

## P44. Innovative bioinformatic tools for the analysis of MS based imaging dataset in plant metabolomics

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### Abstract

The investigation of the spatial distribution of metabolites and bioactive compounds in tissues is an asset to increase our understanding of metabolic and biological processes occurring in plants. In the specific case of fruits this can have important technological, nutritional and economical implications.

MS based techniques represent an excellent tool to study the distribution of small molecules in tissue, but in view of possible high-throughput applications it is necessary to develop innovative bioinformatic tools for data analysis and interpretation.

Among the different critical aspects, metabolite identification is particularly challenging because with direct ionization techniques it has to be based only on (high resolution) mass to-charge ratios. Single mass-to-charge values are not sufficient for chemical identification, but the co-localization of characteristic molecular fragments can be used to overcome such limitation. Image segmentation and signal clustering is another promising research field in view of an automatic mining of MS imaging datasets.

In this communication we will present how advanced image analysis tools can be used to increase the selectivity of MS imaging experiments [1] and to visualize the asymmetric distribution of relevant metabolites in Golden Delicious apples.

Preliminary results on the automatic segmentation of DESI and MALDI datasets will be also discussed.

### References

[1] P. Franceschi, Y. Dong, K. Strupat, U. Vrhovsek, F. Mattivi: Combining intensity correlation analysis and MALDI imaging to study the distribution of flavonoid glycosides in Golden Delicious apples. *J. Exp. Bot.*, 63, 1123-1133 (2012).

### Figures

