

Supporting Information

Flavor profiling by comprehensive mass spectrometry analysis of metabolites in tomato soups

Simon Leygeber¹, Justus L. Grossmann², Carmen Diez-Simon³, Naama Karu¹, Anne-Charlotte Dubbelman¹, Amy C. Harms¹, Johan A. Westerhuis², Doris M. Jacobs⁴, Peter W. Lindenburg^{1,5}, Margriet M.W.B. Hendriks⁶, Brenda Ammerlaan⁶, Marco A. van den Berg⁷, Rudi v Doorn⁷, Roland Mumm^{1,8}, Robert D. Hall^{1,3,8}, Age K. Smilde², Thomas Hankemeier^{1*}

¹Leiden Academic Centre for Drug Research, Leiden University, Einsteinweg 55, 2333 CC Leiden, The Netherlands

²Swammerdam Institute for Life Sciences, University of Amsterdam, Science Park 904, 1098 XH, Amsterdam, The Netherlands

³Laboratory of Plant Physiology, Wageningen University and Research, Droevendaalsesteeg 1, Wageningen, 6708 PB, The Netherlands

⁴Unilever Foods Innovation Centre, Bronland 14, Wageningen, 6708 WH, The Netherlands

⁵Leiden Center for Applied Bioscience, University of Applied Sciences Leiden, Zernikedreef 11, 2333 CK Leiden, The Netherlands

⁶DSM Biodata & Translation, Alexander Fleminglaan 1, Delft 2613 AX, The Netherlands

⁷DSM Food & Beverages, Alexander Fleminglaan 1, Delft 2613 AX, The Netherlands

⁸Wageningen Research (Bioscience), Wageningen University and Research, Droevendaalsesteeg 1, The Netherlands

*Thomas Hankemeier, hankemeier@lacdr.leidenuniv.nl

List of figures

Figure S1 Original sensory scores of all samples and flavor attributes

Figure S2 Quality control of LC-MS, GC-MS data by PCAs

Figure S3 MS/MS spectra of Asp-Leu in tomato soup 05-1 mirrored against a pure standard

Figure S4 MS/MS spectra of Met-Pro in tomato soup 19-2 mirrored against a pure standard

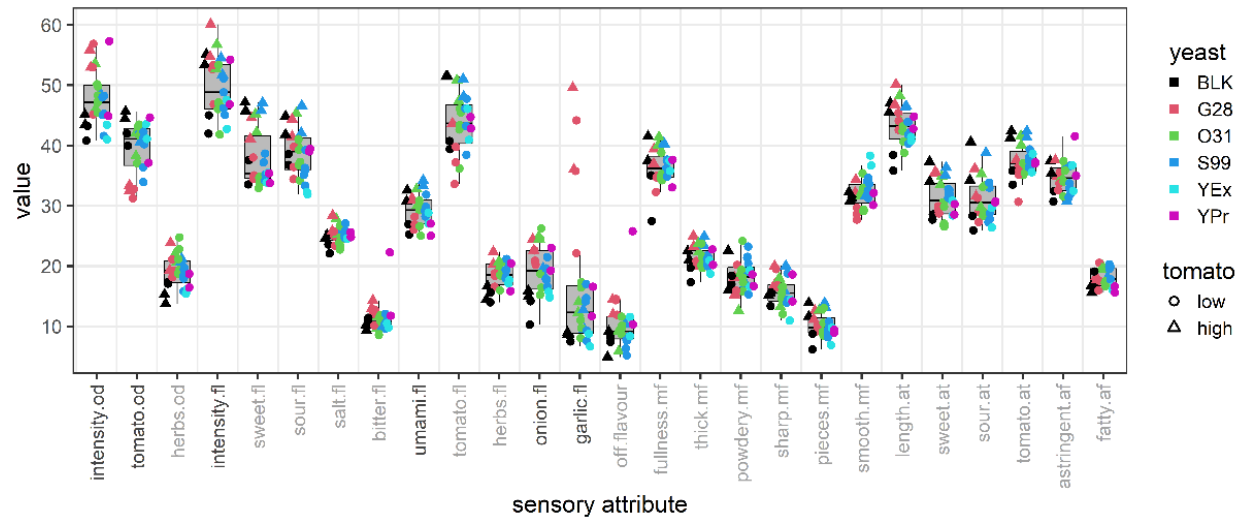


Figure S1: Original sensory scores of all samples and flavor attributes. Colors represent the added yeast derived process flavors and shapes represent tomato dosage. BLK= tomato soup without yeast derived products.

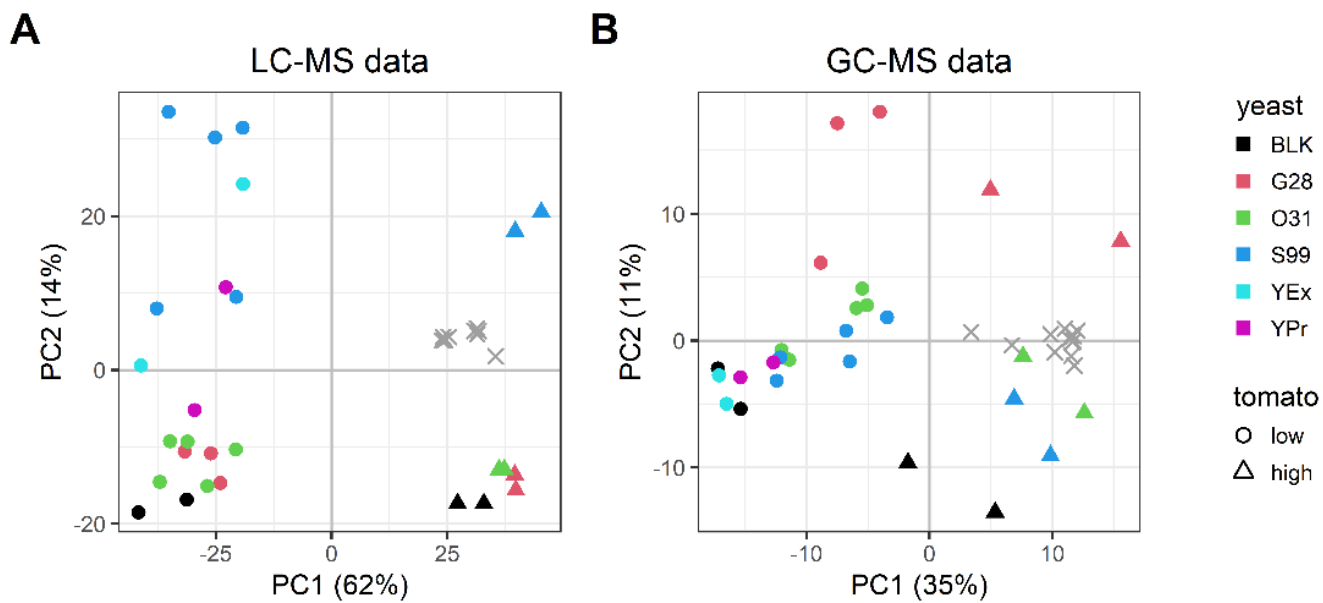


Figure S2: PCA score plots including the quality control samples (QC samples) as grey crosses which were produced as indicated in table S1. Colors represent the added yeast derived process flavors and shapes represent tomato dosage. BLK= tomato soup without yeast derived products. A: Log-transformed, autoscaled LC-MS data. B: Log-transformed, autoscaled GC-MS data.

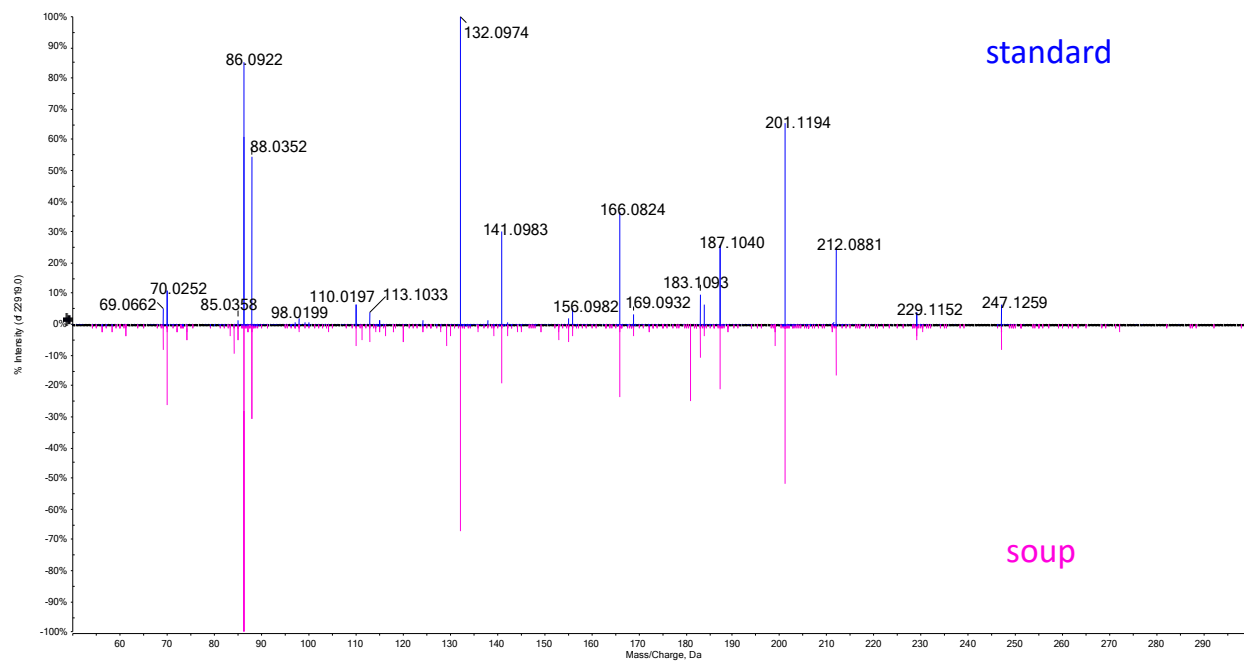


Figure S3 MS/MS spectra of Asp-Leu in tomato soup 05-1 mirrored against a pure standard

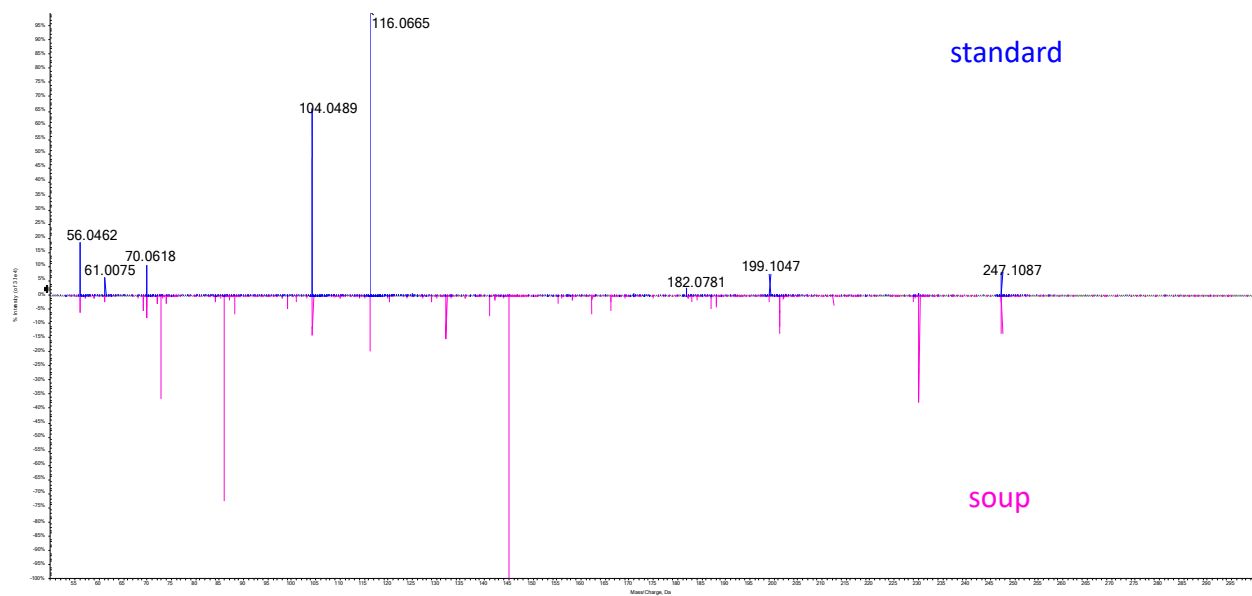


Figure S4 MS/MS spectra of Met-Pro in tomato soup 19-2 mirrored against a pure standard