

Supplementary Materials

Chiral Trapped-Headspace GC-QMS-IMS: Boosting Untargeted Benchtop Volatilomics to the Next Level

Lukas Bodenbender ^{1,2}, Sascha Rohn ², Simeon Sauer ³, Markus Jungen ⁴ and Philipp Weller ^{1,*}

¹ Institute for Instrumental Analytics and Bioanalytics, Mannheim University of Applied Sciences, Paul-Wittsack-Str. 10, 68163 Mannheim, Germany; l.bodenbender@hs-mannheim.de

² Department of Food Chemistry and Analysis, Institute of Food Technology and Food Chemistry, Technische Universität Berlin, Gustav-Meyer-Allee 25, 13355 Berlin, Germany; rohn@tu-berlin.de

³ Faculty of Biotechnology, Mannheim University of Applied Sciences, Paul-Wittsack-Str. 10, 68163 Mannheim, Germany; s.sauer@hs-mannheim.de

⁴ SGF International e.V., Marie-Curie-Ring 10a, 55291 Saulheim, Germany; markus@sgf.org

* Correspondence: p.weller@hs-mannheim.de; Tel.: +49-(0)621-292-6484

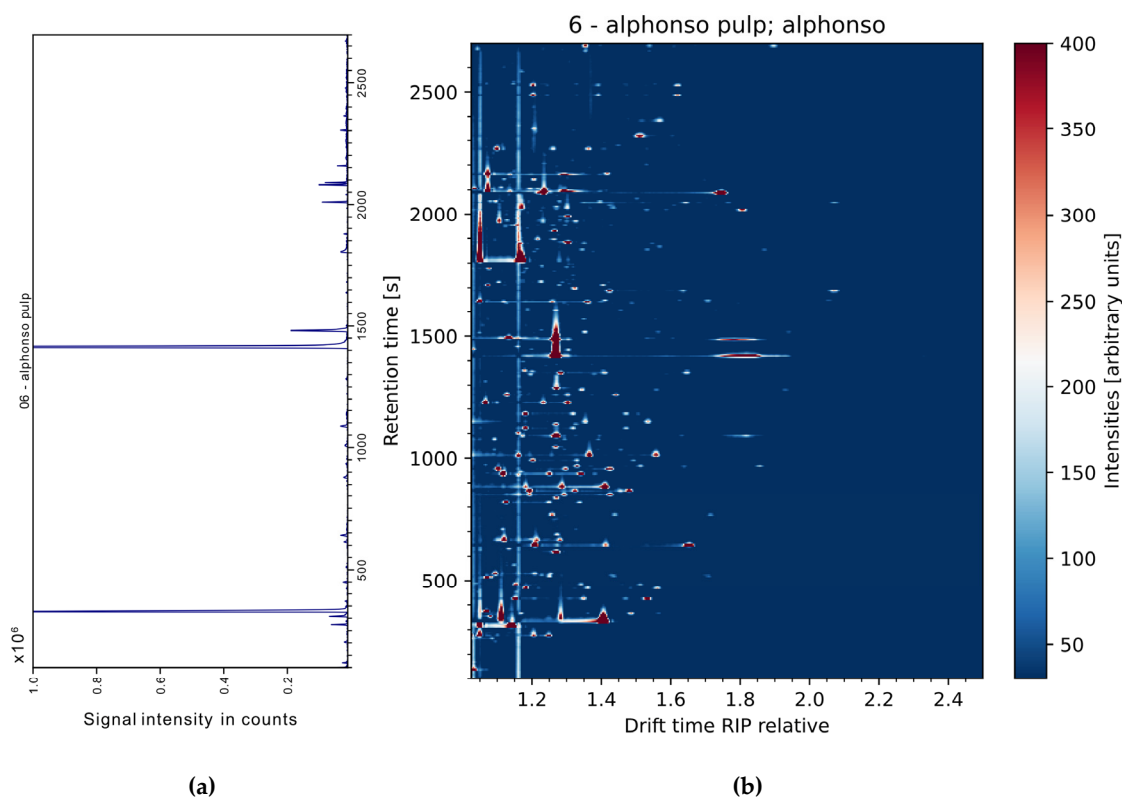


Figure S1. Exemplary visualization of an 'Alphonso' mango sample and the simultaneous sample data of QMS (a) and IMS (b)

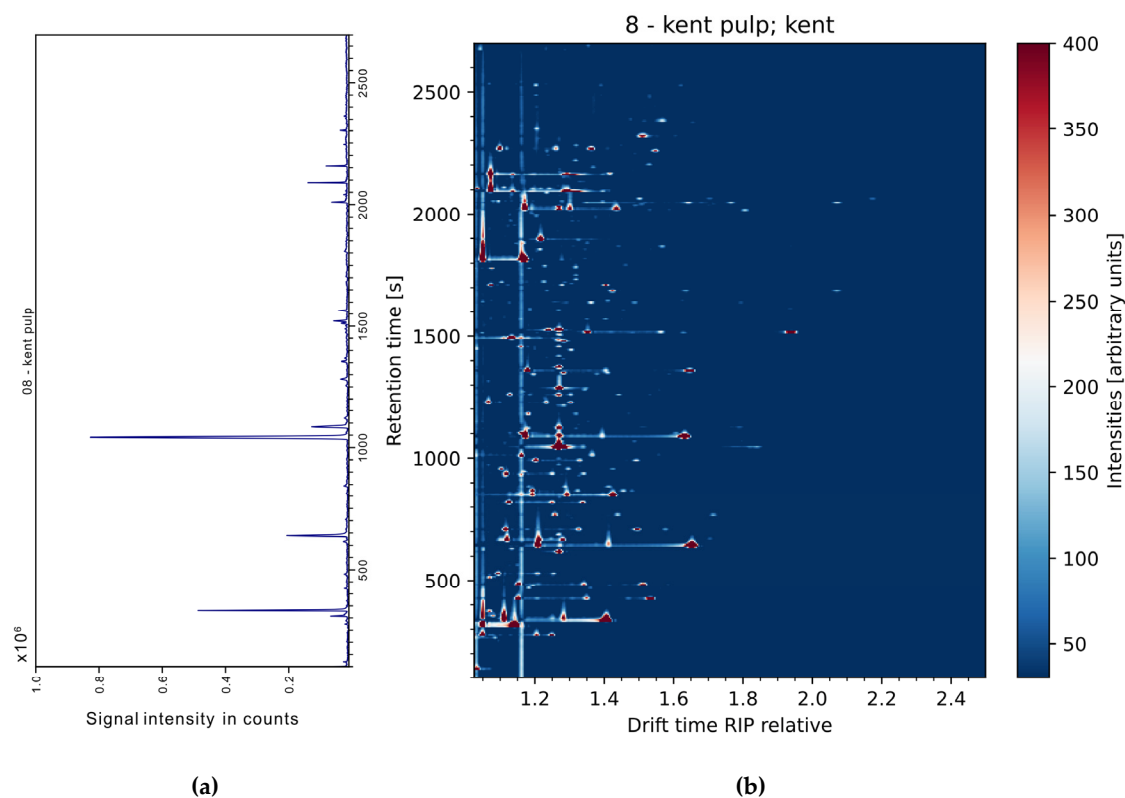


Figure S2. Exemplary visualization of a 'Kent' mango sample and the simultaneous sample data of QMS (a) and IMS (b).

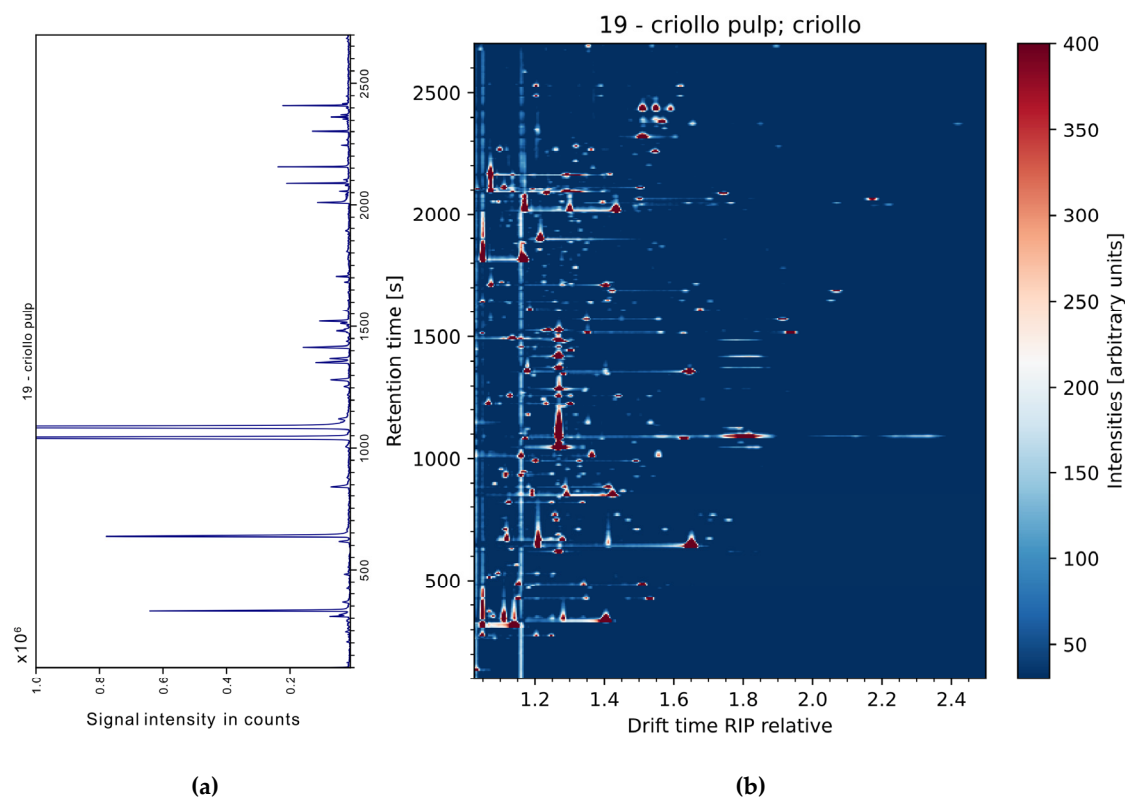


Figure S3. Exemplary visualization of a 'Criollo' mango sample and the simultaneous sample data of QMS (a) and IMS (b).

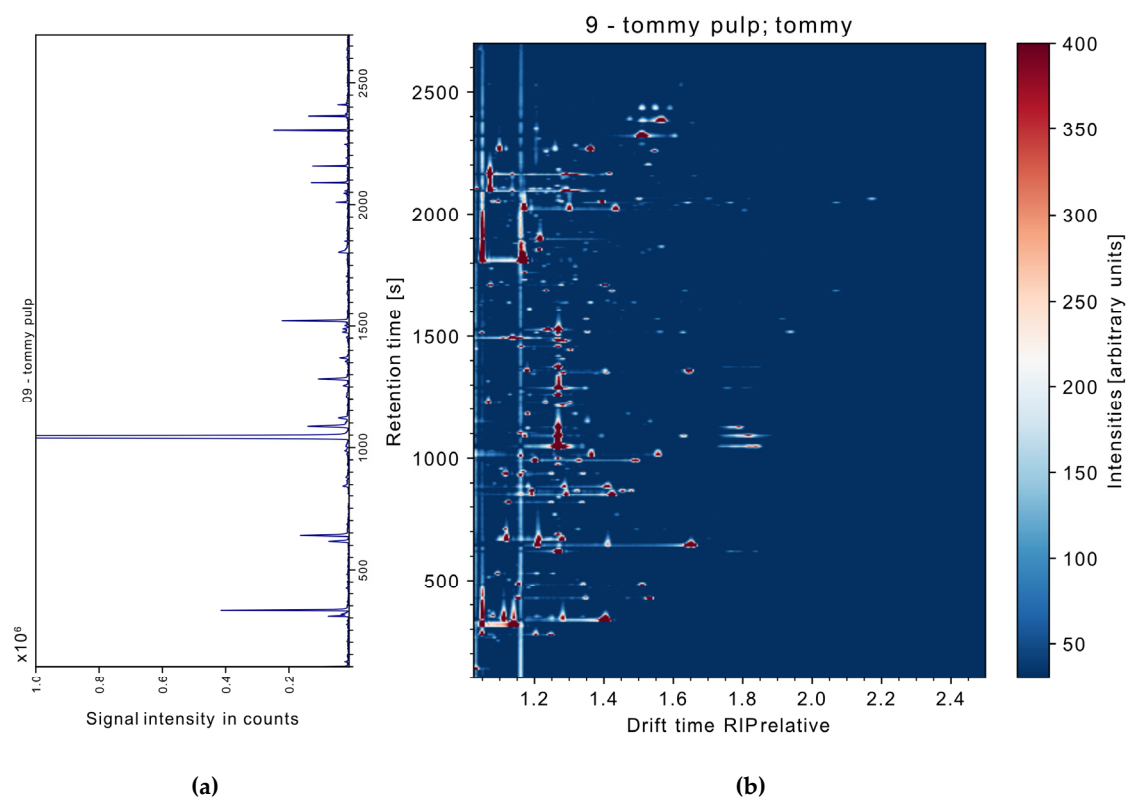


Figure S4. Exemplary visualization of a 'Tommy' mango sample and the simultaneous sample data of QMS (a) and IMS (b)

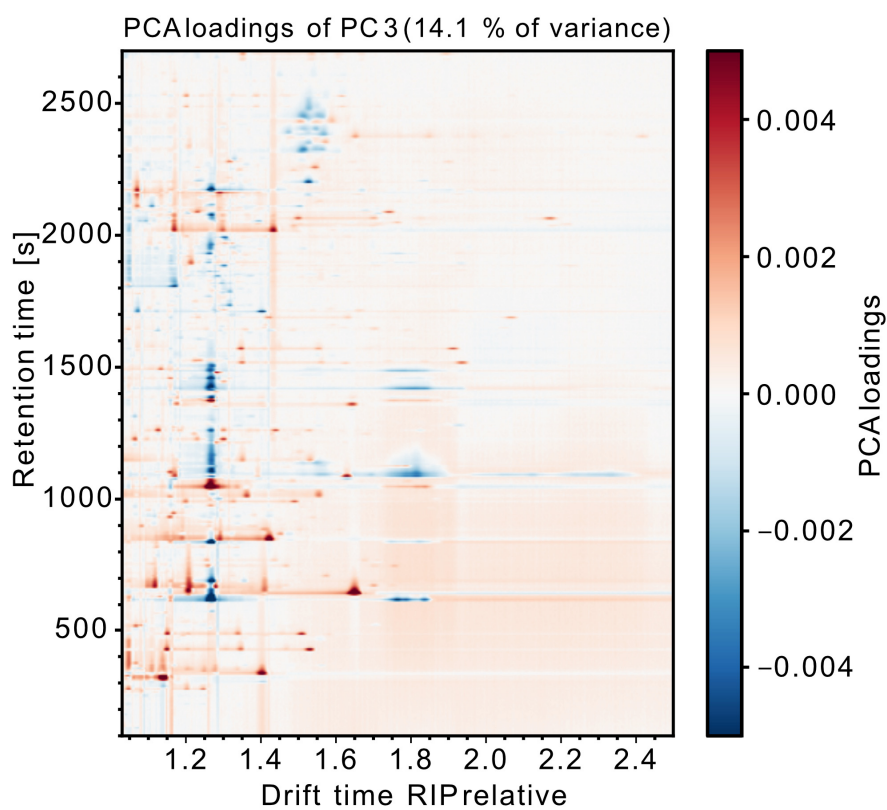


Figure S5. PCA loadings of PC3

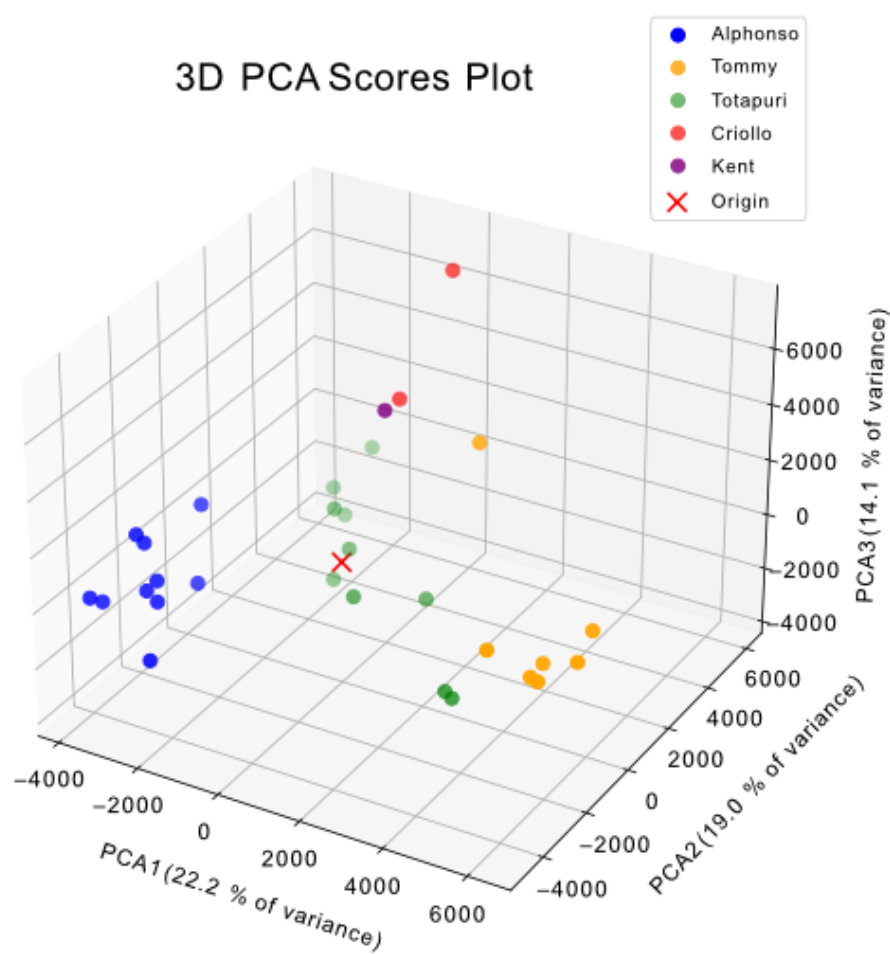


Figure S6. 3D PCA scores plot of PC1, PC2 and PC3