

# Metabolomics for quality research

---

Linking metabolites to your trait of interest



WAGENINGEN **UR**

*For quality of life*

---



## Metabolomics for quality research

Metabolomics is the science of small molecules. These determine key plant features such as nutritional value, flavour, fragrance, colour, pharmaceutical activity, pest and disease antagonism – and much, much more. State-of-the-art technologies allow high throughput comprehensive analyses of complex metabolite mixtures typical of extracts of biological and food materials. Metabolomics links your key characteristics of interest with the causal compounds. Hence, metabolomics provides direct input into designing novel strategies to advance your understanding of the molecular control points behind metabolite composition and its influence on key traits. Metabolomics is now a significant innovation driver in applied science benefitting both industry and consumer.

### **Applications – what's in it for you?**

Highly sensitive Mass Spectrometry technology, in unison with advanced separation approaches, has found application in a wide diversity of applied science approaches. Metabolomics has provided novel commercial and research leads in many fields of (plant) science and is delivering valuable biochemical markers for important phenotypic traits.

In this brochure, we share some examples of our research and our publications with you.

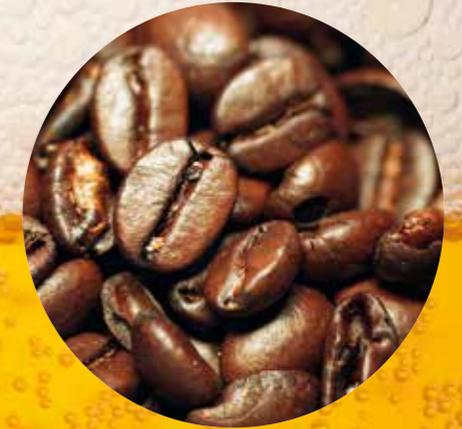
# Biodiversity screening

## Our key publications:

- *Firdaus, S. et al (2013) Identification and QTL mapping of whitefly resistance components in Solanum galapagense Theoretical and Applied Genetics 126, 1487;*
- *Fu et al. (2009) System-wide molecular evidence for phenotypic buffering in Arabidopsis Nature Genetics 41, 166;*
- *Carreno-Quintero et al. (2012) Untargeted metabolic quantitative trait loci analyses reveal a relationship between primary metabolism and potato tuber quality, Plant Physiology 158, 1306.*

Metabolomics has provided us with a unique insight into biodiversity in plant metabolism and the impact of genetics and environmental perturbation. Already we have gained deep knowledge of natural and induced diversity and the genetic and environmental influences on crop quality. Our methods are fully applicable in other crops. Some of our recent achievements:

- Characterising the untapped richness of wild plants
- Genome-wide mapping (GWAS) of metabolites in crops e.g. tomato, Brassica, pepper
- Screening for new pharmaceuticals from medicinal plants
- Demonstrating the influence of genetic integration on rice quality
- Identifying genetic control elements of plant metabolism



# The taste of success

Taste and flavour are primarily determined by the metabolites present in our food. They are complex features requiring broad, detailed analyses. Despite this biochemical complexity, just one 'off flavour' is enough to convert a commercial product into a profit liability. Metabolomics provides novel insights into a diversity of food related issues in both fresh and processed products. Our recent achievements:

- Integrating taste panel and metabolomics analyses to identify coffee off-flavours
- Identifying the compounds and genes behind food quality traits in tomato
- Identifying metabolite changes associated with vegetable cultivation strategies
- Defining the key fragrance differences between Jasmine and Basmati rice
- Defining compositional changes from food processing strategies in cocoa

## Our key publications:

- *Lindinger et al. (2009) Identification of ethyl formate as a quality marker of the fermented off-note in coffee JAFC 57, 9972;*
- *Tikunov, Y.M. et al. (2013) NON-SMOKY GLYCOSYLTRANSFERASE1 Prevents the Release of Smoky Aroma from Tomato Fruit. The Plant Cell 25, 3067;*
- *Calingacion, M.N. et al (2015) Delving deeper into technological innovations to understand differences in rice quality. Rice 8, 10.*



## Development, ripening and shelf life

Plant and fruit development, ripening, time of harvest, storage and shelf life are all defined by coordinated and (pre)programmed paradigm shifts in metabolite composition. Metabolomics generates unique knowledge of these changes giving us the tools with which to design improvements. Some of our recent achievements:

- Characterising the metabolic dynamism of fruit ripening in apple
- Multi-platform analysis of climatic influences on broccoli quality
- Revealing the basis of quality changes during shelf life depreciation in melon cubes
- Deciphering the metabolic differences between tomato ripening mutants
- Spatial and temporal dynamics of metabolism during plant organ development

*Our key publications:*

- Moing et al. (2011) Novel metabolic cross talk in melon fruit *New Phytologist* 190, 683;
- Pedreschi, R. et al (2014) Metabolomics analysis of postharvest ripening heterogeneity of 'Hass' avocados. *Postharvest Biology and Technology* 92, 172;
- Lopez-Sanchez, P. et al (2015) Comprehensive metabolomics to evaluate the impact of industrial processing on the phytochemical composition of vegetable purees. *Food Chemistry* 168, 348.

## Metabolomics for seed-based industries

Seeds are a key food component and also the basis of most crop production strategies. Seed quality, uniformity and viability are therefore key traits determining commercial value and agricultural success. Metabolomics provides novel insights into seed development, maturation and seed treatments. Some of our recent achievements:

- Following metabolic changes during Brassica seed development
- Determining the metabolic basis of loss of viability of seed with limited shelf-life
- Defining the link between seed composition and roasted coffee bean quality
- Characterising the molecular basis of vegetable seed priming
- Identifying the influence of fertilizer application on rice grain quality



*Our key publications:*

- Groot et al. (2012) Seed storage at elevated partial pressure of oxygen, a fast method for analysing seed ageing under dry conditions *Annals of Botany* doi:10.1093/aob/mcs198;
- Calingacion et al. (2012) A genomics and multi-platform metabolomics approach to identify new traits of rice quality *Metabolomics* 8,771;
- Pino del Carpio, D. et al. (2011) The patterns of population differentiation in a Brassica rapa core collection *Theoretical and Applied Genetics* 122, 1105.

# Early warning systems

## Our key publications:

- Snoeren et al. (2010) *Natural variation in herbivore-induced volatiles in Arabidopsis thaliana* *J Ex Bot* 61 3041;
- Villafort Carvalho, M.T. et al (2015) *Gomphrena clausenii, a novel metal-hypertolerant bioindicator species, sequesters cadmium, but not zinc, in vacuolar oxalate crystals.* *New Phytologist* DOI: 10.1111/nph.13500;
- Etalo, D.W. et al. (2013) *System-Wide Hypersensitive Response-Associated Transcriptome and Metabolome Reprogramming in Tomato.* *Plant Physiology* 162, 1599.

Plants are continually interacting with their environment. Furthermore, pest and pathogen attack are usually accompanied by a biochemical response from either plant and/or attacker. Metabolomics can identify the chemicals produced which can be exploited in designing novel resistance strategies as well as developing early (remote) detection systems of infection or attack. Some of our recent achievements:

- Identifying biochemical markers for fungal infection of mushroom compost
- Early detection of pest – induced plant volatiles in greenhouses
- Monitoring and developing markers for food spoilage
- Defining the biochemical changes induced by fungal attack of tomato
- Thrips and white fly resistance and plant interaction mechanisms



# Tackling the terabytes

Metabolomics is a hugely data-rich science requiring tailor-made bioinformatics and biostatistics strategies. Optimal data management facilitates the identification of metabolite features correlating with the trait of interest. Our established track record covers data management and mining approaches:

- Data processing workflow for both targeted and untargeted metabolite analyses
- Establishing in-house databases of metabolites found in important crops
- Designing data mining tools and statistical strategies for determining discriminatory sample differences
- Writing scripts and software for (semi-)automated data storage and retrieval
- Designing tools for metabolic network analysis

## Our key publications:

- Moco et al. (2006) *A liquid chromatography-mass spectrometry-based metabolome database for tomato.* *Plant Physiology* 141, 1205;
- Mihaleva et al. (2009) *Automated procedure for candidate compound selection in GCMS metabolomics* *Bioinformatics* 25, 787;
- van der Hooft et al (2011) *Polyphenol identification based on systematic and robust high-resolution accurate mass spectrometry fragmentation.* *Analytical Chemistry* 83, 409

# Our track record and expertise

- Over 150 publications on a diversity of metabolomics technology development and application topics
- Two books on metabolomics
- Organiser 1st International Metabolomics Congress (Wageningen, 2002) and the 5th Metabolomics Society Conference (Amsterdam 2010)
- Past President and Honorary Fellow International Metabolomics Society
- Coordinator international ([www.meta-phor.eu](http://www.meta-phor.eu)) plant metabolomics research programmes
- Multiple bilateral projects with industrial partners from the breeding, food, pharmaceutical and agro-chemical sectors
- Integrated approaches for both wet and dry science
- Volatile analysis of natural products
- Solid Phase MicroExtraction, TENAX trapping, organic extraction
- Static and dynamic headspace trapping
- Primary and secondary metabolite analysis
- Metabolite identification
- Large scale metabolite profiling and comparative metabolomics
- Metabolite databases, data management and statistical analysis
- Polyphenols, terpenoids, alkaloids, sugars, amino acids, glucosinolates, fatty acids and many more...

Metabolomics for **quality** research



# Our metabolomics platforms

- UPLC, HPLC and GC separation technologies
- Photodiode Array, ElectroChemical and Fluorescence detection
- Q-Exactive and QTOF Mass Spectrometer with MS/MS capabilities
- LTQ-Orbitrap FT Mass Spectrometer with MSn capabilities
- 3 GCQ Mass Spectrometers for extract & volatile analysis
- GC-Triple Quad MS with automated on line derivatization
- HPLC with on-line Anti-oxidant detection
- Full set of bioinformatics and biostatistics tools
- In-house and commercial metabolite databases
- Access to NMR, LC-triple Quad MS and preparative LC-MS machines
- Nanomate LC fractionation with chip-based ESI nanospray direct infusion

## We offer

A unique combination of multiple analytical platforms fully supported by biochemical, bioinformatics and biostatistics expertise with on-hand biological knowledge to identify the biological relevance of metabolomics results in a commercial context.

---

### Contact Information

Wageningen UR

Professor Dr. Robert Hall

Phone: +31 317 48 04 41

E-mail: [robert.hall@wur.nl](mailto:robert.hall@wur.nl)

[www.wageningenur.nl](http://www.wageningenur.nl)

Droevendaalsesteeg 1,

6708 PD Wageningen,

The Netherlands



**WAGENINGEN UR**  
*For quality of life*