

Materials List for:

PTR-ToF-MS Coupled with an Automated Sampling System and Tailored Data Analysis for Food Studies: Bioprocess Monitoring, Screening and Nose-space Analysis

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Materials

Name	Company	Catalog Number	Comments
PTR-TOF 8000 High-Resolution PTR-TOF-MS	Ionicon Analytik Ges.m.b.H.	PTR-TOF 8000	An detector for volatile organic compounds (VOCs) that allows for continuous VOC quantification with a very high mass resolution
GERSTEL MPS 2XL	Gerstel		A multifunctional autosampler
Gas Calibration Unit	Ionicon Analytik Ges.m.b.H.	GCU-s / GCU-a	A dynamic gas dilution system that provides variable but known quantities of different standard compounds in a carrier gas stream
TofDaq	Tofwerk AG	free available at http://soft.tofwerk.com/	A data acquisition software (for spectra acquisition)
MATLAB	MathWorks	http://it.mathworks.com/products/matlab/	A technical computing language and interactive environment for algorithm development, data visualization, and data analysis
R	The R Foundation	free available at https://cran.r-project.org/mirrors.html	A language and environment for statistical computing and graphics