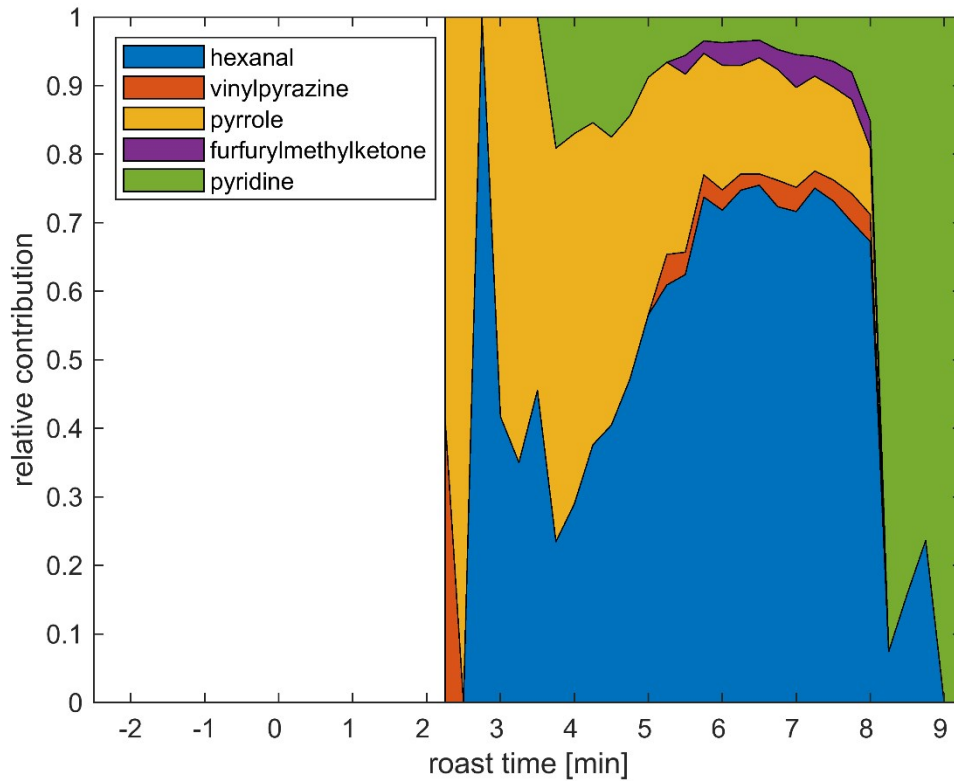


Fig. S4 Relative contribution of individual VOCs in the roast gas during the coffee roast. The drop of the coffee beans happened at approximately 10min.

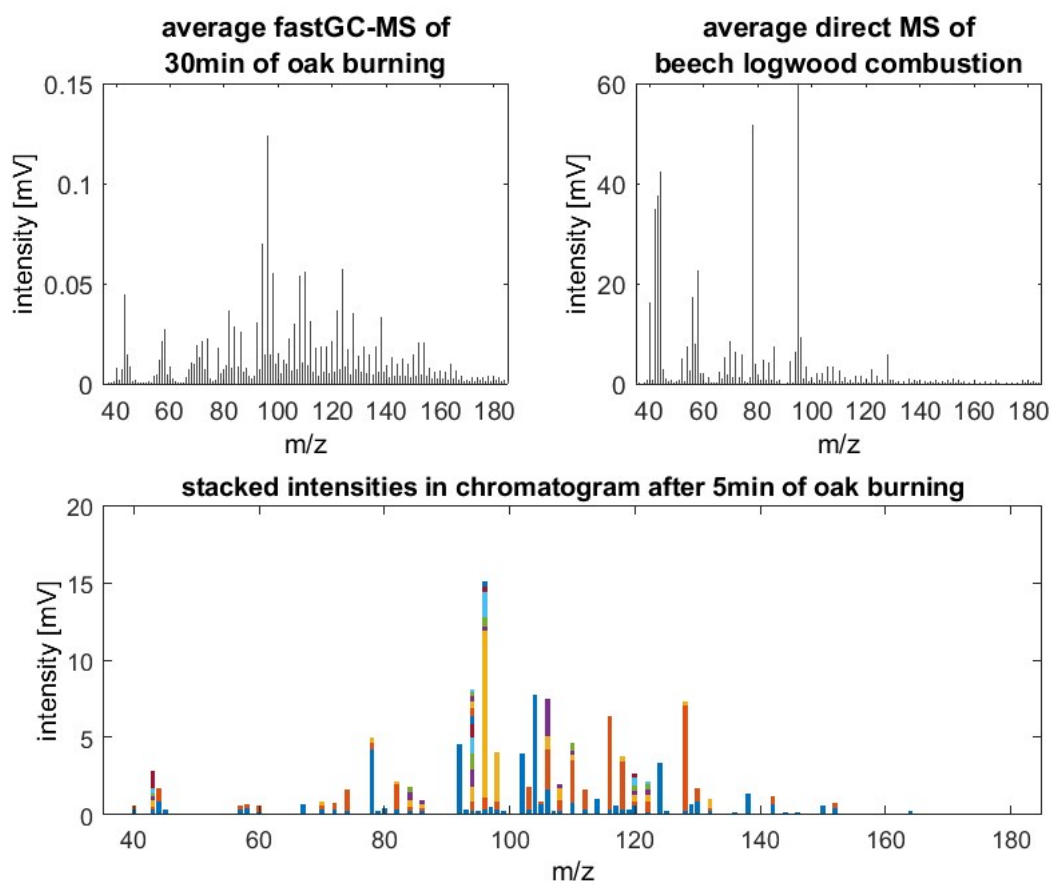


Fig. S5 Top: Comparison of SPI mass spectra obtained from averaged chromatograms of open oak burning emissions using photons from a D_2 -lamp with peak emission at 122 nm and 126 nm (left) and beech logwood burning in a stove using photons from a laser providing 118 nm radiation (Czech 2016 Fuel); peak at m/z 95 results from D_3 -toluene used as internal standard (right). Bottom: Stacked intensities of chromatographic peaks occurring at the same nominal m/z for open oak burning emissions approximately 5 min after ignition. At each nominal m/z , a different colour represent another chromatographic peak.