# **PRIMESOFT**

Development of innovative priming technologies safeguarding yield security in soft fruit crops through a cutting-edge technological approach



**Topic: VOC Workshop Agenda** 

Dates: February 5-7, 2024

Organised and hosted by: KU Leuven, BE

Venue: Willem de Croylaan 42, Leuven





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Day1 (Februari 5)	Day2 (Februari 6)	Day3 (Februari 7)
08:30 Welcome/ General introduction 08:45 Bart Nicolai	Gathering/ evaluating practical work	Gathering/ evaluating practical work
09:00 Sampling techniques for VOC analysis 09:15 Joeri Vercammen (IS-X / UGent) 09:30 09:45 10:00 10:15 10:30	Optimal Experimental Design Peter Goos	Multivariate statistics  Bart De Ketelaere
10:45 coffee	coffee	coffee
11:00 A short introduction to GC-MS 11:15 Maarten Hertog 11:30 11:45	Optimal Experimental Design (cnt'd) Peter Goos	Multivariate statistics (cnt'd)  Bart De Ketelaere
<ul><li>12:00 A short introduction to SIFT-MS</li><li>12:15 Maarten Hertog</li><li>12:30</li></ul>	Case study experimental design PhD Bart De Ketelaere	Case study multivariate statistics PhD Matthias Corion
12:45	Lunch	Lunch
13:15 13:30 Hands on experience 13:45 SPME-GC-MS / SIFT-MS	Case study TDU-SIFT-MS PhD Cecilia Cardinez	Case study SIFT-GC/MS PhD Amina Benchennouf
14:00 Elfie Dekempeneer / Tessa Vanempten 14:15 14:30 14:45 15:00	Hands on experience SPME-GC-MS / SIFT-MS Elfie Dekempeneer / Tessa Vanempten	handson experience DOE Peter Goos
15:15 <mark>coffee</mark>		
15:30 Hands on experience (cnt'd)		coffee
15:45 Elfie Dekempeneer / Tessa Vanempten 16:00 16:15 16:30 16:45 17:00	coffee Hands on experience (cnt'd) Elfie Dekempeneer / Tessa Vanempten	handson experience MV  Bart De Ketelaere
17:15		Final evaluation/closing
17:30		

Workshop Dinner Voltaire











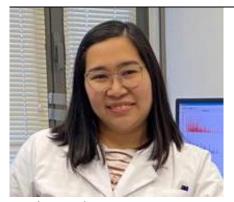


Amina Benchennouf
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Amina Benchennouf is a Ph.D. researcher from the division of MeBioS in the Faculty of Bioscience Engineering at KU Leuven. She holds two master's degrees, one in food industry engineering (Algeria) and the second in food quality and chemistry of natural products (Greece). She worked as a research assistant for 3 years before her PhD journey began. Her Ph.D. was part of a project called "TarOMAAT", funded by the Agency for Innovation and Entrepreneurship (VLAIO). During the 4 years of PhD, she worked on the quality aspects of tomatoes, mainly flavour, which is the combination of taste and aroma. Correspondingly, she explored the potential of SIFT-MS as a fast technique to characterize the aroma of tomato. In collaboration with TarOMAAT partners, she developed a flavour model that can help tomato breeders make selections for improved flavour.

## SIFTing through tomato flavor: Prediction of tomato overall liking

From this presentation, you will have an idea of how to develop a method based on fingerprinting using SIFT-MS. You will learn how to prepare a sample and what are the parameters affecting sampling.



Cecilia Cardinez
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Cecilia Cardinez is a PhD student from the division of MeBioS in the Faculty of Bioscience Engineering at KU Leuven. In collaboration with the Citrus Research Institute in South Africa, she explores the potential of TD-SIFT-MS on false codling moth detection in citrus. Ultimately, she aims to develop a postharvest tool based on SIFT-MS principles for the packhouse detection of false codling moth in citrus.

# Detection of false codling moth infestation in citrus using TD-SIFT-MS

In this presentation, the basic principles of thermal desorption and the challenges for method optimization in tandem with the SIFT-MS will be discussed. In addition, the applicability of TD-SIFT-MS for the detection of false codling moth infestation in citrus will be presented.













Ir. Matthias Corion
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Matthias Corion is a former PhD student from the division of MeBioS in the faculty of Bioscience Engineering at KU Leuven. There, he performed research on the development of in ovo sexing approaches based on optical and non-optical techniques. The research aims to create a reliable solution that answers the poultry industry's needs. Awaiting the defense of his PhD, Matthias started as a scientific researcher in the division of Animal and Human Health Engineering performing research on intestinal health in poultry and pigs.

## **Multivariate Statistics in VOC Measurements of Eggs**

In this session, we will explore the application of multivariate statistics in the analysis of VOC measurements in eggs. This case study delves into utilizing techniques such as principal components analysis (PCA), partial least squares-discriminant analysis (PLS-DA), and hierarchical clustering analysis (HCA). The focus will be set on preprocessing the datasets, preparing the cross-validation splits, applying different variable selection techniques, and interpreting the results.



Elfie Dekempeneer
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Elfie Dekempeneer started her professional career in 1995 at KU Leuven and is since 2003 part of the BIOSYST-MeBioS postharvest group of Prof Nicolai. She's highly experienced in GCMS work and specializes in VOC analyses and metabolomics of fruit and vegetables. She is the principal contact for the postharvest laboratory and takes quality, safety and wellbeing as a high priority.

# Hands on experience SPME-GCMS

This hands-on training will give you a practical insight in the world of HS-GCMS. We'll go through all the different aspects which need to be taking in account for an optimal working GCMS system. We'll have a look at all the parameters which have influence on optimizing a HS-SPME\_GCMS protocol.













Dr. Ir. Bart De Ketelaere KU Leuven, BIOSYST-MeBioS (BE) Innovation Manager bart.deketelaere@kuleuven.be

Bart De Ketelaere combines a master in Bioscience Engineering and a master in Statistics. He holds a PhD in Bioscience Engineering and developed a keen interest in industrial quality control, combining sensor technologies with advanced data processing. He is (co-) author of more than 130 journal papers and (co-)inventor of several patents. Moreover, he is the co-founder of two start-up companies. He currently holds a position as innovation manager at the division for Mechatronics, Biostatistics and Sensors, working together with researchers towards valorization of the basic research.

#### **Multivariate Statistics: an introduction**

In this session I will provide a basic introduction to important techniques for analysing multivariate data. Rather than providing the mathematical background I will explain the intuition behind these techniques, how they can be applied and how to interpret the results. Topics covered will range from dimension reduction to clustering and prediction.



Prof. Dr. Peter Goos
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Peter Goos is a full professor at the Faculty of Bio-Science Engineering of KU Leuven, and at the Faculty of Business and Economics of the University of Antwerp, where he teaches various introductory and advanced courses on statistics and probability. His main research area is the statistical design and analysis of experiments. Besides numerous influential articles in various kinds of scientific journals, he published the books The Optimal Design of Blocked and Split-Plot Experiments, Optimal Experimental Design: A Case Study Approach, Statistics with JMP: Graphs, Descriptive Statistics and Probability and Statistics with JMP: Hypothesis Tests, ANOVA and Regression. For his work, Peter has received four Shewell Awards, two Lloyd S. Nelson Awards, the Youden Award and a Brumbaugh Award from the American Society for Quality, the Ziegel Award and the Statistics in Chemistry Award from the American Statistical Association, and the Young Statistician Award of the European Network for Business and Industrial Statistics (ENBIS). Peter is also cofounder of EFFEX™ which provides software for design of experiments and the analysis of experimental data.

#### An introduction to optimal design of experiments

Design of experiments or DOE is a key tool for researchers as well as for product and process improvement and innovation. However, experimenters often have to deal with a mismatch between standard experimental designs, such as factorial and fractional factorial designs, central composite designs, and the features of their problems. This introductory course motivates the











standard and routine use of a fully flexible approach to design of experiments, named optimal design of experiments, by showing several examples. The increasing computing power and the availability of user-friendly software for the tailor-made design of experiments has made optimal experimental design a key tool for the industrial statistician in the 21st century.



Dr. Maarten Hertog
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Research leader computational plant
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Maarten Hertog has been working in the area of postharvest research in The Netherlands, New Zealand and Belgium. He is known for his research in the area of quality change modelling of the postharvest behaviour of fruits and vegetables. As research leader computational plant biology at the KU Leuven BIOSYST-MeBioS postharvest group, Maarten is responsible for the applied system biology projects in the area of postharvest biology. As part of recent and ongoing projects The MeBioS group has accumulated valuable expertise in the area of VOC analyses on fresh fruits and vegetables in response to fruit ripening and storage.

#### An introduction to GC-MS and SIFT-MS

This contribution will provide you with a condensed overview of both GC-MS and SIFT-MS for VOC analyses. Focus will be on the fundaments of chromatography to improve your understanding of the underlying principles of the analysis. After this lecture you should be better equipped to interpret its outcomes and to troubleshoot your protocols.



Tessa Vanempten
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Almost three years ago, in 2021, fresh from school and with a thirst for knowledge, Tessa Vanempten stepped into the postharvest research as a lab technician at the KU Leuven BIOSYST-MeBioS postharvest group.

Beyond her instrumental role with SIFT-MS, Tessa extends her expertise to assist PhD students, creating a collaborative and supportive atmosphere in the lab.

#### Hands on experience with SIFT-MS

This hands-on training will guide you through the steps involved in setting up and fine-tuning experiments. You will learn the handling and preparing of samples for optimal VOC extraction and learn more about the SIFT-MS technology.













Dr. Joeri Vercammen
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Vercammen has been working frontstage chromatographic innovation for more than two decades. After his Ph.D., which he obtained from Ghent University (Belgium) in 2002, Joeri worked as operational manager of a large environmental laboratory in Belgium. Since 2008, he is R&D manager at Interscience, a leading integrator of GC&MS based solutions in the Benelux countries, where Joeri leads the IS-X competence center. In addition to his extensive analytical background, Joeri is ISO/IEC 17025 quality assessor and certified Lean Black Belt. Since 2017, Joeri is visiting professor at Ghent University where he aims to inspire the new generation of young scientists regarding the exciting ecosystem of chromatography.

## Sampling techniques for aroma analysis

Introducing basic principles of headspace sampling techniques, such as static and dynamic headspace and fibertrapping. In case of time, slides are available on multiple headspace extraction, which is particularly useful to quantify volatile constituents in solid matrices without matrix effects.







