# Direct injection and chromatography, mass spectrometry and ion mobility: a synergic approach for strawberry volatilome analysis

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**VOC phenotyping** is currently a limiting step in **breeding programs** (high costs; complex analytical techniques; complicated interaction between fruit genetics and environmental effects). Most plant breeding programs have historically neglected the flavour variation within fruit species which caused the drop-off in flavor quality perceived by consumer.
To **incorporate flavour** into breeding program routines: **i)** identify the sources of flavor variability, **ii)** understand the role of genetic and environmental factors, and **iii)** define cost-effective methods of selection.


PTR-ToF-MS
(Ionicon, Austria)


SHS-GC-IMS
(G.A.S., Dortmund, Germany)

SPME-GC-MS
(Perkin-Elmer, USA)

## Experimental setup and dataset

Nine ripe strawberry fruits of ten commercial cultivars were sampled singolarmente for each type of measurement

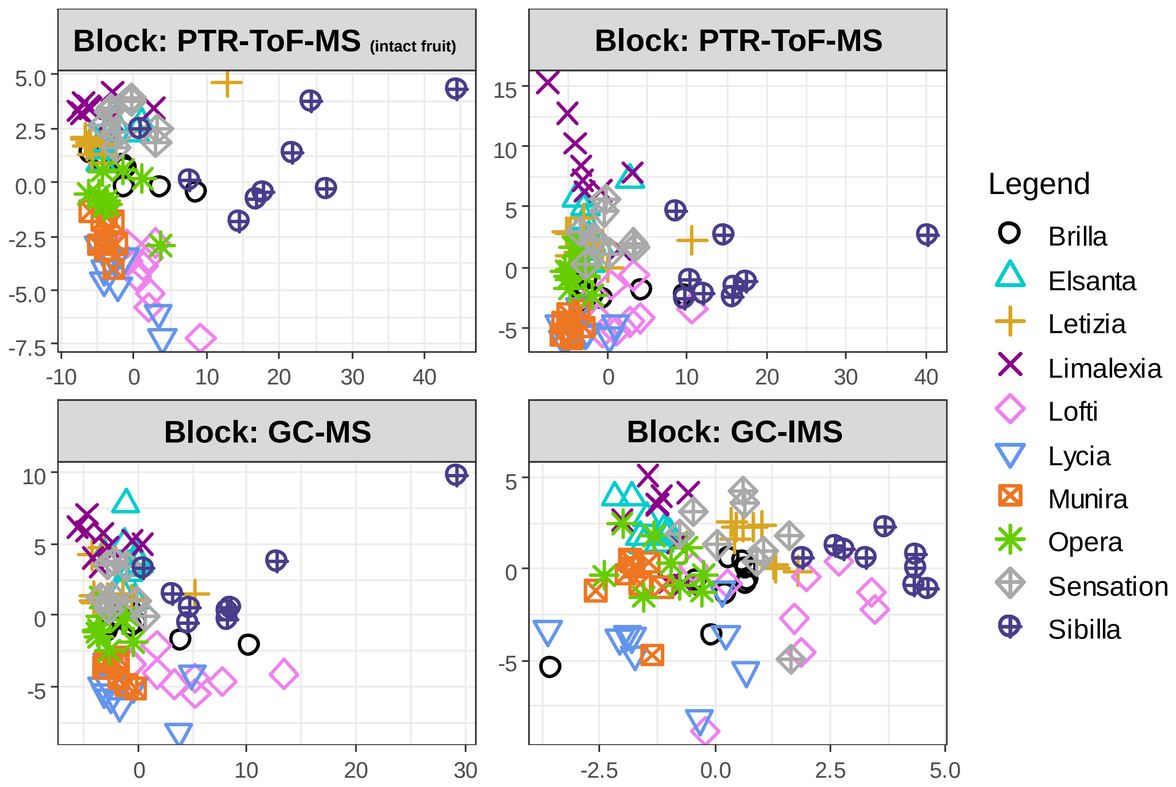
| Sampling | PTR-ToF-MS | GC-MS | GC-IMS |
|---|---|---|---|
| Single intact fruit in 250 mL jar | x | | |
| Single fruit frozen, grinned in liquid nitrogen and sampled in 20 mL vial | x | x | x |

Data extraction were performed separately for each type of measurement

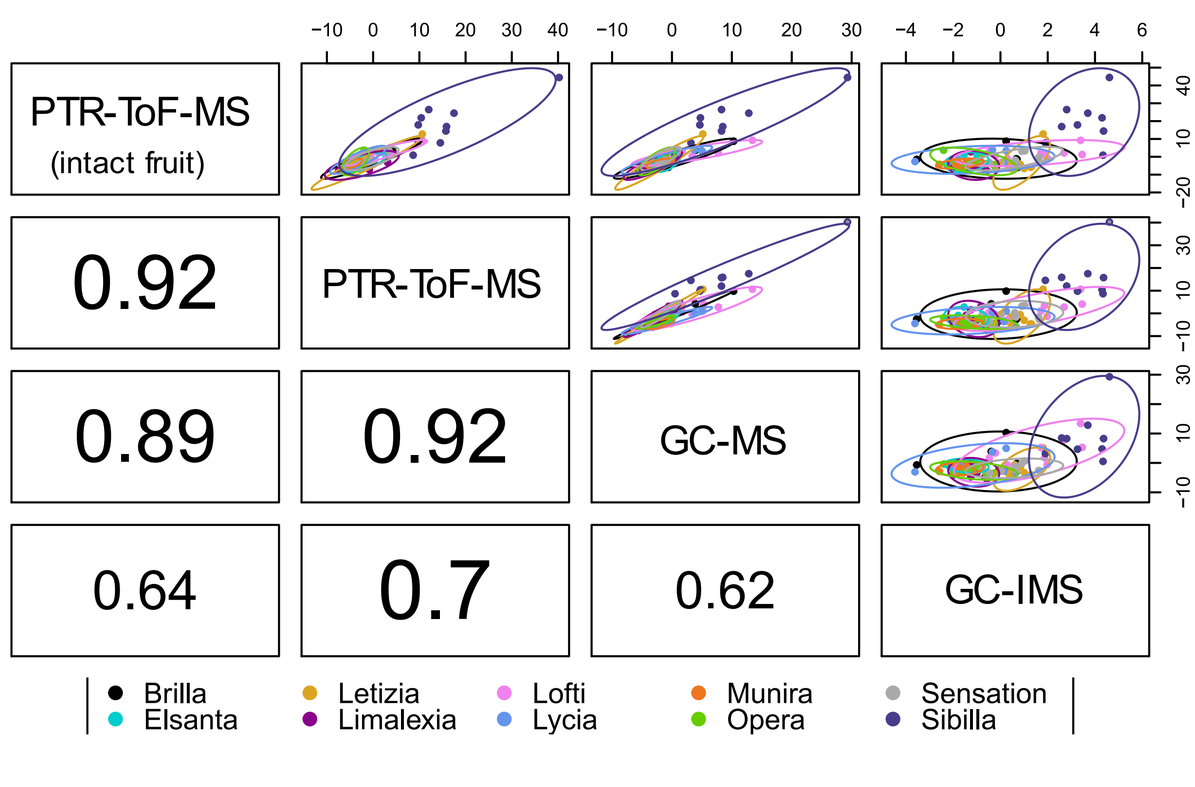
| Dataset | Dimention | Information |
|---|---|---|
| PTR (intact fruit) | 90 x 131 | mass peaks |
| PTR-ToF-MS | 90 x 151 | mass peaks |
| GC-MS | 90 x 119 | compounds |
| GC-IMS | 90 x 69 | monomers and/or dimers of compounds |

## N-Integration Discriminant Analysis with DIABLO (*mixomics*, R)

**DIABLO** stands for **D**ata **I**ntegration **A**nalysis for **B**iomarker discovery using **L**atent variable approaches for **O**mics studies (Multiblock (s)PLS-DA). DIABLO is the supervised approach with the *mixOmics* N-integrative framework models and allows to integrate multiple datasets while explaining their relationship with a categorical outcome variable




Sample plot from multiblock sPLS-DA performed on the strawberry study. The samples are plotted according to their scores on the first 2 components for each data set. Samples are coloured by cultivar




Diagnostic plot from multiblock sPLS-DA applied on the strawberry study. Samples are represented based on the specified component (here ncomp = 1) for each data sat. Samples are coloured by cultivar and 95% confidence ellipse plots are represented

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This study demonstrated the complementarity of three analytic methodologies and two types of sampling and the prospect to apply them both for broad volatilome screenings and for fruit quality assessment