

# Recent developments in plant metabolomics

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## 1. Introduction

Plant metabolomics in general is a challenging topic, not only because plants contain a large set of so-called secondary metabolites, next to the primary metabolites common to other living organisms. These secondary metabolites function as bioactives against biotic and abiotic stress effectors, like pathogens and excess light. Being part of our diet, many of these plant secondary compounds also exert bioactive effects in human, thereby determining for instance taste, aroma and healthiness of our food. However, for most of these compounds their exact role in plant life is still unknown, as is their bioactivity in human. In this presentation we provide examples of our research on this topic, which we call *functional metabolomics*.

## 2. Approach

Since authentic standards of plant secondary metabolites are hardly available or compounds detectable are yet unknown, we usually apply untargeted MS-based metabolomics. We use an in-house developed workflow from unbiased peak picking towards (putatively) annotated compounds, batch correction<sup>1</sup> and correlation analyses tools. Metabolite profiles of contrasting crude extracts are linked to bioactivity results, in order to identify the key bioactive compounds. If possible we also link to genomics and transcriptomics data, in order to identify molecular markers for breeding and isolate genes for production of the bioactive compounds in expression platforms.

## 3. Results

With regards to functional metabolomics in crop plants, examples related to plant-insect interactions will be provided. In the Brassicaceae family, including the plant model *Arabidopsis* and cabbages, cyanide-containing glucosinolates play a key role in defence against caterpillars, while the Solanaceae family, including tomato and eggplant, accumulate acylated sugars in their leaf hairs as defence against pest insects<sup>2</sup>. By means of untargeted metabolome comparison of mutants, breeding lines or GWAS populations, loci and underlying genes regulating the biosynthesis of these compounds can be identified. These studies may result in new phytochemical or genetic markers for breeding towards improved varieties.

With regard to potential bioactivities in human, we aim to couple metabolomics approaches to relevant *in vitro* and

cell assays in 96-wells format and, if possible, to online post-column assays. We recently developed a microfluidic biosensor with human cells expressing an array of membrane-bound receptors, in order to identify plant compounds interacting with taste or pharmaceutical-relevant receptors. For instance, using this platform in combination with LCMS-based metabolomics enabled the identification of novel compounds in pepper interacting with the pain and heat perception-related TRPV1 receptor<sup>3</sup>.

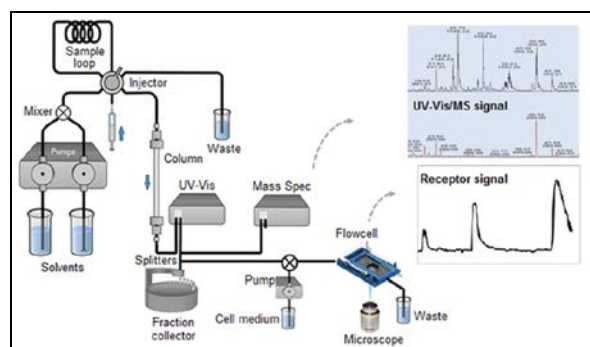


Figure 1. scheme of an online functional metabolomics setup.

## 4. Discussion

Elucidating bioactive activities of plant metabolites, either in the plants themselves or in human upon intake, can be elucidated by different approaches. Untargeted metabolomics analyses of large series of plant tissues or products with contrasting bioactivities followed by dedicated correlation analyses, enabled us to identify phytochemicals that are key in biotic stress resistance, taste and aroma, and in several cases also the genes involved in their biosynthesis. In identifying compounds having impact in human, our final aim is to couple the receptoromics platform online to analytical LCMS separation (Figure 1).

## References

1. R. Wehrens et al. "Improved batch correction in untargeted MS-based metabolomics". *Metabolomics* 12: 88, 2016
2. B. Vosman et al. "Broad spectrum insect resistance and metabolites in close relatives of the cultivated tomato". *Euphytica* 214: 46, 2018.
3. M. Henquet et al. "Metabolomics meets functional assays: coupling LCMS and microfluidic cell-based receptor-ligand analyses". *Metabolomics* 12: 115, 2016