15th **Weurman Flavour Research** Symposium

18–22 September 2017 • Graz University of Technology • Austria

Book of Abstracts

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18-22 September 2017

Graz, Austria

www.weurman2017.at

TU Graz

Graz University of Technology

15^{th} Weurman Flavour Research Symposium

Book of Abstracts

Schlossberg Uhrturm @ Graz Tourismus - Harry Schiffer

Graz University of Technology
Austria

organised by

TU Graz
Graz University of Technology

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Impressum
15^{th} Weurman Flavour Research Symposium

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Graz University of Technology
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WEURMAN 2017

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Dear delegates,
Dear colleague and friends,

On behalf of the members of the organising committee, it is our great pleasure to welcome you to the 15th Weurman Flavour Research Symposium. Since 1975, the Weurman Flavour Research Symposium has been a unique platform for flavour scientists from all over the world offering the opportunity to discuss recent trends and developments in the field of flavour research. It is a great honour for us to be the host of the 15th edition of this important conference.

We would like to thank the scientific committee for their dedicated involvement in arranging the scientific program as well as for their support during the conference by taking chairs and evaluating posters for the poster awards.

We would like to greatly acknowledge the generous support of our sponsoring companies listed in alphabetic order on the back cover of the Book of Abstracts. Their financial support greatly assisted us in organising this conference. With their support, it was possible to provide a significantly reduced student fee for 35 research students. The participation at the symposium will hopefully encourage them to continue their research in flavour chemistry.

Finally, we would like to thank all scientists for their contributions in terms of lectures and poster contributions.

We wish you a successful conference with a lot of interesting and rewarding discussions and we hope that you will enjoy the 15th Weurman Symposium!

Barbara Siegmund
On behalf of the organising committee

General Information

Name Badges

Attendees are asked to wear their name badges at all times to gain admission to all sessions, exhibits and social events.

Wireless Internet Access

Wifi access is provided at the conference venue. Access is provided via eduroam. If you do not have access to eduroam, please receive your wifi access data at the registration desk.

Mobile Phones

As a courtesy to our speakers and other attendees, please turn off your mobile phones during the sessions.

Video Recording

Video recordings are not allowed in the sessions, poster presentations and the exhibit area.

Oral Presentation Guidelines

Projectors and computers are available for your presentation. Please be sure to provide your presentation on a USB flash drive in time. It is not possible to connect your own laptop. Stephan Lippitsch, who is responsible for technical issues throughout the conference, will be present in the lecture hall to receive your presentation.
The following time slots are scheduled for your presentations: (i) keynote lectures: 30 minutes + 5 minutes for discussion, (ii) contributed lectures: 20 minutes + 5 minutes for discussion, (iii) flash presentations: 5 minutes WITHOUT discussion. Attendees with flash presentations will present their results also on their posters and will be available for discussion during the poster sessions. We kindly ask all presenters to keep the time. The schedule will be followed strictly!

Poster Presentation Guidelines

Posters will be presented throughout the whole conference. Adhesives are provided at the poster boards as well as at the registration desk. Posters are divided into two poster sets. For details on the poster program as well as on the selection of the best posters, please see the technical program.

Poster Talks

20 posters were selected for a short poster talk. The poster presentation will be 3 minutes maximum and without questions from the audience. The presentation must not be longer than three slides and no videos are allowed. We ask the presenters to check for their presenting time at the poster talk list on page 68 and be in time. The schedule will be followed strictly! Speakers not showing up in time will be skipped. The presentation files (ppt(x) or pdf) will be collected at the registration desk on Monday from 9.00 till 14.00 h.

Information on Social Events

Guided Tour through the Historic Centre of Graz

'Graz City Guides' will await you on Wednesday after the afternoon session in front of the university building (Rechbauerstraße 12) and take you on the tour through the historic centre of Graz. The tours will last about 1.5 hours.

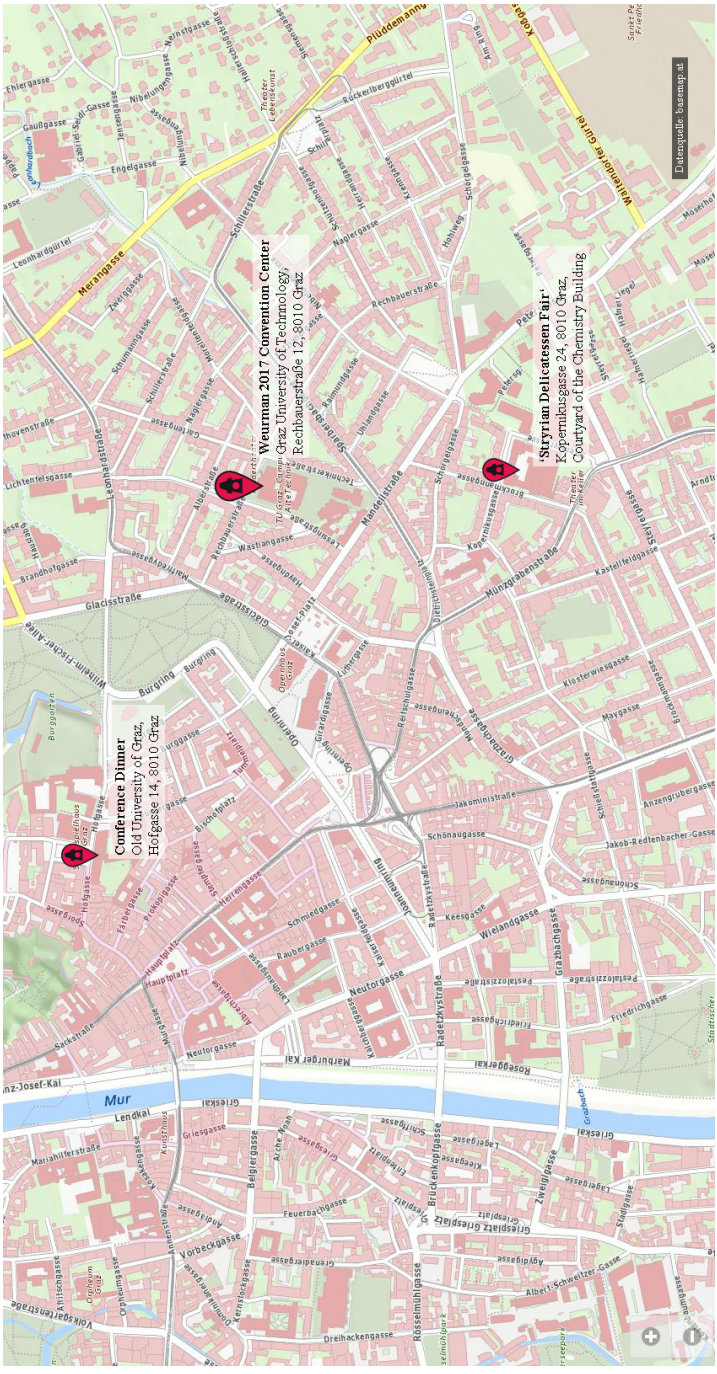
'Styrian Delicatessen Fair'

On Wednesday evening, a special event is waiting for you where local food and drinks will be prepared. The 'Styrian Delicatessen Fair' will take place in the courtyard of the Chemistry Building, Kopernikusgasse 24. After the guided tour through the historic centre, you can either walk back or you can take the tramway line 3 or 6 to the station 'Dietrichsteinplatz' or line 6 until the station 'Neue Technik'. Drinks will be served from 6 p.m., the food court will open at 7 p.m.

Conference Dinner

The conference dinner will be served in the former library hall of the Old University located in the historic city centre (Hofgasse 14). The Old University is in about 15 minutes walking distance from the conference centre. You find a map in your conference bag or on the backside of your voucher for the conference dinner.
Be sure to bring your voucher that you can find in the personalised envelope handed out at the registration. You will need it to get admission to the conference dinner. Doors to the Old University will open at 7 p.m.

City Map



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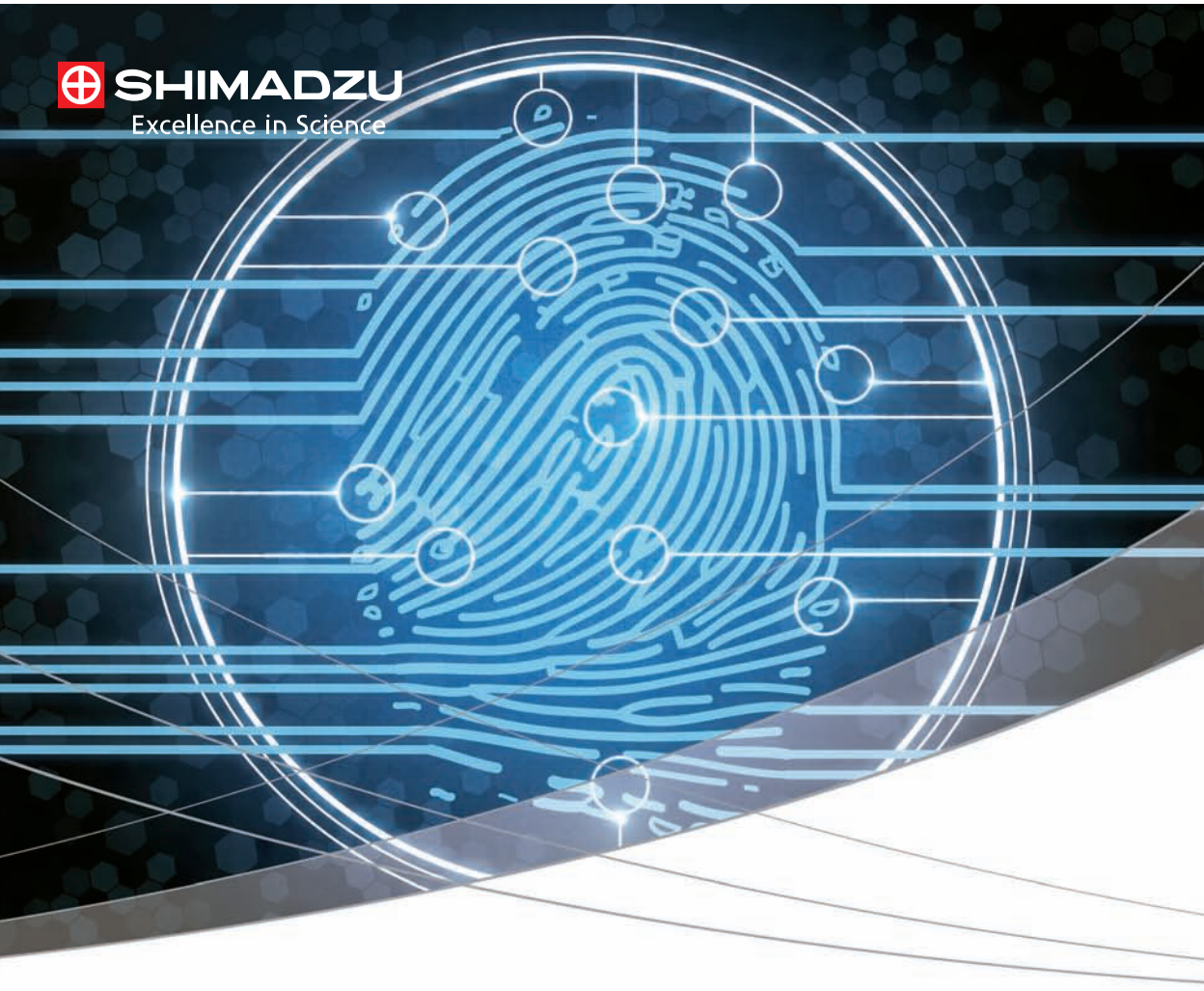

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Conference Schedule

Monday, 18.9.2017

13:00 - 17:00	**Satellite Symposia** (in parallel) Session I: Interactive Symposium on real-time Flavour Release Analysis with PTR-TOFMS (hosted by Ionicon) Session II: Analysis of Flavour Compounds by Advanced Chromatographic Methods (hosted by Shimadzu) Location: Kopernikusgasse 24/II, 8010 Graz Seminar Rooms: Chemistry II and Chemistry IV
17:00 - 20:00	**Registration** Location: Graz University of Technology, Old Campus Rechbauerstr. 12, 8010 Graz
19:00 - 21:00	**Welcome Reception**

Tuesday, 19.9.2017

08:00	Registration
08:30 - 09:00	Welcome and Conference Opening Ceremony
09:00 - 09:45	Opening lecture Olfactory loss and neuroplasticity *Veronika Schöpf, University of Graz, Institute of Psychology, Graz, Austria*

Session 1: Impact of Flavour Compounds on Humans

Chair: Veronika Somoza, Austria

09:45 - 10:20	Keynote lecture Taste Receptors and Upper Airway Immunity *Noam A. Cohen, University of Pennsylvania, Otorhinolaryngology - Head and Neck Surgery, Philadelphia, USA*
10:20 - 10:45	Bitter taste: prediction, relation to toxicity, and effect on emotions *Masha Niv, The Hebrew University, The Institute of Biochemistry, Food Science and Nutrition, Rehovot, Israel*
10:45 - 11:15	Coffee break

Session 1 continued: Impact of Flavour Compounds on Humans

Chair: Jean Luc LeQuéré, France

11:15 - 11:40	Can cross-modal flavour enhancement modulate appetite and food intake? *Ian Fisk, University of Nottingham, Sutton Bonington Campus, United Kingdom*
11:40 - 12:05	Implicit processing of relaxing - energizing effects of flavors *Isabelle Cayeux, Firmenich, Geneva, Switzerland*
12:05 - 12:30	Implications of flavor-active compounds for lipid metabolism *Barbara Lieder, University of Vienna, Dep. of Nutritional & Physio. Chem. & CDL f. Bioactive Aroma Compounds, Vienna, Austria*
12:30 - 13:45	Lunch break

Session 2: Flavour Generation & Release

Chair: Harald Pichler, Austria

13:45 - 14:20 Keynote lecture
Terpenoid biosynthesis in plants
Harro Bouwmeester, University of Amsterdam, Swammerdam Institute for Life Sciences, Amsterdam, The Netherlands

14:20 - 14:45 Heliotropin preparation by a carboxylate reductase in resting cells
Daniel Schwendenwein, acib GmbH, Graz, Austria

14:45 - 15:10 Flash presentations I (Flavour Generation & Release)

P1 Enhancing (+)-nootkatone production in Pichia pastoris and Saccharomyces cerevisiae through cytochrome P450-mediated conversions
Sandra Moser, Austrian Centre of Industrial Biotechnology, Graz, Austria

P12 The impact of plant proteins on vanilla flavour
Lizeth Lopez Torrez, V MANE Fils, Flavours R& D, Le Bar-sur-Loup, France

P40 Sensory and physicochemical quality attributes of honeys from native plants: a sensometric approach
Eduardo Dellacassa, Facultad de QuÃmica-UdelaR, Laboratorio de BiotecnologÃa de Aromas, Montevideo, Uruguay

P50 Unravelling the effects of interindividual variability of human saliva (flow and composition) on aroma compounds
Carolina Muñoz-González, Centre des Sciences du Goût et de l'Alimentation, UMR1324 INRA, UMR626, Dijon, France

P29 Revisiting the role of glycosidic aroma precursors on wine aroma: effects of microorganisms and of slow hydrolytical processes
Ines Oliveira, University of Zaragoza, Analytical Chemistry, Zaragoza, Spain

15:10 - 16:30 **Poster Session 1** - **Poster Set A** & Coffee break
Coffee break sponsored by AKRAS FLAVOURS GmbH

Session 2 continued: Flavour Generation & Release

Chair: Elisabeth Guichard, France

16:30 - 16:55	Two distinct volatile biosynthetic pathways are linked through alcohol acyl transferase 1 in apple fruit *Ross Atkinson, The New Zealand Institute for Plant & Food Research Limited, Auckland, New Zealand*
16:55 - 17:20	Microbial production of novel C11-terpenes *Jens Schrader, DECHEMA Research Institute, Industrial Biotechnology, Frankfurt-Main, Germany*
17:20 - 17:45	Shedding light on the modulation of key Riesling wine aroma compounds in a changing climate *Josh Hixson, The Australian Wine Research Institute, Urrbrae, Australia*
17:45 - 18:10	Flavor composition of cheddar cheeses made from different milk sources and heat treatments *Elizabeth Tomasino, Oregon State University, Food Science & Technology, Corvallis, USA*

Free evening

Wednesday, 20.9.2017

Session 2 continued: Flavour Generation & Release

Chair: Don Mottram, UK

08:30 - 08:55	From culinary chemistry to food-grade and high-yield generation of Maillard-derived taste modulators in NADES *Thomas Hofmann, TU Munich, Food Chemistry and Molecular Sensory Science, Freising, Germany*
08:55 - 09:20	Changes in key aroma compounds during cocoa powder process *Ondrej Novotny, Nestec Ltd., Nestle Product Technology Center Beverages, Science and Technology, Orbe, Switzerlan*
09:20 - 09:45	A food revolution powered by heme *Celeste Holz-Schietinger, Impossible Foods, Redwood City, CA, USA*
09:45 - 11:15	**Poster Session 2 - Poster Set A** & Coffee break Coffee break sponsored by AUSTRIA JUICE GmbH

Session 2 continued: Flavour Generation & Release

Chair: Christian Lindinger, Austria/Switzerland

11:15 - 11.40	Flavour release from wine glycosides during tasting *Mango Parker, The University of South Australia / The Australian Wine Research Institute, Adelaide, Australia*
11:40 - 12:05	New insight on the role of the oral mucosa in aroma release *Francis Canon, INRA - CSGA, Dijon, France*
12:05 - 12:30	Understanding fat, protein and saliva impact on aroma release from flavoured ice creams *Charfedinne Ayed, Institute National De La Recherche Agronomique (INRA), Centre for taste and feeding behaviour, Dijon, France*
12:30 - 13:50	Lunch break

Session 3: Flavour and Off-Flavour of Non-Food Products

Chair: Erich Leitner, Austria

13:50 - 14:25	Keynote lecture Odorants in non-food products - is there more to them than just smell? *Andrea Büttner, Fraunhofer Institute for Process Engineering and Packaging, Sensory Analytics, Freising, Germany*
14:25 - 14:50	The toilet maldodor challenge *Christian Starkenmann, firmenich, analytical innovation, Geneva, Switzerland*
14:50 - 15:15	Key odorants in the artificial leather of car interiors *Martin Steinhaus, Deutsche Forschungsanstalt für Lebensmittelchemie (German Research Centre for Food Chemistry), Freising, Germany*
15:30 - 17:00	**Guided Tour** through the historic centre of Graz
17:00 - 22:00	**Styrian Delicatessen Fair** Courtyard of the Chemistry Building, Kopernikusgasse 24

Thursday, 21.9.2017

Session 4: Flavour Perception & Psychophysics

Chair: Klaus Dürrschmid, Austria

08:30 - 09:05	Keynote lecture Influence of genetic variation on flavour perception *John Hayes, The Pennsylvania State University, Sensory Evaluation Center, University Park, USA*
09:05 - 09:30	Investigating liking and perception of non-nutritive sweeteners according to taste genotype *Lisa Methven, University of Reading, Food and Nutritional Science, UK*
09:30 - 09:55	A human odorant receptor for food-relevant pyrazines *Patrick Marcinek, Deutsche Forschungsanstalt für Lebensmittelchemie - Leibniz Institut, PBIII - Physiologie, Freising, Germany*
09:55 - 11:15	**Poster Session 3** - **Poster Set B** & Coffee break Coffee break sponsored by IONICON Analytik GmbH

Session 4 continued: Flavour Perception & Psychophysics

Chair: Dietmar Krautwurst, Germany

11:15 - 11:40	The robustness of aroma-induced taste enhancement in foods *Peter de Kok, NIZO food research, Flavour & Texture, Ede, The Netherlands*
11:40 - 12:05	Valence, and its modulatory role in mediating the effects of visual and auditory stimuli on taste *Qian Wang, University of Oxford, Department of Experimental Psychology, Oxford, UK*
12:05 - 12:30	The perception of odor mixtures: the next challenge in flavor analysis *Thierry Thomas-Danguin, Centre des Sciences du Goût et de l'Alimentation, INRA, CNRS, AgroSup Dijon, Université Bourgogne Franche-Comte, Dijon, France*
12:30 - 13:45	Lunch break

Session 5: Industry related Flavour Issues

Chair: Tomas Davidek, Switzerland

13:45 - 14:20	Keynote lecture Safety assessment of flavourings in the European Union *Karl Heinz Engel, Technical University Munich, Chair of General Food Technology, Freising, Germany*
14:20 - 14:45	Impact of Nagoya Protocol on flavour research *Robin Clery, Givaudan AG, Flavour Science, Dübendorf, Switzerland*
14:45 - 15:10	Acetals in food flavourings *Jan Petka, Austria Juice, R& D, Allhartsberg, Austria*
15:10 - 16:30	**Poster Session 4 - Poster Set B** & Coffee break

Session 5 continued: Industry related Flavour Issues

Chair: Jan Petka, Austria

16:30 - 16:55	Trends in flavour research - a food industry perspective *Imre Blank, Nestle Research Center, Lausanne, Switzerland*
16:55 - 17:20	Effect of muscle, ageing and packaging on marker volatiles for beef flavour *Linda Farmer, Agri-Food and Biosciences Institute, Food Research Branch, Belfast, UK*

17:20 - 17:45 Flash presentations II (mixed topics)

P94 Impact of enzyme treatment on flavour of aronia juice
Mari Sandell, University of Turku, Functional Foods Forum, Turku, Finland

P78 The role of salivary proteome in salt sensitivity
Theresa Stolle, Technical University of Munich, Chair of Food Chemistry and Molecular Sensory Science, Freising, Germany

P76 Biotransformation, transmission and excretion processes of garlic odorants in humans: impact on human milk, urine and exhaled
Laura Scheffler, Friedrich-Alexander-University, Chemistry and Pharmacy, Erlangen, Germany

P77 Flavor peptides of Takifugu obscurus and Takifugu rubripes from China
Yuan (Raymond) Liu, Shanghai Jiaotong University, Department of Food Science and Technology, Shanghai, China

19:30 **Conference Dinner**
Old University Graz
Hofgasse 14

Friday, 22.9.2017

Session 6: Recent Developments in Analytical Techniques

Chair: Andy Taylor, UK

08:30 - 09:05	Keynote lecture Measuring smell - challenges and strategies *Erich Leitner, Graz University of Technology, Institute of Analytical Chemistry and Food Chemistry, Graz, Austria*
09:05 - 09:30	PARADISe - a ground-breaking tool to treat complex GC-MS datasets *Mikael Agerlin Petersen, University of Copenhagen, Department of Food Science, Frederiksberg, Denmark*
09:30 - 09:55	Exploring 2-acetyl-1-pyrroline loss by high resolution mass spectrometry and nuclear magnetic resonance *Bethany Hausch, University of Illinois at Urbana-Champaign, Food Science and Human Nutrition, Urbana, United States*

09:55 - 10:20 Flash presentations III (mixed topics)

P122 Selected Ion Flow Tube Mass Spectrometry (SIFT-MS) for real time flavour analysis- sampling possibilities and automation
David Hera, Syft Technologies Ltd, Middleton, Christchurch 8242, New Zealand

P45 Research on the aroma characteristics and impacts of the non-volatile matrix composition on the aroma release of Vidal icewine based on sensomics
Yue Ma, Jiangnan University, Biotechnology, Wuxi, P.R.China

P101 Characterization of Odorants in wood
Linda Schreiner, Fraunhofer Institute for Process Engineering and Packaging, Sensory Analytics, Freising, Germany

P66 Elucidating the mechanisms of individual variation in fat perception and preference
Xirui Zhou, University of Reading, Department of Food and Nutritional Sciences, Reading, United Kingdom

P107 Investigation of odor-active compounds in grapefruit (Citrus paradisi)
Akihiro Kawaraya, Takasago International Corporation, Corporate Research & Development Division, Hiratsuka city, Kanagawa, Japan

10:20 - 10:50 Coffee break

Session 6 continued: Recent Developments in Analytical Techniques

Chair: Jonathan Beauchamp, Germany

10:50 - 11:15	A sophisticated setup for rapid, sensitive and selective food and flavor analysis *Philip Sulzer, IONICON Analytik GmbH., Innsbruck, Austria*
11:15 - 11:40	DOLC-NMR: Differential off-line LC-NMR analysis of nutrient-induced metabolome alterations in S. cerevisiae and their taste impact *Richard Hammerl, TU Munich, Food Chemistry and Molecular Sensory Science, Freising, Germany*
11:40 - 12:05	Process control in flavour generation: NIR-MVA as a tool to monitor key odorants formation *Antonio Cesar da Silva Ferreira, Universidade Catolica Portuguesa - Escola Superior de Biotecnologia, Porto, Portugal*
12:05 - 12:30	End of the Symposium - Closing Ceremony
12:30 - 14:00	Farewell Lunch

SCIENCE AND INNOVATION AT MARS incorporated

Mars has been in business since 1911—and we want to still be thriving another 100 years from now. How are we going to achieve this? Through scientific research and innovation. Our innovation teams are working on transformational projects that could change the way we farm and eat in the future. We have our own network of labs and research facilities, where our scientists conduct fundamental and applied research in flavor science, health & nutrition, food safety science, plant science, materials science and computational science.

COCOA FLAVANOLS

For more than 20 years, Mars has been conducting research together with several scientific collaborators to advance understanding of cocoa flavanols and their effects on human health.
A significant body of research now shows that cocoa flavanols can promote healthy blood vessel function.

GLOBAL FOOD SAFETY CENTER

Our Global Food Safety Center opened in September 2015 in Huairou, China. The aim is to increase understanding and raise food safety standards on a global scale through research, training, and knowledge sharing.

CONSORTIUM FOR SEQUENCING THE FOOD SUPPLY CHAIN

Mars, IBM and other partners recently began sequencing microbial DNA and RNA samples from entire food supply chains to establish what normal microbial communities look like. Food companies will be able to use this data to spot deviations from the norm and prevent food safety issues before they occur.

AFRICAN ORPHAN CROPS CONSORTIUM

A consortium co-founded by Mars is currently sequencing the genomes of 101 African crops previously neglected by research and development. Plant breeders will use the results to breed varieties that are higher yielding, more nutritious and more resilient.

FOR MORE INFORMATION, VISIT MARS.COM

Poster Program

There will be two sets of posters. During the announced poster sessions, the organisers kindly ask the presenting authors to be present at their posters for discussion with other conference attendees.
Authors with posters in Poster set A are kindly asked to remove their posters by Wednesday afternoon, at the latest to make the boards available for authors with posters in poster set B. Posters that are not removed until Wednesday evening will be removed by members of the organising committee and can be collected at the registration desk.

Poster Session

Poster set A	Posters with **ODD** poster numbers Tuesday, September 19, 2017, 15:10-16:30 Wednesday, September 20, 2017, 9:45-11:15
Poster set B	Posters with **EVEN** poster numbers Thursday, September 21, 2017, 9:55-11:15 Thursday, September 21, 2017, 15:10-16:30

Best Poster Awards

Two posters per session will be awarded.

(i)	Two posters will be selected as best posters by the scientific committee (one per poster set)
(ii)	'Audience award': Selected by all conference attendees Please select your personal best poster per session and use the voting cards that you find in your conference bag. blue card: to vote for your favoured poster from poster set A green card: to vote for your favoured poster from poster set B Please leave your cards in the boxes at the registration desk.

The posters will be awarded in the course of the conference dinner on Thursday evening.

Flavour Generation and Flavour Release

P 001 **Aroma Active Compounds of Pontianak Orange**
Dharmawan J, Curran P

P 002 **Screening of yeast strains with flavour potential for meat products under reduced concentration of preservative nitrifying agents**
Flores M, Moncunill D, López-Díez JJ, Belloch, C

P 003 **New insight into the role of free amino acids upon coffee roasting**
Poisson L, Auzanneau N, Schaerer A, Mestdagh F, Blank I, Davidek T

P 004 **Modifications of raw beef odor under different periods of retail display**
Lopez R, Espada L, de la Fuente A, Escudero A, Bueno M, Resconi V C, Campo M M

P 005 **Identification of odor-active trace compounds in roses and fruits**
Ohashi T, Miyazawa Y, Shibuya T, Ishizaki S, Kurobayashi Y, Saito T

P 006 **Characterisation of aroma active compounds in horseradish (Armoracia rusticana)**
Kroener E-M, Buettner A

P 007 **Effect of nitrate reduction on dry fermented sausage aroma during vacuum storage**
Perea-Sanz L, Belloch C, Flores M

P 008 **Shelf-life model: Useful tool to predict sensory and nutritional quality of infant formulas**
Kersch C, Vossenberg P, de Wit R, Timmermans W, Cruijsen H, Rallapalli J, Deckers P

P 009 **Milk fat globule membrane and its role in flavour development in cheese during ripening**
Haddadian Z, Eyres G T, Bremer P J

P 010 **The effect of sugar type on VOC generation in a model baked system**
Silcock P, Brecheteau J, Toupin L, Heenan S

P 011 **Understanding the role of sodium in biscuits**
Ayed C, Lim M, Macnaughtan W, Linforth R, Fisk I D

P 012 **The impact of plant proteins on vanilla flavour perception**
Lopez Torrez L, Van Belzen L, Michalet M, Janinet O

P 013 **Decoding the Unique Peaty Aroma of Islay Scotch Single Malt Whisky by Means of the Sensomics Concept**
Mall V, Schieberle P

P 014 **Flavour generation from microalgae in mixotrophic cultivation**
Santos A B, Vieira K R, Pinheiro P N, Paulino B N, Bicas J L, Jacob-Lopes E, Zepka L Q

P 015 **Unraveling the complexity of savory biohydrolysate using a holistic sensory-analytical approach**
Arne Glabasnia, Joséphine Charve

P 016 **Enhancing (+)-nootkatone production in Pichia pastoris and Saccharomyces cerevisiae through cytochrome P450-mediated conversions**
Moser S, Wriessnegger T, Emmerstorfer-Augustin A, Wimmer-Teubenbacher M, Engleder M, Leitner E, Müller M, Schürmann M, Mink D, Pichler H

P 017 **Effects of Drying Methods on the Composition of Volatile Compounds in Fruits and Vegetables**
Karabacak A Ö, Özcan Sinir G, Çopur Ö U

P 018 **In Vivo Flavor Release From Foods**
Karabacak A Ö, Özcan Sinir G, Suna S

P 019 **Wine aroma persistence during wine intake is affected by differences in human oral physiology and on wine matrix composition**
Pérez-Jimenez M, Rocha-Alcubilla N, Chaya C, Pozo-Bayón M A

P 020 **Unexpected pungent effects from aldol products of hydroxymethylfurfural**
van der Schatte Olivier A, Kaouas A, Winkel C

P 021 **Aroma-active compounds in canned tuna fish by aroma extract dilution analysis**
He F, Qian Y P, Dewitt C, Qian M C

P 022 **Formation of volatile compounds and carotenoids degradation products in red pepper fermented by Lactobacillus parabuchneri**
Lee J Y, Lee S M, Kim Y-S

P 023 **Extrusion on aroma compounds in brown and polished rice**
He F, Qian Y P, Zhang Y, Zhang M W, Qian M C

P 024 **Citral-like Thiophenes in Chicken Thigh Meat**
Cannon R J, Curto N L, Esposito C M, Payne R K, Agyemang D O, Cai T

P 025 **Aroma profiles and proximate composition of Roselle seeds: Effects of different origin and different sample preparation methods**
Juhari N H, Juhari N H, Petersen M A

P 026 **Effects of Sodium Chloride, Potassium Chloride and Calcium Chloride on the Flavor Formation during Heating of Wheat Flour-Glucose Model System**
Kocadagli T, Balagiannis D, Gökmen V, Parker J

P 027 **An assessment of the effect of cinnamon spice on cocoa nibs (Theobroma cacao L.) - An approach to change flavor in stored roasted cocoa nibs**
Escalante M, Meerdink G, Umaharan P

P 028 **Impact of Water-Soluble Precursors Leaching from Green Beans on Aroma Generation during Coffee Roasting**
Liu C, Yang N, Linforth R, Fisk I D

P 029 **Revisiting the role of glycosidic aroma precursors on wine aroma: effects of microorganisms and of slow hydrolytical processes**
Oliveira I, Ferreira V

P 030 **Organoleptic properties of dark chocolates investigated by direct-injection mass spectrometry (PTR-ToF-MS) and GC-Olfactometry**
Deuscher Z, Andriot I, Gourrat K, Sémon E, Repoux M, Guichard E, Preys S, Boulanger R, Labouré H, Le Quéré J-L

P 031 **Elucidation of the pattern of volatile compounds responsible of the odor profile in a fermented meat product (chorizo) during ripening time.**
Carmona-Escutia R P, Escalona-Buendía H B, Villanueva-Rodriguez S J, Ponce-Alquicira E

P 032 **Influence of salt reduction on flavour release in ready-to-eat meal**
Rannou C, Texier F, Courcoux P, Cariou V, Prost C

P 033 **Apple Flavour Characterisation from Skin to Flesh - On Basis of the Old Apple Variety 'Ilzer Rose'**
Tauber I, Innerhofer G, Leitner E, Siegmund B

P 034 **Analytical mapping of a Swiss Gruyère Cheese to highlight the distribution of aroma compounds using HS-ITEX-GC-MS-PFPD**
Fuchsmann P, Tena Stern M, Guggenbühl B

P 035 **Aronia melanocarpa - the Styrian 'Super-Berry' - A Flavour Characterization of Black Chokeberry NFC Juice**
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Abstracts Oral Presentations

[O 01] Olfactory loss and neuroplasticity

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Anosmia, the complete loss of odor perception, is a common disorder that has far reaching consequences on everyday life, particularly on nutritional health and personal safety and overall well-being. For the visual and auditory senses, an array of studies has reported on neuronal reorganization processes after sensory loss. In contrast to this, neuroplasticity processes have been investigated only scarcely after loss of the olfactory sense. Neuroimaging magnetic resonance techniques offer the opportunity of capturing different characteristics of the brain, such as morphology, functional connectivity, metabolism and structural connectivity. In the past, those modalities have served a great part in understanding the neural pathways of the human brain in health and disease. The huge potential that lies in these data, is the combination of the modalities coupled with behavioral and clinical measures. Based upon its special characteristics, the olfactory system allows the investigation of functional networks in patients with smell loss. In the future this knowledge of neuroplasticity effects of olfactory loss and regain combined with new biobehavioral measures have the potential to offer new approaches into personalized medical treatment of patients with olfactory dysfunction.

[O 02] Taste Receptors and Upper Airway Immunity

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Taste receptors were first identified on the tongue, where they initiate a signaling pathway that communicates information to the brain about the nutrient content or potential toxicity of ingested foods. However, recent research has shown that taste receptors are also expressed in a myriad of other tissues, from the airway and gastrointestinal epithelia to the pancreas and brain. The functions of many of these extra-oral taste receptors remain unknown, but emerging evidence suggests that taste receptors in the airway are important sentinels of innate immunity. We will discuss our recent findings demonstrating that a subset of bitter taste receptors expressed in human ciliated cells regulate rapid nitric oxide production in response to microbial factors. We have also demonstrated that bitter and sweet taste receptors expressed in human sinonasal solitary chemosensory cells regulate a complimentary arm of innate immunity, the release of antimicrobial peptides. Lastly, common genetic polymorphisms of the taste receptor genes that render these receptors non-functional appear to result in a weakened respiratory innate defense contributing to therapeutically recalcitrant upper respiratory infections.

[O 03] Bitter taste: prediction, relation to toxicity, and effect on emotions

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The bitter taste sensation in humans is elicited by molecules of widely varying chemical structure, summarized in BitterDB http://bitterdb.agri.huji.ac.il/dbbitter.php. This enables us to explore the bitter chemical space: Are there chemical properties of a compounds that predict if it is bitter or not? Are all bitter compounds toxic? Does bitter taste impart emotional effects compatible with signaling danger?
We developed a machine-learning (decision trees-based) tool BitterPredict that correctly classifies 80% of the compounds in the hold-out test set and in three independent external sets, into bitter and non-bitter compounds. The total charge, the hydrophobic component of the saturated carbons and descriptors of molecular surface are the most important contributors to the classifier. To estimate the bitterness-toxicity paradigm, we analyzed large repositories of toxic compounds. Only 30% of the toxic compounds are either known or predicted to be bitter. In comparison, 70% of FDA-approved drugs, and 10% of compounds found in food are predicted to be bitter. We next used sensory tests with close to 300 participant to examine the effect of oral exposure to bitter compounds (quinine and PROP) on risk-taking behavior and trust measures (no effect was found), and on mood: bitter mouth-rinse led to lower mood scores and the effect depended on perceiving the solution as bitter.
In summary, using BitterDB and BitterPredict we show that the bitterness-toxicity overlap is partial, supporting the idea that activation of bitter taste receptors has physiological roles beyond alerting against poisons. Interestingly, bitter compounds negatively affected emotion as measured by the PANAS mood questionnaire, leading to further questions about bitterness in the context of food consumption.

[O 04] Can cross-modal flavour enhancement modulate appetite and food intake?

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Aroma and taste modalities are key drivers in the perception of food flavour. They can be perceived individually, but when presented together, they can synergistically enhance food flavour through cross-modal flavour enhancement. In complex foods, this play a significant role in regulating food liking and enjoyment. Food liking is known to regulate hunger and appetite but to date there has been no systematic study investigating the role of cross-modal (aroma and taste) flavour enhancement on satiety / satiation. In this study the effects of aroma (strawberry aroma) and taste (sugar and citric acid) on appetite sensation and subsequent food intake were studied. When both taste and aroma were consumed together there was a synergistic enhancement in their perceived flavour and the combined flavour suppressed hunger for 20 minutes (over the control sample) from the start of consumption (15 minutes consumption + 5 minutes after consumption had been completed). This study suggests for the first time that cross-modal flavour enhancement modulates short term feelings of hunger.

[O 05] Implicit processing of relaxing- energizing effects of flavors

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'Self-report' measures provide important information about the explicit processing of relaxing/energizing feelings induced by flavors. These direct measures may rely on individual introspective abilities and are subject to biases.
The main objective of this series of studies is to investigate the implicit nature of the relaxing/energizing processing of flavors. Response times were used as indirect measures of relaxing/energizing processing in an adapted version of the implicit association test (IAT). In this IAT, participants were requested to categorize as quickly and accurately as possible relaxing or energizing target words that were presented simultaneously with relaxing or energizing odors. In compatible trials energizing odors were presented with energizing target words (or relaxing odors with relaxing words) whereas in incompatible trials energizing odors were presented with relaxing target words (or relaxing odors with energizing words). We selected odors that were explicitly reported as relaxing or energizing (e.g., vanilla, peppermint or more complex flavors) and they were delivered via a computer controlled olfactometer to record accurate response times. Three types of experiments were conducted for which the target words were associated with the odors associated with their names, the odors alone and their names alone.
Results showed that the participants responded statistically more rapidly in the compatible response blocks (e.g., vanilla and relaxing; peppermint and energizing) than in the incompatible ones, thus confirming the existence of stronger implicit associations between compatible stimuli.
Those results provide evidence that odors-feelings associations are stable enough to influence not only deliberate, but also spontaneous behavior. Furthermore, this convergence between direct and indirect measures is indicative that subjects are able to provide accurate self-reports on their feelings. Moreover, indirect measures could bring some key insights for the prediction of implicit processing when self-report is not enough discriminant which is often the case for pleasant feelings elicited by flavors.

[O 06] Implications of flavor-active compounds for lipid metabolism

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Beyond their actual taste- and aroma activity, flavor-active compounds may have potential health benefits on humans, which has been of increasing research interest in the past years. Beside beneficial effects on mood, immune responses and satiety, also advances have been made for flavor compounds targeting outcome measures of the metabolic syndrome, for example body weight, body fat and type 2 diabetes. In this context, promising effects towards maintaining a healthy body weight and reducing an excess of body fat have been demonstrated for trigeminally active compounds that unfold activity via members of the transient receptor potential (TRP) channels family. In general, TRP channels have been described as the vanguard of our sensory system, responding to ligands, but also to noxious ambient temperatures in order to avoid tissue damage. Well-known representatives of the TRP channel family are TRP-V1, which is responsible for the pungent sensation after the consumption of capsaicin-containing food, and TRP-A1, responding to, e.g., flavoring ingredients of mustard oil. This presentation will review latest advances made with naturally occurring trigeminally active flavor compounds such as capsaicinoids, alkamides, or cinnamaldehyde, and related compounds in regulating mechanisms of lipid metabolism. Studies of our own group have demonstrated a less-pungent TRP-V1 agonist than capsaicin, nonivamide, to impact adipogenesis and fatty acid uptake in cells in culture. In addition, a long-term human intervention study also showed that daily consumption of 0.15 mg nonivamide prevented a dietary-induced body fat gain in healthy, moderately overweight subjects [1]. More recent work also presented that treatment with the alkamide *trans*-pellitorine reduces lipid accumulation in developing adipocytes via targeting TRP-V1. The same study also demonstrated an involvement of the cation channel TRP-A1 in earlier, but not later stages of adipogenesis. This novel role for the TRP channel A1 may also explain the anti-adipogenic potential of cinnamaldehyde, a well-known TRP-A1 agonist and key aroma compound of cinnamon oil, which was demonstrated for cells in culture and in an animal study [2].

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2. Bo Huang, et al. Journal of Agricultural and Food Chemistry 2011 59(8), 3666-3673

[O 07] Terpenoid biosynthesis in plants

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Plants produce terpenoids as a means of communication with and response to the outside world. This includes the production and emission of volatiles to repel harmful or to attract beneficial organisms, such as pollinators and natural enemies of herbivores. But also the secretion of terpenoids from the roots into the soil to attract symbiotic organisms or repel pathogens. Some examples of such relationships will be given. The production of specific signals for friends and the abuse of these signals by enemies has caused an arms race between plants and their enemies which has resulted in the enormous diversity of secondary metabolites present in the plant kingdom. My group studies the regulation of the production of these chemical signals including their structural diversity. This requires that we elucidate biosynthetic pathways and characterize the genes and enzymes that constitute these pathways. With the genes in hand we can use metabolic engineering approaches to change the production of certain terpenoids and study the consequences of these changes for the biology of the plant to try to underpin their biological role. On the one hand, this research on biosynthesis by us and by others has resulted in the elucidation of a multitude of biosynthetic pathways and increasingly better tools to unravel other as yet uncharacterized pathways. On the other, the research on metabolic engineering of plants and micro-organisms, is creating new opportunities for biotechnological production of terpenoids for the flavor, fragrance and pharamaceutical industry. The advances in our understanding of the biosynthesis of terpenoids and their biological role will be discussed, as well as the growing opportunities for the industry to use this knowledge for the (biotechnological) production of economically attractive terpenoids.

[O 08] Heliotropin preparation by a carboxylate reductase in resting cells

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Carboxylate reductases (CARs, E.C. 1.2.1.30) reduce carboxylic acids to the corresponding aldehyde at the expense of ATP for substrate activation and NADPH for the actual reduction. Probably the best known compound which can be produced with a CAR is vanillin [1]. However, this compound is not the only aromatic aldehyde that is accessible with these enzymes. We recently identified and characterized a fungal CAR, which has a relaxed substrate spectrum and is able to generate various aromatic aldehydes from their corresponding acid. We demonstrated the preparation of Piperonal (Heliotropin) from piperonylic acid quantitatively on gram scale. The bioconversion was achieved with a whole cell approach by expressing the CAR in *E. coli* RARE (Reduced Aldehyde REduction) [2]. The cells were subsequently used as resting cells for the bioconversion. Since the enzyme needs two different cofactors, this kind of application allowed us to avoid costly and often difficult to achieve cofactor recycling by utilizing the bacterial recycling system. The product was isolated directly from the reaction mix by extraction with hexane as solvent with a yield of 92% and $>$ 98% purity [3].

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[O 09] Two distinct volatile biosynthetic pathways are linked through alcohol acyl transferase 1 in apple fruit

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Fruit such as apple, banana, kiwifruit, melon and pineapple produce high levels of volatile esters where they contribute characteristic 'fruity' notes to the aroma. In 'Gala' apples, the major odour-active esters are hexyl acetate (fruity, green, apple notes), butyl acetate (ethereal, solvent, fruity) and 2-methylbutyl acetate (2MBA; overripe, fruit, sweet). Phenylpropenes are typically found at much lower levels in fruit, and impart flavour notes associated with aromatic spices. In apple, estragole (anise, licorice notes) is the most widely described odour-active phenylpropene; with eugenol (sweet, spicy, clove) and chavicol (clove, spicy) also being reported. Volatile esters are synthesised via fatty acid degradation or from amino acid precursors with the final step being catalysed by alcohol acyl transferases (AATs). In contrast, phenylpropenes are produced as a side branch of the general phenylpropanoid pathway. We have shown for the first time via genetic, molecular and biochemical analyses that these two distinct pathways are linked through a single enzyme (MdAAT1) in apple [1]. The major QTLs in apple for production of the phenylpropene estragole and volatile esters both co-located with the *MdAAT1* gene. Fruit from transgenic 'Royal Gala' *MdAAT1* knockdown lines produced significantly reduced ester and phenylpropene levels. Biochemical analysis showed that *MdAAT1* was required to produce *p*-hydroxycinnamyl acetates that serve as substrates for a bifunctional chavicol/eugenol synthase (*MdoPhR5*) in ripe apple fruit. Manipulation of the phenylpropanoid pathway using *MdCHS* (chalcone synthase) knockout and *MdMYB10* over-expression lines increased phenylpropene production. Finally we showed that AATs from ripe strawberry and tomato fruit could also utilise *p*-coumaryl and coniferyl alcohols, indicating that ripening-related AATs are likely to link volatile ester and phenylpropene production in many different fruit. These results significantly increase our understanding of volatile synthesis in fruit and provide the basis for breeding new apple varieties with improved flavour profiles by marker assisted selection.

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[O 10] Microbial production of novel C11-terpenes

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The isoprene rule states that all terpenes are composed of the C_5-compounds isopentenyl diphosphate (IPP) and dimethylallyl diphosphate (DMAPP). In this way the substrates and the products of terpene synthases are always composed of a multiple of five carbon atoms [1]. By discovery and elucidation of the reaction mechanisms of a 2-methylisoborneol and 2-methylenebornane synthases the first exception to the isoprene rule and the first C_{11}-terpene synthases were described [2-4].
We set out to further investigate the product spectra of C_{11}-terpene synthases by engineering *Eschericha coli* cells for *de-novo* bioproduction of these compounds. To optimize the carbon flux to the precursor geranyl diphosphate (GPP), genes of the mevalonate pathway and a GPP synthase were overexpressed in *E. coli*. Additionally, genes of a GPP methyltransferase and one of four different C_{11}-terpene synthases were co-expressed in the production strain. Solid phase micro extraction from the headspace of production cultures and subsequent GC/MS-analysis combined with ^{13}C-isotope-labeling revealed diverse product spectra. Beside eight previously described products [3] 23 novel C_{11}-terpenes could be detected. So far the structure of four new C_{11}-terpenes have been elucidated: (*E*)- and (Z)-2-methyl-citronellol, 3,4-dimethylcumene and 2-methylnerol.
The odours of the new C_{11}-derivatives differ clearly from those of the corresponding conventional monoterpenes. Making available naturally methylated monoterpenes, the diversity of this important flavour and fragrance class is increased considerably. Enzyme engineering will allow to further adjust the product spectra of the synthases. Furthermore, high-yielding microbial production strains may offer a sustainable supply of these compounds from cheap renewable feedstocks via fermentation. The C_{11}-terpenes could add interesting new notes to aroma and scent compositions made in the flavour and fragrance industry.

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[O 11] Shedding light on the modulation of key Riesling wine aroma compounds in a changing climate

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Riesling is among the most significant white grape varieties globally, with much of Riesling cultivated in Germany (44 % of global production) and Australia (10 %). Recognized as a floral variety, typical young Riesling wine aroma is dominated by monoterpenes, however as Riesling ages the development of 1,1,6-trimethyl-1,2-dihydronaphthalene (TDN) can lead to a distinct 'kerosene' or 'petrol' note. The production of TDN, and indeed a host of other volatile carotenoid breakdown products, can be modulated by the environmental factors encountered during the growing season resulting in remarkably different wine aroma profiles. A partnership between L'Institut des Sciences de la Vigne et du Vin, **B**ordeaux, the **A**ustralian Wine Research Institute (AWRI), and Hochschule **G**eisenheim (BAG alliance), has allowed researchers in Australia and Germany to collaboratively investigate how environmental factors impact the development of such a key aroma compound in Riesling wine. This presentation will detail the role that light exposure can play on the concentration of important aroma compounds and related glycosidic analogues, in the context of a potential climatic shift towards 2 °C hotter growing conditions.

Treatments were applied to modulate grape bunch light exposure in two Riesling vineyards, situated 14 km apart with an approximate 2 °C difference in Mean January Temperature (MJT). Chemical data from vintage 2015, showed significantly different levels of TDN, linalool and b-damascenone in grapes where light exposure was modulated. But no major variance between the vineyards, despite differences in MJT and viticultural management practices. Carotenoid quantification in the developing grapes also showed differences for a number of carotenoids, which are known to give rise to TDN. Preparatory HPLC followed by LC-MS/MS assessment of fractions has provided a tentative assessment of the glycosidically bound TDN derivatives present in grapes, which have the potential to give rise to TDN during storage and ageing.

Different light modulating treatments were assessed in further viticultural experiments. Agricultural sprays designed to protect from UV radiation and shade cloth were used to limit light exposure, and hence TDN production in both vineyards, with significant changes to the grape and wine composition observed for some light modulating treatments.

[O 12] Flavor composition of cheddar cheeses made from different milk sources and heat treatments

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Terroir is a term that builds off the idea that a food's organoleptic properties are defined by the environment, climate, and production practices. The impact of *terroir* and heat treatment effect on *terroir* to Oregon cheddar flavor were explored. Cheddar was produced with raw and low-temperature long-time (LTLT) pasteurized milk at Oregon State University. Milk was sourced from three individual farms (Dallas, Lafayette and Corvallis) with similar herd management systems and two comingled sites in different eco-regions of Oregon (Coastal and High Desert). Milk collection occurred within a four week period while the Jersey herds were on a pasture-based diet. Cheddar was aged at 5°C and samples were extracted at five and nine months of aging. Flavor compounds were analyzed using Gas-Chromatography Mass-Spectrometry (GCMS). At five and nine months 45 and 30 flavor compounds were identified respectively. Principle component analysis (PCA) showed that samples were separated based on milk source location and for many compounds a location by treatment interaction occurred. At five months cheeses were very clearly differentiated by location. Differentiation by milk origin still occurred at 9 months with the Coastal raw cheese very different from all other cheeses. Heat treatment had a greater impact at 9 months than 5 months, with several compounds showing a significant treatment by location interaction. Results suggest that the flavor of cheddar is impacted by terroir even when a heat treatment is used and suggest that *terroir* is part of what characterizes a Cheddar cheese.

[O 13] From culinary chemistry to food-grade and high-yield generation of Maillard-derived taste modulators in NADES

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The development of healthier food products, for example, reduced in fat, sugar, or salt, respectively, is well-known to induce nonacceptable flavor defects in the products and has, thus, created unexpected flavor challenges for the food industry. In response to the consumers demand for healthy but tasty foods, novel ingredient discovery is essential to overcome such flavor challenges associated with the production of, in particular, sugar, salt or fat-reduced products. Varying widely across the world, reflecting unique environmental, economic, and cultural traditions, various drying, fermentation, cooking and roasting procedures have been empirically developed during the last millenniums and, since then, the alluring flavor of the dishes prepared do attract consumers on a global scale. In particular, the food manufacturing techniques leading to the most premium tastes promise to contain essential taste compounds and/or taste modulators generated from sensory inactive precursors upon processing of the raw materials. This evolutionary refinement of food manufacturing procedures is, therefore, expected to open an interesting avenue towards the discovery of natural orosensory modulators, which might be applied as natural solutions to enhance culinary authenticity of convenience products or to overcome flavor challenges associated with the production of, in particular, sugar, salt or fat-reduced products. The presentation will highlight the identification of taste modulators in processed food by means of a Sensomics approach and present novel approaches for the food-grade and high-yield production of taste enhancers ex-food, e.g. by using natural deep eutectic solvents (NADES).

[O 14] Changes in key aroma compounds during cocoa powder process

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Flavour character of cocoa powder originates from genotype and origin of cocoa tree, post-harvest treatments (e.g. fermentation and drying) and from the manufacturing processes such as alkalization, roasting and pressing.
Changes in key aroma compounds during the cocoa bean roasting [1] as well as the impact of alkalization-roasting interaction [1, 2] on the aroma content were described. Yet, there is no comprehensive study clarifying the origin of key cocoa odorants in whole cocoa powder process. Moreover, majority of reported studies were performed under laboratory conditions that do not exactly match the conditions of industrial process.
To extend our knowledge, content of 15 key cocoa odorants was quantified in different stages of cocoa powder process, i.e. in raw fermented cocoa nibs, in cocoa nibs after the alkalization, in cocoa nibs after the roasting, and finally in cocoa powder and cocoa butter obtained after the pressing of cocoa mass. The study was conducted in parallel in two scales using laboratory equipment (1.5 kg batch) as well as pilot plant facilities (15 kg batch).The objective of the study was to evaluate the contribution of intrinsic aroma content of fermented cocoa and the impact of individual processing steps on the aroma content in cocoa powder. In addition, impact of the scale (batch size) on the origin of the odorants was assessed.

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[O 15] A Food Revolution Powered By Heme

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Raising animals for food is the most environmentally destructive industry. However, for thousands of years and in cultures all around the globe, humans have had the desire to eat meat, and the demand for meat is only rising. To date, meat substitutes have tried to mimic the flavor of meat through the use of flavor additives - e.g. isolated or synthesized aroma compounds, processed flavors from high temperature reactions, and/or herbs and spices. In all of these cases, the added flavors are incorporated into the product as the final cooked flavor. But these products have failed to appeal to the larger consumer population that is accustomed to eating meat. In order to feed the growing human population with its love for meat at the same time as we turn the clock back on climate change, we need new solutions. Our approach was to examine the flavor-generating processes and components in meat, and then to apply these learnings to create a plant-based beef burger that has the same desirable flavors of beef-particularly during and after cooking.
The heme cofactor is an iron-containing porphyrin found in myoglobin and hemoglobin, the two proteins in mammals that are responsible for the red color. And we discovered that heme proteins lead to the metallic flavor of raw meat and upon cooking, heme proteins act as a catalyst to generate hundreds of aroma compounds from their structural precursors-simple nutrients like sugars, amino acids, and vitamins. These aroma compounds are responsible for meat flavor: they bind to the olfactory receptors in our nose, and our brains integrate these hundreds of signals into a distinct perception of the identity of the meat, as well as our pleasure response to the experience. Excitingly, we discovered that heme proteins in plants are also capable of meat aroma generation activity; one example is leghemoglobin from the root nodules of soybeans. Our research shows how heme proteins are the catalyst for the flavor transition in meat: upon cooking, the bland and metallic flavors of the raw state are transformed into the roasted, caramelized, meaty, gamey, and nutty flavors of the cooked state. Our newly identified plant based flavor system enable the creation of meat products that carnivores crave with a fraction of the environmental impact; opening up the possibility to feed our growing human population while expanding forested land, increasing freshwater, and reversal of greenhouse gases.

[O 16] Flavour release from wine glycosides during tasting

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Grape-derived glycosides contribute some of the most important varietal characteristics to the aroma of wine, with volatiles released from glycosides during fermentation, processing and storage. Wine can retain high concentrations of these non-volatile flavour precursors. Juice and wine made from aromatic varieties such as Gewurztraminer and Riesling are particularly rich in glycosides of the monoterpenes geraniol, linalool, nerol and alpha-terpineol. Monoterpene glycosides were analysed directly by LCMS, and a range of wines surveyed. Glycosides from these varieties were extracted and purified to remove phenolics and free volatiles, and extensively characterised. GCMS analysis following beta-glucosidase enzyme hydrolysis, hydrolysis by human saliva, and analysis of breath after tasting glycosides showed that monoterpene glycosides can release monoterpenes upon hydrolysis in vivo and in vitro. The possibility that this hydrolysis could contribute to flavour via retronasal odour perception was investigated in a series of sensory experiments. Time-intensity sensory studies showed that significant fruity flavour resulted from assessors tasting pure glycosides, as well as glycosides isolated from wine, when tasted in model wine at elevated concentrations. The effect was not significant at wine-like concentrations. However, there was substantial variability in response to glycosides, with about half of the panel reporting flavour from the glycosides. A larger study of 39 people showed that 77% could reproducibly detect flavour from at least one glycoside, from several different glycosides assessed over a number of days. Close examination of the results revealed a complex pattern of response. This study has provided evidence that non-volatile glycoconjugates can contribute previously unrecognised flavour during tasting, as well as contributing to aftertaste, a sought-after aspect of wine quality.

[O 17] New insight on the role of the oral mucosa in aroma release

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When you are drinking a glass of wine, you perceive aroma over a certain length of time. A greater length is generally considered as a positive organoleptic characteristic of food products. This phenomenon, called aroma persistence, is generally thought to be due to a two-stepped mechanism. In a first step, aroma compounds adsorb onto the oral mucosa, then, in a second step, they are released before reaching the olfactory receptors. If the persistence of aroma release from the buccal cavity has been demonstrated, the molecular mechanisms involved in adsorption onto the oral mucosa are still unclear.The aim of the present study is to gain a deeper understanding on these mechanisms.
We mimicked the *in vivo* condition using an innovative model of oral mucosa, taking into account for the first time the thin layer of salivary proteins covering the mucosal pellicle, called the mucosal pellicle. Interestingly, it has been reported that some salivary proteins have the ability to interact with aroma compounds and modify their release. Therefore, aroma adsorption onto the mucosa could be due to the binding of aroma compounds onto this layer of salivary proteins. Fifteen aroma compounds representing different chemical families and a large range of physico-chemical properties have been introduced in the presence of the oral mucosa model. Their release has been studied both in static and dynamic conditions using GC/FID and PTR-MS.
Static headspace analysis revealed a decrease of aroma compounds release in the presence of the oral mucosa depending on their molecular structure. This effect may be attributed, in part, to the ability of oral mucosa to metabolize aroma compounds. Both oxidation and reduction of aroma compounds by the epithelial cells have been observed depending on their structure.
In parallel, dynamic experiments have shown that the mucosa can also modify the kinetic of release of aroma compounds depending also on their structure.
The result revealed that molecules with a higher log P value are more affected.The present results give a new insight on the role of oral mucosa on aroma release and on aroma persistence.

[O 18] Understanding fat, protein and saliva impact on aroma release from flavoured ice creams

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Ice cream is a complex aerated emulsion composed, amongst other, of protein and fat which play an important role in the stabilisation of its structure, flavour release and perception. In the present study different ice creams were made by varying fat and protein, type and level. The release of fourteen aroma compounds was followed using a saliva reactor [1] allowing temperature control and addition of human saliva. The effect of fat type and fat level on either aroma release or sensory perception in ice creams has been the subject of different studies [2]. It demonstrated that a modification of fat type and level induced differences in the perceived rate of melting and in flavour release of different aroma compounds which were partly explained by hydrophobicity. Proteins on the other hand are known to interact with aroma compounds according to both the nature of aroma and the nature of the protein [3]. Even if general trends of flavour release from ice cream during eating have already been reviewed [4], these do not necessarily explain the differences observed in perception. In the present study the outcome was expected to reproduce as faithfully as possible the principal phenomena occurring in the mouth during eating (i.e. stirring, saliva flow, and temperature) by using data from real measurements in subjects consuming the same products. The obtained results, clearly showed an effect of the addition of saliva in ice creams with a high fat level. Of particular interest, the significant effect of fat on the initial rate of release was overserved as function of flavour compounds physical chemical properties, where the LogP was also not enough to justify the obtained differences. The combined effects of food composition, human saliva and aroma physical chemical properties on the release of a wide range of aroma compounds from ice creams were determined. This work will provide innovative tools to guide food industries to reformulate ice-creams with less fat while maintaining their sensory acceptability.

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[O 19] Odorants in non-food products - is there more to them than just smell?

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Contemporary products often emanate unusual or unpleasant smells that people are repeatedly confronted with in their everyday lives [1,2,3]. As with many unpleasant smells, consumers might be concerned over associated health risks, yet equally, an increasing number of consumers no longer react to such warning signals due to their belief that some smells, for example, 'plastic', are entirely normal and should not be a cause for concern. In most cases, such smells indeed might be simply harmless by-products of production processes that dissipate quickly after purchase. Conversely, however, odourless is not synonymous with harmless.The continual development and global ubiquity of contemporary materials and associated products presents an increasingly pressing need to monitor and control their quality. In view of this it is interesting to note that the issue of non-intentionally added substances (NIAS) has received increasing attention in product quality control screenings [4,5]. This lecture will present an overview of odorous artefacts associated with the modern materials and products including those derived from wood, plastics, polymers, regrinds, colouring agents, glues, adhesives and binders. Knowledge of the underlying chemical structures of contemporary smells provides an essential basis to elucidate their formation pathways and is a primary premise for the development of targeted avoidance strategies. The presentation will explore the challenges relating to how emissions from such products can be monitored [6] and will discuss analytical risk assessment strategies for those who are exposed to such odorous emissions, not only consumers, but also people that regularly handle such products vocationally.

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[O 20] The toilet malodor challenge

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Firmenich joined the project of the Bill & Melinda Gates Foundation initiative about reinventing the toilet challenge. At the same time, a receptor based discovery of malodor antagonists was developed to bring to market affordable and effective toilet cleaning and freshening products. Globally 2.5 billion people have no access of proper sanitation. When integrated into cleaning products, and used as part of a regular hygiene and maintenance regime, our malodor counteracting technologies aim to promote sanitary environments.
This presentation will focus on the malodor analysis. It will explain how pit latrine headspace analyses were performed in crowded slums in Africa and India. From the dozens of diverse volatiles found, a rigorous sensory analysis allowed us to develop fecal reconstitutions based on 4 molecules. The appreciation of odors (like or dislike) are driven by diverse factors including cultural heritage. We therefore validated this hypothesis through sensory surveys with more than 400 subjects in Switzerland, Africa and India. In the meantime these 4 molecules were used to identify odorant receptors and to screen for their antagonists. From these results, we were able to recreate the exact toilet conditions in terms of temperature, humidity and ventilation in model latrine cabins. These cabins are equipped with devices that deliver malodors, including H_2S and methyl mercaptan. We can concurrently monitor perfume release by solid supported delivery systems gravimetrically, analyze the concentrations of antagonists in the air and conduct sensory analyses.

[O 21] Key odorants in the artificial leather of car interiors

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Car manufacturers are facing an increasing number of consumer complaints about the interior odor of new vehicles. Plastic materials are considered a major source of odor-active compounds. Among them are PVC based artificial leathers, which are widely used as material for seats and covers.To get a deeper insight into the compounds contributing to the characteristic odor of artificial leathers, a representative sample provided by a German car manufacturer was cryomilled and extracted with dichloromethane. Volatiles were isolated by solvent-assisted flavor evaporation and subjected to GC-O and aroma extract dilution analysis [1]. Thirty odor-active compounds were detected in the FD factor range of 1-128, among which 2 compounds revealed high FD factors in combination with a characteristic plastic-like smell. On the basis of their retention indices determined on two GC columns of different polarity (DB-5, FFAP) and their mass spectra recorded by GCxGC-TOFMS analysis, the compounds were tentatively identified as 1-hexen-3-one and acetophenone, and structure assignments were finally confirmed by analysis of reference compounds. A third compound also showing a high FD factor and a mushroom-like smell was identified as 1-octen-3-one.Using ($^2H_2$)-1-hexen-3-one, ($^2H_4$)-1-octen-3-one, and ($^2H_5$)acetophenone as internal standards, the concentrations of 1-hexen-3-one, 1-octen-3-one, and acetophenone in the artificial leather were determined by stable isotope dilution assays. An odor reconstitution model based on the 3 compounds dissolved in a lipophilic matrix in exactly the concentrations determined clearly exhibited the typical odor of the artificial leather. Omission tests showed that 1-hexen-3-one contributed most to the overall odor, but 1-octen-3-one and acetophenone modified the sensory impression of the mixture.

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[O 22] Influence of genetic variation on flavour perception

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At the December 1931 meeting in New Orleans for the American Association for the Advancement of Science (AAAS), Albert Blakeslee and Arthur Fox stated: '*Thomas Jefferson said all men are created equal, but he had not tried [phenylthiocarbamide]crystals. Taste tests show people are different. Our world is what our senses tell us. Each [of us]lives in a different world*.' Seven decades later, the molecular mechanism behind 'taste blindness' for certain thiourea compounds was finally elucidated. Over the last 15 years, application of modern psychophysics and molecular genetics have made it clear that this heritable dimorphism is only one of many, some of which are directly relevant to ingredients in the food supply (e.g., *TAS2R31* alleles and sulfonyl amide sweeteners). Nor are these differences restricted to taste, as other sensory modalities involved in flavour perception (i.e., smell, chemesthesis, oral touch) each show genetic variability. This talk will review various molecular mechanisms involved in systematic variation in chemosensation across individuals, and highlight a few key examples across multiple modalities that are relevant to ingestive behavior, food choice, and consumer behavior.

[O 23] Investigating Liking and Perception of Non-Nutritive Sweeteners according to Taste Genotype

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Differences exist between individuals in their liking and perception of sweetness. This study investigates whether variation in taste genotype is a factor that can account for some of these differences, looking specifically at sweetness from the non- nutritive sweeteners sucralose and Rebaudioside A (a steviol glycoside). Single nucleotide polymorphisms (SNPs) of both the sweet taste receptors T1R2 and T1R3 (6 SNPs), and bitter receptors T2R4 and T2R14 (2 SNPs) were investigated. The T1R2/T1R3 SNPs chosen had previously been found to have a significant effect on sweetness liking and perception of natural sugars and the T2R4/T2R14 on bitterness perception of stevia. Additionally, a polymorphism in the Gustin (CA6) gene was included as this has previously been found to significantly affect taste cell proliferation. Liking and intensity perception of apple squash samples varying in concentration of either sucralose or, separately, Rebaudioside A were measured with 62 consumers. Their taste genotypes were identified from DNA extracted form buccal swabs. From both sweetener types, participants could be grouped into different clusters depending on their liking of the samples, and depending on their perception of samples. Significant associations were found between the taste receptor polymorphisms. Liking and perception, of apple squash with both sweetener types, were significantly influenced by taste receptor genotype.

[O 24] A human odorant receptor for food-relevant pyrazines

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Pyrazines are nitrogen-based heterocyclic aromatic compounds that are responsible for a wide array of natural odors, their function ranging from animal- and plant-based intra- and interspecies communication to food-relevant aromas. Currently, there are six pyrazines identified as key food odorants, further emphasizing their importance with regards to human assessment of aromatic quality. Yet, despite their ubiquitous nature, human odorant receptors (ORs) that recognize pyrazines have not been described, so far. Here we present, to our knowledge for the first time, OR5K1 as a strong candidate for human pyrazine perception. By employing our standardized, bi-directional, and high-throughput molecular screening procedure, we identified OR5K1 as the sole and highly responsive OR at 30 μM of 2-ethyl-3,5(6)-dimethylpyrazine and 2,3-diethyl-5-methylpyrazine in a library containing 600 OR genetic variants. These two compounds are amongst the pyrazines with the lowest odor threshold concentrations in the picograms per liter of air range. In our hands they activated OR5K1 each with EC_{50}-values in the low micromolar range. Moreover, a food aroma recombinate (liver) containing 2-ethyl-3,5(6)-dimethylpyrazine at food-typical concentrations activated OR5K1. In summary, our data suggest OR5K1 as a receptor for the chemosensory detection of food-related key-aroma pyrazines.

[O 25] The robustness of aroma-induced taste enhancement in foods

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The consumer interest in healthier food is still growing and with it the demand for low salt and sugar products . These aspirations are not new and many food products have already been reformulated. Sodium salts have been replaced by e.g. potassium salts, taste enhancers, amino acids etc and sugar by sweeteners such as stevia. Technologically, this now has reached its limit, while significant reductions are still demanded. And at the same time, the consumer does not accept any compromise in taste and asks for label-free and natural solutions. This calls for an innovative approach. One option that is hardly exploited yet is the use of cross-modal effects to enhance taste perception. The last decade NIZO food research has invested heavily in exploiting taste enhancement by adopting the texture and aromas of food products.

Although the application of cross-modal effects have been shown to be very attractive, one of the basic questions still needs answering; is the effect stable enough to support long-time application in food products? Batenburg er al. (2011) already showed that trained descriptive panels were able to differentiate between the aroma and the taste effect (salt) which resulted in a loss of the multisensory saltiness enhancement. Native, i.e. untrained panels however, were more suitable for establishing the taste-aroma integration effect. One could expect that consumer would also learn to differentiate between the two different modalities taste and aroma. If so, the strategy would be unsuitable for salt/sugar reduction purposes.

To test the robustness of such cross-modal effects for sweetness enhancing purposes, we used the system developed by Knoop (2011); apple juice sweetness was increased by adding ethyl hexanoate, an odorant synthesized in apples during ripening. To re-confirm that the panel experienced sweetness enhancement, we first monitored the effect of adding ethyl hexanoate to apple juice over repeated exposures during a 6-month period. In a next sequence of exposures, the panellists were given explicit feedback on sucrose-calorie content intermittently in dedicated sessions. After a block of repeated sucrose-feedback sessions, we reverted to the procedure in which no sucrose feedback was given.This lecture will present the results of this study and will discuss the consequences for salt/sugar enhancement strategies using these cross-modal effects.

[O 26] Valence, and its modulatory role in mediating the effects of visual and auditory stimuli on taste

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Recent research demonstrates that taste evaluation of food/beverages can be modulated by means of visual and auditory stimuli such as colours, shapes, and music. The aim of the study reported here was to assess the role of the emotional valence of the extrinsic stimuli in such taste modulation effects. The participants in the present study evaluated samples of mixed fruit juice whilst being simultaneously presented with auditory or visual stimuli of positive or negative valence. The soundtracks had either been harmonised with consonant (positive valence) or dissonant (negative valence) musical intervals. The visual stimuli consisted of images from the International Affective Picture System (IAPS) with matched valence ratings as the soundtracks. Each sample of juice was rated on two computer-based scales: One scale was anchored with the words sour and sweet, while the other scale required hedonic ratings of the sample. Those participants who tasted the juice sample while presented with the positively-valenced stimuli rated the juice as tasting sweeter compared to negatively-valenced stimuli, regardless of whether the stimuli were visual or auditory. These results are discussed in terms of the possible mechanism(s) underlying the auditory modulation of taste.

[O 27] The perception of odor mixtures: the next challenge in flavor analysis

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The olfactory dimension of food flavor is critical to the food identity and typicality. Food odor and aroma result from the processing of complex mixtures of volatiles reaching the sense of smell either orthonasally or retronasally. From a perceptual point of view, such processing allows the recognition and categorization of familiar smells, but also unknown ones, which are encoded as odor objects. The perceptual properties of odor mixtures have been explored from both the aroma analysis point of view and the psychophysical point of view, thus revealing perceptual effects such as masking, synergy, or perceptual blending. However, the neurophysiological mechanisms underpinning the processing of complex mixtures are still to be determined. Whereas the psychophysical approach focused on combinations of two or a few odorants, the aroma analysis approach started with very complex mixtures trying to identify the most contributing single odorants through the GC-MS-O procedure. Nevertheless, considering odorants separately, this approach misses the central role of perceptual integration in odor mixture processing. Therefore, the challenge of food flavor analysis is now to integrate the mechanisms of complex odorants mixture perception, and to develop recombination strategies and tools that could be advantageously included within the aroma analysis path. In this context, this presentation aims to gather the recent findings on the processing of odorants mixtures, thus showing selected examples of flavor analysis and sensory evaluation results, but also data obtained in animal studies, which support the idea that the challenge is now winnable. Indeed it will be highlight that efficient tools and original strategies are already available or under study to go one step forward. Finally, this presentation will emphasize the fact that, beyond the expected results in terms of food flavor analysis, the study of odor mixtures is an original window allowing the investigation of olfaction-specific mechanisms certainly crucial to interpret and afford an efficient representation of our food and more broadly our environment.

[O 28] Safety assessment of flavourings in the European Union

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In the European Union (EU) the regulatory framework for the use of flavourings in and on foods is provided by Regulation (EC) No 1334/2008. The implementation of a Union list, i.e. a list of flavouring substances that are authorized to be used in and on foods to the exclusion of all others, constituted a basic change in paradigm regarding the use of flavouring substances in foods in the EU. Prior to their inclusion in the Union list, flavouring substances had to be subjected to a safety assessment performed by the European Food Safety Authority (EFSA). The applied procedure used a group-based approach, with a decision-tree as central element. It considered information on structure-activity relationships, metabolism, dietary intake and toxicity data. Features, such as unsaturated aldehyde and ketone structures that are considered as structural alerts for genotoxicity, were specifically taken into account.
The established Union list is open-ended and can be amended in the light of scientific and technical developments. An EFSA guidance on the risk assessment of flavourings newly submitted after the adoption of the Union list has been provided. In addition, principles for the safety assessment of flavourings others than flavouring substances have been outlined. This includes, for example, flavouring preparations obtained from material of vegetable, animal or microbiological origin other than food, thermal process flavourings for which ingredients for their production are source materials other than food and/or for which the conditions of their production and/or the maximum levels of undesirable substances set out in Regulation 1334/2008 are not met, or flavour precursors obtained from source materials other than food.

[O 29] Impact of Nagoya Protocol on Flavour Research

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On 12^{th} October 2014 the Nagoya Protocol on *Access to Genetic Resources and the Fair and Equitable Sharing of Benefits Arising from their Utilization* came into effect on being ratified by the 50^{th} party. So, three years after ratification, what has happened and what impact can be expected on commercially orientated flavour research ?
The overall aims and intentions of the Nagoya Protocol are relatively clear in principle; researchers who obtain biological materials from a Nagoya country with ABS legislation in place, and develop and launch a new ingredient based on that research, now have an obligation to establish a benefit sharing agreement with the provider.
However the specific national laws and regulations are often complex and unclear. On the provider side, where national access legislation exists it is variable in its scope and application while the official processes and documentation are still evolving in many countries. On the user side, the EU has enacted the first compliance legislation and is currently working on the guidance documentation and the processes for making the declarations as required by the legislation.
The main impact for those involved in Flavour Research appears to be more paperwork, a need to carry out additional due diligence concerning the origin of natural materials, and in some cases additional agreements or contracts when obtaining biological materials for use in research programs. At present there are many more questions than answers and most of the activity is in the realm of industry associations and corporate legal departments but as the obligations under the EU legislation become clearer it is now beginning to impact at the research laboratory level.
The case studies and examples given in the presentation address some of the common and increasingly urgent questions arising in the Flavour and related industries; Does this affect my research program? Does it apply to all naturals ? What do I have to do? What are the risks of non-compliance?

[O 30] Acetals in food flavourings

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Matching of competitor flavours is one of the most common tasks for the majority of flavour chemists working in a flavour house. It is very obvious to find various artefacts in those flavourings, where carbonyl compounds, alcohols and acids are together part of the recipe. Nevertheless, mass spectra of many of these compounds are not available in the commercial mass spectral databases. We decided to systematically investigate reaction products of 28 carbonyl compounds with the most common solvents used in the flavour industry, ethanol and propylene glycol, by means of gas chromatography - mass spectrometry. In a second study we focused on alcohols and aldehydes naturally occurring in apple FTNFs. In our contribution we will present the results of these studies, we will show typical examples of mass spectra and we will discuss the reactivity of the involved flavouring compounds and stability of acetals and ketals in a standard beverage base.

1. Woelfel, K. and Hartman, T.G.: Mass Spectrometry of the Acetals Derivatives of Selected Generally Recognized as Safe Listed Aldehydes with Ethanol, 1,2-Propylene Glycol and Glycerol. In: Flavor Analysis, Ed. Mussinan, C.J. and Morello, M.J., ACS Symposium Series, American Chemical Society, Washington, 1998, pp. 193-210

[O 31] Trends in Flavour Research - A Food Industry Perspective

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Flavour research has been a key activity in academia as well as in the flavour and food industry. Many key odorants and taste compounds have been identified, their sensory characteristics described, their formation mechanisms studied using thermal and/or bio-assisted approaches, and means for their formulation and release developed. For a long time, discovery of new molecules has been the focus, using analytical and synthetic chemistry, and recently high-throughput receptor-based assays have been designed for the screening of odour- and taste-active components. While identifying new sensorially relevant molecules will remain an area of interest, generating and delivering the desired complex and well-balanced flavour profile by natural and mild processing has become a major focus. Given the global trends in the food and flavour industry, i.e. naturality, organic food, authenticity, transparency as well as 'clean label', etc., it has become essential to revisit the way flavour is imparted in foods and beverages. Flavour addition as commonly used in the past is often not anymore the most preferred option to obtain the desired sensory profile. This may even apply to natural flavours, depending on the food category, customer needs, and consumer expectations. Hence, the food industry requires alternative concepts responding to consumers needs, based on kitchen-type preparations, natural flavour extracts and known ingredients. Furthermore, flavour generation may increasingly become part of food processing and structuring, thus resulting in final food products with desired flavour properties. The talk will elaborate on a few current issues and on how the food industry is transforming challenges into opportunities. Overall, approaches inspired by nature, including home-style cooking and mild processing, offer new opportunities to deliver nutritious food with delicious taste. This trend, however, needs to be supported by academic research adapted to the new context.

[O 32] Effect of muscle, ageing and packaging on marker volatiles for beef flavour

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Beef is an expensive food item and is expected to deliver a high quality eating experience. Evidence suggests that some beef products are inconsistent in eating quality and that flavour can be as important as tenderness for consumers. Many of the key flavour impact compounds for cooked beef are present at very low concentrations and are challenging to analyse. Therefore, marker compounds for desirable flavour have been identified. In this study, these marker compounds are used to follow the impact of muscle, ageing and packaging on grilled beef flavour.

Beef samples from four muscles, three packaging methods and three ageing periods from a study in Australia were transported to Northern Ireland and were stored at -80^{o}C. Beef was grilled according to a standard protocol and were the volatiles collected using Solid Phase Micro Extraction, prior to analysis by electron impact GC-MS.

Differences between muscles and ageing periods are significant for some compounds, while those caused by packaging are more extensive. Benzaldehyde ($P < 0.001$) was lowest in modified atmosphere packed (MAP) beef and highest in vacuum packed beef. Other Strecker aldehydes followed the same pattern (though non-significantly), as did dimethyltrisulphide ($P < 0.01$). MAP is alleged to inhibit proteolysis which may reduce the concentrations of free amino acids available for the formation of these compounds. Strecker aldehydes have been found to be markers for desirable beef flavour.

Amongst the n-aldehydes, pentanal shows a significant difference with at least 5 times more in MAP-packed beef than the other two packaging treatments. Vacuum-packed beef has significantly lower concentrations than overwrapped beef of 3-heptanone, 5-methyl-3-hexanone, 2-pentyl furan and 2-ethyl-1-hexanol. All these compounds are likely to be formed by oxidation pathways and it is possible that the reduced oxygen in vacuum-packed beef and higher oxygen permeability of overwrapped beef has caused this effect.

This approach is yielding a new understanding of the factors affecting the formation of flavour compounds in cooked beef, which could enable new processing methods to be proposed to manage flavour formation in commercial beef products.

[O 33] Measuring Smell-Challenges and Strategies

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Odors and odor impressions both in a positive and in a negative way have drawn the attention of mankind since ancient times. Not only the positive changes of food smell by the cooking process but also the smell of certain plants and oils have played an important role since centuries.One important requirement for odor activity is volatility and by the molecular weight range it is limited to 400 Dalton, as a consequence the 'Gold Standards' for the analysis of odorants are gas chromatographic based methods.But there are some limitations and restrictions which can make the identification and quantification process quite tricky. One of these limitations is the sensitivity of the human nose. Beside the fact that humans can cover a concentration range of up to 10 or 12 orders of magnitude, some molecules can be perceived down to the picogram per kilogram range.Even in the limited molecular weight range there are thousands of possible volatile molecules with different functional groups which are covering a wide concentration range. In addition only a small proportion of up to 3% of the volatiles show odor activity [1]. So there is a strong demand for methods which are highly selective and sensitive.For the optimization purposes all parameters from the sample preparation to the separation and the detection should be taken into consideration.
In this presentation several analytical approaches and latest developments will be presented and critically discussed. Different sample preparation regimes in combination with one and two dimensional chromatographic separations and mass selective detection can push the limits of detection down to even the most challenging concentration ranges. The feasibility of these methods will be demonstrated on the identification and quantification of odor and off odor substances in different matrices.

1. A. Dunkel et al., Natures Chemical Signatures in Human Olfaction: A Foodborne Perspective for Future Biotechnology, Angewandte Chemie International, Vol 53, 28 (2014), 7124-7143

[O 34] PARADISe - a ground-breaking tool to treat complex GC-MS datasets

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Modern GC-MS systems combined with efficient sampling techniques produce chromatograms with a large number of peaks of which many are not well-resolved. Well-designed experiments and screening investigations include many samples and replicates. The result is unavoidably heavy workload on the investigator to treat this data and extract all the chemical information. Many approaches have been used from simple analysis of total ion chromatograms over single-ion techniques to different kinds of deconvolution techniques, but they all have significant draw-backs: Most are very time-consuming, results can be user-dependent to different degrees, and by almost all techniques chromatograms are treated independently of each other. Furthermore, many approaches can only handle moderately overlapping peaks and often experience problems with low signal-to-noise peaks. Non-detects remain an issue as well.Here, a completely different approach using the so-called PARAFAC2 modelling (PARAllel FACtor analysis 2) is demonstrated. Until now, PARAFAC2 modelling has only been available for mathematical users and has required extensive coding for efficient use. An integrated approach called PARAFAC2 based Deconvolution and Identification System (PARADISe) has, however, become available. The solution is user-friendly, extremely time-saving, and produces reliable results that are less user-dependent. It is developed by a group of chemometricians around the 'Chemometrics and Analytical Technology' group at Department of Food Science, University of Copenhagen, and is freely available. PARADISe benefits from the ability of PARAFAC2 to resolve co-eluted chromatographic peaks for all investigated chromatograms simultaneously. It overcomes the limitation of PARAFAC2 which only works on time intervals, and it can perform all the necessary steps from visualization of data to generation of a final table of identified compounds for an entire set of chromatograms. Examples will be shown comparing data treatment of real datasets done with a commonly used vendor software (Agilent Chemstation) and PARADISe. It will be demonstrated how the two techniques perform with regard to deconvolution, integration/baseline-modelling, peak identification, and user's time-consumption. It is concluded that treatment of large datasets with PARADISe results in extraction of more information, the information is more reliable, and user's time-consumption when treating datasets with numerous complex samples/chromatograms is dramatically reduced.

[O 35] Exploring 2-Acetyl-1-Pyrroline Loss by High Resolution Mass Spectrometry and Nuclear Magnetic Resonance

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2-Acetyl-1-pyrroline (2AP) is the characterizing odorant in foods such as aromatic rice and popcorn and is an important odorant in many other foods including corn, crustaceans, cooked meat and roasted nuts. 2AP is a potent odorant with a detection threshold of 0.1 ppb and contributes a roasted, cracker-like or popcorn-like aroma character. As such, 2AP would be appealing as an added flavoring but this poses a challenge due to the molecule's unstable nature. This molecule was first discovered in 1982 by Ron Buttery and his group, who noted its unstable nature in their first report [1]. When 2AP is neat or in a concentrated aqueous solution, the color will rapidly change from colorless to red as 2AP reacts. Mass spectral data from our lab show a decline in a 25 mg/mL aqueous solution of 2AP in only 5 minutes. Buttery et al. hypothesized in 1983 that this molecule undergoes a polymerization process [2]. Yet, little information is available in the literature to support this hypothesis. Conversely, the literature is rich with reports on 2AP's biological formation, its formation via the Maillard reaction, synthetic routes to generate 2AP, its occurrence in various foods and methods for quantitation. Therefore, the significance of this compound is clear, but knowledge about its loss/degradation is lacking. Our research has probed 2AP loss in water by high resolution mass spectrometry (HR-MS) and NMR (1D and 2D) and confirmed that 2AP undergoes a polymerization reaction. We have observed that 2AP polymerization is a complex process, generating many unstable intermediates. The intermediates are highly unsaturated molecules which contain increasing numbers of 2AP moieties, accompanied by the loss of water. NMR showed an increase of other small molecules in the first 2-6 hours of reaction. We have assembled a list of structural features of the polymeric species via 2D NMR and MS^2. The research presented will focus on the insights gained about 2AP's reactions products. Stabilization strategies for 2AP will also be briefly mentioned.

1. Buttery, R. G.; Ling, L. C.; Juliano, B. O. 2-Acetyl-1-Pyrroline: An Important Aroma Component of Cooked Rice. *Chem. Ind.* 1982, 958-9.
2. Buttery, R. G.; Ling, L. C.; Juliano, B. O.; Turnbaugh, J. G. Cooked Rice Aroma and 2-Acetyl-1-Pyrroline. *J. Agric. Food Chem.* 1983, *31*, 823-6.

[O 36] A Sophisticated Setup for Rapid, Sensitive and Selective Food and Flavor Analysis

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Here we present a proof-of-concept study utilizing a sophisticated setup developed for rapid food and flavor analysis with high selectivity based on Proton-Transfer-Reaction - Mass-Spectrometry (PTR-MS). Established technologies in flavor and aroma research, such as Gas Chromatography coupled with Mass Spectrometry (GC-MS), require laborious sample preparation and are time-consuming, particularly if large numbers of samples have to be analyzed. PTR-MS on the other hand is a direct injection method, which is very sensitive and capable of real-time quantification. However, so far in complex matrices (e.g. wine) selectivity has been somewhat limited and setups for automated sampling have not been commercially available.In order to overcome these limitations we equipped a Time-Of-Flight (TOF) based PTR-TOFMS instrument with an optimized fastGC inlet system and coupled it with a state-of-the-art autosampler. The entire inlet line, from the autosampler syringe to the newly developed injection interface and all the way to the PTR reaction chamber, can be heated, which improves sample transfer and effectively suppresses condensation. The PTR-TOFMS instrument can be automatically switched between real-time direct injection and highly selective fastGC mode. In order to conduct a proof-of-concept study we operated the autosampler with vials filled with 5 mL of nine different red wines from various grapes and origins, respectively. Additionally, by conducting measurements on interjacent standards we observed an excellent reproducibility within an error margin of about 5 % .

Although the mass spectra obtained from the headspaces of the different wine samples are very complex, we found that by switching to fastGC mode, compounds can be identified at a high level of confidence (e.g. isoamyl acetate, ethyl octanoate). Moreover, even when standards are not available, the fastGC mode offers the crucial advantage to differentiate between mass spectral peaks originating from compounds present in the sample and from fragmentation processes upon PTR ionization.

We conclude that the autosampler - fastGC-PTR-TOFMS instrument combination is a powerful tool for rapid, sensitive and selective food and flavor analysis, which produces considerably more high quality data at the a higher sample-throughput than established methods.

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[O 37] DOLC-NMR: Differential Off-line LC-NMR Analysis of Nutrient-Induced Metabolome Alterations in S. cerevisiae and their Taste Impact

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Metabolome investigations by means of mass spectrometry are often limited in structure elucidation of unknown and new metabolites. A novel Differential Off-Line LC-NMR approach (DOLC-NMR) was developed to record and quantify nutrient-induced metabolome adjustments in *Saccharomyces cerevisiae*. Off-line coupling of preparative high performance liquid chromatography separation and ^{1}H NMR spectroscopy supported by automated comparative NMR bucket analyses, followed by quantitative ^{1}H-NMR using ERETIC II has been successfully utilized to monitor significant quantitative changes in the metabolome of *S. cerevisiae* upon intervention with the aromatic amino acid L-tyrosine. Among the 33 metabolites identified by means of exact mass and 1D/2D-NMR experiments, glyceryl succinate, tyrosol acetate, tyrosol lactate, tyrosol succinate, and *N*-acyl-tyrosine derivatives like *N*-(1-oxooctyl)-tyrosine have not been earlier reported as yeast metabolites. Depending on the chain length of the fatty acid, *N*-(1-oxooctyl)-, *N*-(1-oxodecanyl)-, *N*-(1-oxododecanyl)-, *N*-(1-oxomyristinyl)-, *N*-(1-oxopalmityl)-, and *N*-(1-oxooleoyl)-tyrosine imparted a kokumi taste enhancement above their human recognition thresholds ranging between 145 and 1432 μ mol/L in a savoury model broth.

[O 38] Process Control in Flavour Generation : NIR-MVA as a tool to monitor key odorants formation

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Sensors suitable to monitor chemical reactions leading to the formation of potent odorants in foods and consequently enabling process control are on increasing demand.In the present work real time kinetic analyses were made by developing new methodologies combining near infrared spectroscopy (NIR). These were applied to study the dynamics in phenylacetaldehyde formation through a number of reactions, namely (i) glucose and phenylalanine, (ii) gallic acid and phenylalanine and iii) gallic acid, phenylalanine and glucose.Phenylacetaldehyde as well as other reaction intermediaries were monitored during 60 min with a frequency for data acquisition of 3 spectra/min. A 10 minutes' reaction intervals samples were collected and target analysis was performed using mass spectroscopy (GC-ITMS and LC-qTOF).
For comparison, the spectral data were analysed in a conventional way fitting kinetics for specific wavelengths, and then by soft-modelling multivariate alternative least squares (MCR-ALS) method for modelling spectral data with quantification of reaction compounds, and perform deconvolution of spectral data. The method developed allows to unlock chemical information related with specific compounds present in the reaction (phenylacetaldehyde, benzaldehyde, quinones and dicarbonyls). Different reaction rates were observed according to the perturbation, i.e. metals addition, temperature increasing and substrate class. A database for feature comparison has been developed to classify each new set of 'individuals' taking into account their ability to form potent odorants. In conclusion the method allows for a real time, high-throughput and low cost analysis for process monitoring.

Nestlé, founded in 1866, is the world's leading Nutrition, Health and Wellness Company employing over 360 000 people worldwide. With unrivalled research and development capabilities, Nestlé has a rich heritage in food and nutrition science. At the heart of the Nestlé Research Network lies the Nestlé Research Center (NRC), based in Lausanne, Switzerland, with additional locations in the USA and Asia. Its core purpose is to provide the scientific knowledge and research base needed for the renovation of our existing foods and beverages, as well as the creation of new, innovative products.

As the world's largest private food and nutrition research institute, the NRC is home to a staff of over 600 people, with more than 300 researchers from 50 nationalities representing a diverse range of scientific competencies. The NRC plays an important role in providing the science behind healthier products with lower levels of sugar, salt and fat, and an increase in vitamins, minerals and fibre. The expertise of NRC scientists is complemented by more than 40 R&D centres worldwide, as well as a wide-reaching network of external partners such as universities, private research institutes and start-up companies. With 47 key academic partners and 16 innovation partners, in 2016, Nestlé Research published about 270 scientific publications in peer-reviewed journals and filed 320 patents.

Food products usually deliver several quality attributes such as aroma, taste, colour, texture and nutrition. A major part of product renovation and innovation involves delivering authentic taste and aroma freshness using the latest developments in flavour science. The Weurman Flavour Research Symposium has been since ever an excellent forum for high-level scientific exchange and a rich source of inspiration and state-of-the-art research.

Abstracts Poster Contributions

[P 001] Aroma Active Compounds of Pontianak Orange

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The aroma active compounds of Pontianak orange peel oil (*Citrus nobilis* Lour. var. *microcarpa* Hassk.) were characterized by using gas chromatography-olfactometry (GC-O) and aroma extract dilution analysis (AEDA) techniques. Forty-one compounds were found to be aroma-active, which were mainly dominated by saturated and unsaturated aldehydes. The flavor dilution (FD) factor was within the range of 2-2048, and compounds having the highest FD factor were pinene, linalool, and 2-methoxy-3-(2-methylpropyl) pyrazine, including a few unknown compounds. On the basis of GC-O results, odor activity value (OAV) and relative flavor activity (RFA) were determined for aroma model reconstitution. These resembled the original aroma of the peel oil for the green, fatty, fresh, peely, floral, and tarry attributes, with the model solution derived from OAV being the closest to Pontianak oil. Omission tests were carried out to verify the significance of (Z)-5-dodecenal and 1-phenylethyl mercaptan as key compounds in the aroma of Pontianak orange peel oil.

[P 002] Screening of yeast strains with flavour potential for meat products under reduced concentration of preservative nitrifying agents

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During sausage manufacturing amino acid degradation into aroma compounds depends largely on microbial metabolism during fermentation where yeasts play an important role (Flores et al., 2015). Aroma characteristics of fermented sausage will depend not only on the yeast strain used but also on the processing factors (raw material, meat ingredients, preservatives, technological parameters, presence of starter cultures). Despite the role of nitrites and nitrates in meat product safety and technological properties, there is a trend to reduce its use (Alahakoon et al., 2015). So, to meet this demand without changes in sausage aroma, the objective is to search towards yeast with flavor capabilities and determine the effect of reduced preservative concentrations on their amino acid metabolism.

Nine strains of *Debaryomyces hansenii* were isolated from fermented sausages produced using pork and llama meat (Flores et al., 2017). These strains were evaluated in a model system after 16 d of incubation at 25°C resembling the sausage formulation containing free amino acid and additives (salt, glucose and nitrite agents) and a variable concentration of the preservatives agents (nitrite and nitrate).

After incubation, volatile compounds and free amino acids were determined. The study revealed the ability of *D. hansenii* yeast to produce differential aroma compounds based on the type of meat used. Yeast strains from Llama sausages were related to the production of propanoate ester compounds and branched alcohols while those from pork sausages to branched aldehydes and acids. One of the pork yeast has a distinct volatile character characterized by the production of ethyl esters. The nitrate-nitrite reduction affected the yeast ability to produced volatiles. Specially two of the yeasts (L1 and L5) from pork sausages increased the production of branched acids (L1) and ethyl ester compounds (L5) under reduced nitrifying agent content. These yeast strains isolated from sausages manufactured with different raw materials (meat from pork or llama) have different ability to produce volatile compounds with a significant effect on the overall sausage flavor. They may be used to study the metabolic pathways involved in the generation of aroma compounds in fermented meats.

[P 003] New insight into the role of free amino acids upon coffee roasting

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Coffee roasting represents the key refinement step in the coffee value chain where the green coffee precursors are transformed into roasted coffee constituents giving rise to color, aroma and taste. The soluble low molecular weight fraction in green coffee beans was discussed as the essential precursor pool comprising important flavor generating constituents such as free sugars, amino acids, trigonelline, and chlorogenic acids [1, 2]. These constituents are readily available for manifold reactions, which is demonstrated by their rapid consumption at the early stage of roasting [3].

Coffee roasting is a very complex process as many chemical reactions proceed in parallel and compete for precursors and intermediates. Recently a significant effort was taken to better understand the role of free sugars, namely sucrose, in the formation of key aroma compounds like diketones applying the biomimetic in-bean approach combined with labeling experiments [4]. In addition, kinetic experiments with fully labeled sucrose highlighted that the contribution of low molecular weight precursors can significantly change during the roasting course, shifting the importance to bound precursors. To extend our knowledge to free amino acids, the formation of key aroma compounds like Strecker aldehydes and alkyl pyrazines in coffee was studied by in-bean experiments replacing the free amino acids by their completely ^{15}N and ^{13}C labeled analogues.

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[P 004] Modifications of raw beef odor under different periods of retail display

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The volatile compounds responsible of beef aroma have been extensively studied using cooked samples, but less is known about the volatile composition of raw meat. However, when opening the meat package at home, the odor must be adequate for the consumer, and short or extended periods of acceptability would happen depending on numerous factors, such as the antioxidant status of the meat. Furthermore, some compounds already present or developed in the raw meat will remain after cooking and could affect flavor perception.
In the present work, the changes in the aroma of beef when stored during different periods in retail display under high oxygen conditions have been studied. Samples of knuckle beef steaks were aged for 15 days in vacuum conditions and packed under modified atmosphere (80% O_2, 20% CO_2) for 0, 5 and 9 days.
A composite sample of 30 g of minced meat from the steaks of 3 different animals was prepared for each packing period. Each composite sample was subjected to dynamic headspace extraction and retention in a sorbent bed. The retained volatiles were eluted and the extract used for gas chromatography-olfactometry profiling.
Odor zones were ranked by 6 judges and identified by means of multidimensional gas chromatography-mass spectrometry. Additionally, the samples were analyzed by solid phase microextraction coupled to gas chromatography-mass spectrometry to quantify targeted volatile compounds.
The obtained data have shown a clear change in volatile and odor profile associated to the time on display. The study has also allowed to identify and quantify several odor zones related to oxygen exposure that could influence the perception of the consumer when opening the raw meat package.

[P 005] Identification of odor-active trace compounds in roses and fruits

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The flower scents of *Rosa damascena* were investigated using aroma extract dilution analysis. Along with major compounds, such as 2-phenylethanol, geraniol, and citronellol, two ultra-trace components that showed a high flavor dilution factors were detected as odor-active compounds. One of the trace compounds (woody note) was identified as rotundone by multidimensional gas chromatography-mass spectrometry, whereas the other (citrus note) was identified as 4-(4-methyl-3-pentenyl)-2(5*H*)-furanone (MPF) via purification of the commercial rose absolute from *R. damascena*. MPF was isolated via distillation, silica-gel column chromatography, and two-step high performance liquid chromatography purification. Identification was further confirmed by matching the analytical data and odor qualities of the isolated MPF with those of synthesized MPF. This is the first report that refers to the organoleptic importance of these two compounds for the rose scent. In this study, the odor of MPF was described by panelists as citrus-like (lemon, orange, and grapefruit) and floral (muguet and jasmine); moreover, its threshold was fairly low at 3.6 μg/kg in water.The presence of rotundone and MPF in five other types of roses was examined. While the former was detected in all the roses investigated, the latter was found in three of them. Sensory analyses were carried out to assess the effects of rotundone and MPF on compounded rose perfume. Results revealed that the addition of 50 μg/kg rotundone and 5 μg/kg MPF to the model rose perfume conveyed glamorous and natural aspects to it.The presence of MPF also was detected in fruits (lemon, orange grapefruit, apple, and muscat), black tea, and beer. The findings demonstrate the wide distribution of MPF not only in roses but also in various types of foods.

[P 006] Characterisation of aroma active compounds in horseradish (Armoracia rusticana)

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Horseradish (*Armoracia rusticana* Gaertn., Mey. et Scherb.) is a hardy perennial plant belonging to the family of Brassicaceae and is cultivated in temperate climates in many parts all over the world [1]. In Europe the countries with the main growing areas are Austria, Germany, Hungary and Poland. The main reason for cultivation is its white and fleshy root, which is processed to condiments, mainly spicy pastes or sauces; moreover, horseradish is used in traditional phytomedicine and has been reported in relation to antimicrobial effects [1]. Responsible for the pungent note of the typical horseradish aroma are isothiocyanates, which are released upon cell disruption, when the root is cut or ground [1]. Those isothiocyanates activate branches of the trigeminal nerve and generate a pain sensation. Many studies have dealt with the isothiocyanate composition and content of horseradish roots [2,3], but none of them has ever focused on comprehensively exploring the substances responsible for the whole aroma impression of horseradish.
Accordingly, we applied state-of-the-art methods that cover both sensory and analytical techniques to unravel the composition of horseradish aroma. Therefore ground material of the main root was extracted with dichloromethane, and the aroma fraction was subsequently recovered by solvent-assisted flavour evaporation distillation. The sample extracts were analysed after mild concentration by means of gas chromatography-olfactometry, gas chromatography-mass spectrometry and two-dimensional gas chromatography-mass spectrometry/olfactometry. Aroma extract dilution analysis was applied to determine the relative contribution of every single aroma active compound to the overall aroma of horseradish roots. Besides already reported compounds like allyl isothiocyanate and 2-phenylethyl isothiocyanate, a series of odorous substances, previously unknown and belonging to different structural classes, could be identified that have not been described in horseradish before, some of them having been detected with high odour potency in the samples.

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[P 007] Effect of nitrate reduction on dry fermented sausage aroma during vacuum storage

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Aroma characteristics of fermented sausage depend on processing factors such as raw material, meat ingredients, preservatives, technological parameters and presence of starter cultures. Despite the role of nitrites and nitrates in meat product safety and technological properties, there is a trend to reduce its use (Bolger et al., 2017). However, the effect of nitrite on flavor formation in meat products is essential to develop cured aroma. Thomas et al., (2013) indicated that cured cooked ham aroma is due to the balance of sulfur compounds and oxidation compounds produced during cooking and in the absence of nitrite, the aroma is disturbed due to the excessive formation of oxidation compounds that mask the sulphur meaty notes. In dry fermented sausage aroma nitrite plays a fundamental role in developing the typical dry cured aroma (Flores & Olivares, 2011) although it is not known the effect of nitrite reduction on aroma generation and stability during shelf life. Therefore, our aim is to determine the effect of reduced nitrate concentrations (as a source of nitrite) used as preservatives on the development of sausage aroma in dry fermented sausages after storage at ambient temperature under vacuum. For this purpose, three different sausage formulations have been manufactured with different nitrate contents, control with 250 mg/kg (C), 15% (RN15) and 25% reduction (RN25). The oxidation of sausages has been evaluated by the analysis of TBARS and extraction of the volatile compounds using SPME and gas chromatography mass spectrometry. The sausage oxidation values depended on the fat content of sausages. Regarding volatile compounds derived from lipid oxidation processes several compounds related to oxidation reactions have been identified (linear aldehydes and 2-alkenals) and quantified in the different formulations and storage times. The study examined the relation of nitrate reduction and fat content on aroma compounds related to oxidation process and their effect on sausage aroma perception during vacuum storage.

[P 008] Shelf-life model: Useful tool to predict sensory and nutritional quality of infant formulas

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Shelf life prediction attracts increasing interest in the food industry. It is especially relevant for long shelf-life products where degradations have more time to occur. In this study, we show that it is possible to build a reliable shelf-life kinetics model for infant formula (powder) packed in metal cans. The model varies the following parameters: storage temperature (realistic range: 5-40°C), storage time (0-2 years), oxygen level in the pack (protected or unprotected atmosphere), and the composition of the product (high/low PUFA). The effects of light and moisture were discarded as they cannot penetrate through the metal can. A model was build based on chemical kinetics. The model is able to predict the taste, the level of vitamin C, and the aromas concentrations based on the chemical reactions occurring in the infant formula. The kinetic reactions were fitted based on data of aroma concentrations, oxygen level in the package, and composition of the product. Several examples of accelerated shelf life tests simulating a normal shelf life at 2 years are illustrated. The results are compared to the most common practice in shelf-life: using a fixed Q10 temperature coefficient. It is advised to use multiple accelerated shelf life tests to mimic the normal shelf life of the relevant sensory or nutritional aspects of the product.

[P 009] Milk fat globule membrane and its role in flavour development in cheese during ripening

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The milk fat globule (MFG) plays a vital role in determining the flavour development of cheese during ripening. The MFG consists of a fat core and a three-layer membrane (MFGM). The MFGM has a complex composition of polar lipids, proteins, and enzymes such as xanthine oxidase (XO), which is capable of catalysing the oxidation and reduction of a wide range of substrates. Rearrangement of the MFGM may affect the accessibility of the milkfat and the MFGM components to the enzymes present (coming from the MFGM, milk, and starter bacteria) and thus may play a role in flavour development in cheese. However, research investigating the influence of processing on the MFGM structure and its subsequent effect on the flavour profile of cheese is limited.
This study investigated how the source, composition and XO activity of the MFGM fraction in a Cheddar-like model cheese impacted on the volatile organic compounds (VOC) developed over 6 months. Freeze-dried β -serum and buttermilk powder were used for MFGM isolation. Milkfat emulsions (5%) were prepared using the three MFGM isolates as emulsifiers and used for cheese making. Two reference cheeses were also produced: one containing cream as a source of native MFGs (Control), and one containing recombined MFGs with Tween 80 as an emulsifier. VOCs were measured during ripening at 8°C after 0, 90, and 180 days using headspace solid phase micro-extraction (SPME) with gas chromatography mass spectrometry (GC/MS).
MFGM recombined cheeses had a higher concentration of short chain fatty acids (SCFAs; acetic, butanoic, hexanoic acids), alcohols (e.g. 1-nonanol), methyl ketones (e.g. 2-hexanone) and sulfide compounds; but had lower levels of diacetyl, acetoin and ethyl esters compared to the control and the Tween-containing cheese. This illustrated that rearrangement of the MFGM structure significantly influenced volatile compound development during ripening. Within MFGM recombined cheese samples, a higher XO activity was correlated to higher concentrations of SCFAs. The Tween-containing cheese highlighted the importance of MFGM components on flavour development. This research highlights the potential of using MFGM components from commercial by-products as a functional ingredient to manipulate cheese flavour.

[P 010] The effect of sugar type on VOC generation in a model baked system

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Replacing sugar in baked products is a major challenge Sugar not only imparts sweetness, but contributes to the fresh flavour quality of baked foods during thermal processing and acts as a tenderiser by retarding and restricting gluten formation. Reducing sugars, have a direct influence on the Maillard reaction, which can either promote or reduce Strecker degradation, resulting in the formation of important compounds such as pyrazines that are character impact odorants of freshly baked foods. Sucrose a non-reducing sugar can degrade during baking forming the reducing sugars fructose and glucose.
The effect of sugar type (sucrose, glucose, fructose and lactose) and sugar level (3.7%, 14.7% of batter recipe) on volatile organic compound (VOC) generation in a model muffin system was investigated. Other ingredients in the baked system were wheat flour, water, liquid egg white, canola oil, polydextrose and baking powder. Polydextrose levels were adjusted to maintain a constant carbohydrate content. A sugar-free sample, where all the sugar was replaced with polydextrose was also prepared. After baking for 18.5 min at 200°C each sample (200g) was immediately frozen in liquid nitrogen, ground, then extracted with diethyl ether (1:1), the DE recovered and distilled using a solvent assisted flavour evaporation apparatus. Distillates were reduced in volume to 1 mL and analysed by GC-MS.
The relative concentration of the VOCs generated was dependant upon the sugar type and amount of sugar added. In the absence of sugar (polydextrose only formulation) the amounts of VOCs generated were very low. Overall, fructose produced the highest concentrations of VOCs generated, followed by glucose, lactose, sucrose and finally polydextrose. Detected VOCs include 5-hydroxymethyl furfural, 2-furanmethanol and 2,3-dihydro-3,5-dihydro-4H-pryan-4-one. While lactose produced lower concentrations of total generated VOCs, it did produce the highest concentration of some VOCs, e.g. furfural, butyrolactone and maltol.
In baked products when sugar is removed, even if the sweetness is maintained, the characteristic VOC associated with fresh baked flavour will be substantially decreased. Subsequently incorporating small amounts of glucose and fructose may be sufficient to generate the characteristic fresh-baked flavour.

[P 011] Understanding the role of sodium in biscuits

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Sodium chloride is included in many biscuit products as a functional ingredient as well as a flavour enhancer, whilst many companies have significantly reduced sodium in many products, technical solutions for reducing sodium further are urgently required (WHO recommendations). It may be possible to reduce the need for salt if we can determine how it impacts the global behaviour of biscuits (structure, aroma release, colour, moistening...) and therefore mitigate the effects of its reduction.
It is also known that salt impact sweetness perception at low concentrations within model systems (Liem *et al.*, 2011) so it is important to understand the role of salt in these products where the overall taste is one of sweetness rather than saltiness.
Standard biscuits were prepared with varying levels of sodium reduction (0%, 33%, 66% and 100%) and physicochemical analyses were performed: GC-MS (total aroma, aroma release by headspace dynamic trapping), texture analysis (hardness - three-point bending tests), thermogravimetric analysis TGA (loss of matter during baking), colour (colorimeter, CIELab), moisture content and water activity.
Increasing the amount of salt increases the amount of total available aroma in the biscuit headspace. This phenomenon is greater for more hydrophobic aroma compounds ($p < 0.05$). This may be due to an increased loss of aroma during the baking phase or increased aroma formation through thermal reactions. TGA monitoring showed that the rate of weight loss is higher for low salt biscuits and sodium levels also impacts the final structure of biscuits. Indeed, those containing more salt may impact gluten network formation leading to increased hardness (Tuhumury *et al.*, 2014).
The impact of exchanging sodium for potassium is also studied, initial results suggest that potassium can partially rebalance the aroma release in low sodium biscuits.
These *in vitro* analyses demonstrated that sodium reduction leads to less available aroma and a softer structure. Understanding the interactions between salt, structure and aromas, therefore may allow manufacturers to formulate biscuits with less added salt in a more effective way while maintaining a consumer liking.

[P 012] The impact of plant proteins on vanilla flavour perception

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Interactions between proteins and flavours have been reported to produce flavour retention and to decrease flavour perception in food products. Protein/flavour interactions can be either reversible, such as hydrophobic, hydrogen, and electrostatic interactions or irreversible as covalent binding. Proteins can also transmit to food products undesirable off-flavours, such as bitterness and astringency, affecting their organoleptic properties and thus also altering flavour perception. Vanillin is the main component of vanilla flavour, one of the most popular flavours used in high-protein food products. It has been previously confirmed that vanilla flavour intensity was reduced due to chemical reversible interactions between vanillin and milk proteins. However, less is known about plant protein/flavour interactions. The recent interest on alternative proteins from vegetal sources has brought new challenges to the flavour industry. The aim of this study was then to investigate interactions between vanillin and plant proteins (soy, lupin, pea, potato, and wheat) in aqueous mixtures and their impact on flavour perception. HPLC analysis and dialysis equilibrium methods were used to determinate the percentage of free vanillin lost by chemical interaction with proteins. Descriptive sensory analyses were performed to investigate the perception of vanillin and protein off-notes in mixtures. All proteins interacted with vanillin in different degrees. The loss of free vanillin occurred mainly in mixtures with pea, potato, and wheat proteins. The sensory profile of protein mixtures were evaluated in terms of vanillin, cereal, herbal, and bitterness descriptors, common to all protein profiles. Understanding the protein/flavour chemical interaction and the impact of flavour compounds on flavour perception allow optimising the use of flavours, reducing off-notes, and controling flavour release in food products.

[P 013] Decoding the Unique Peaty Aroma of Islay Scotch Single Malt Whisky by Means of the Sensomics Concept

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Whisky making has a long tradition in Scotland and its islands. After mashing barley malt with yeast, a double-batch distillation yields the raw spirit, which has to age for at least 3 years in second hand-oak casks before being bottled as single malt whisky.
Especially, Whiskies from the island Islay are known to be particularly peaty. The malting process on Islay contains the traditional step of kilning with so-called peat reek (peat smoke) which is responsible for the typical smoky and phenolic aroma of the spirit. But of course the intensity of peatiness is chosen by the different whisky makers and their favorite taste. Heavily peated whiskies usually derive from the south-eastern coast of Islay, while the distilleries on the east coast are known to produce more moderate spirits.
In order to decode the unique aroma of Scotch Single Malt whiskies from Islay on a molecular basis and to elucidate the different grades of peatiness, three whiskies from different distilleries from Islay were investigated by means of the Sensomics concept. The important aroma compounds, identified by mass spectrometry based on results from GC-O and aroma extract dilution analysis, were quantitated by stable isotope dilution assays. Odor activity values (OAVs) were then calculated considering their odor thresholds in 40% ethanol ABV and the results were verified by preparing aroma recombinates to mimic the original whisky aroma profiles.
The peatiness of the whiskies could be correlated to a set of phenolic compounds with quantitative differences, though. While the mildly peated whisky only contained trace amounts of phenol derivatives, the heavily smoky whisky showed the highest OAVs for this substance group, e.g. 3-ethylphenol (940), 2-methoxy-5-methylphenol (380) or 2-methoxyphenol (280). Additionally, the influence of cask maturation was addressed by investigating a raw whisky in comparison to the final product from the same distillery. While typical maturation derived compounds such as 4-hydroxy-3-methoxybenzaldehyde and whisky lactone were only present in the aged whisky, the group of phenol derivatives were found with even higher concentration in the raw spirit.

[P 014] Flavour generation from microalgae in mixotrophic cultivation

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Microalgae are known to produce several volatile organic compounds (VOCs) that can be obtained from the biomass or released extracellularly into the medium. Many of these volatiles present odor descriptors such as floral, fruity, spice, sweet, roasted, and can thus be used as a flavoring agent in the food industry and others used in the pharmaceutical and fine chemicals industries. The objective of this study was to evaluate the generation of VOCs with flavour potential from the microalga *Phormidium autumnale* in mixotrophic cultivation. The experiment was conducted in a New Brunswick Scientific BioFlo®310 bioreactor operating under a batch system, with a 1.5L working volume. The bioreactor including filtration units was sterilized by autoclaving at 121° C for 20min. The experimental conditions were as follows: initial inoculum concentration 100mg.L^{-1}, temperature 25°C, pH adjusted to 7.6 and aeration of 1.0 volume air per culture volume per minute, supplemented with 5g.L^{-1} of sucrose and constant light intensity of 4 klux. The volatiles compounds were isolated by solid phase microextraction applied in headspace every 24 hours of residence time (144 hours), separated by gas chromatography and identified by mass spectrometry (HS-SPME-GC/MS). The major products in the bioreactor are 2,4-decadienal (46.03%), 3-methyl-1-butanol (12.39%), hexanol (4.17%) and 2-ethyl-1-hexanol (3,51%). The descriptor flavor of the compounds detected in experiments was mainly classified as fried food, fruity, spice, and floral compounds. In conclusion, the results have shown that the mixotrophic cultivation of the *Phormidium autumnale* can be a potential biotechnological to produce natural flavours.

[P 015] Unraveling the complexity of savory biohydrolysate using a holistic sensory-analytical approach

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For culinary products taste and flavor enhancement are imparted to a large part by savory umami compounds such as glutamic acid and 5'-nucleotides. As consumers get more and more sensitive to the addition of isolated taste enhancers, alternative natural sources have gained interest in the past years. In the recent years several studies have been conducted to determine the presence of taste active or modifying compounds in such ingredients, mainly in soy sauce [1,2]. The link to the sensory characteristics of the products was, however, studied less intensely and the role of the individual taste compounds on the overall flavour remains in many cases questionable [3].
In the present study we aimed at fully characterizing a biohydrolysate by combination of taste-reengineering experiments, sequential liquid chromatographic-fractionation and sensory assessments. Sophisticated LC/MS techniques by developing multi-methods were used for the quantification of known taste-active compounds, such as peptides, nucleotides, or Amadori compounds. In addition to that, sensory-guided fractionation approaches in combination with HR-LC/MS and NMR were performed to unravel the presence of yet unknown compounds as possible taste-active or taste-modifying candidates. Finally, in-depth sensory evaluations were conducted to determine contribution to the taste-enhancing effect observed in the raw material. To better understand the importance of each of the different compounds, respectively compound classes, and their interplay, taste thresholds in the corresponding matrix were determined and interactive effects investigated by reconstitution and omission tests. Such a holistic approach was found to be crucial to entirely cover and understand the natural complexity and richness of such bio hydrolysates.

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[P 016] Enhancing (+)-nootkatone production in Pichia pastoris and Saccharomyces cerevisiae through cytochrome P450-mediated conversions

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(+)-Nootkatone is a highly demanded and expensive compound naturally found in citrus oils, vetiver grass or cedar trees, and has recently been demonstrated as powerful insect repellent active against a wide range of insects including head lice, ticks, bed bugs, and mosquitoes. Extraction of (+)-nootkatone from plant material or its production by chemical synthesis suffers from low yields and the use of environmentally harmful methods, respectively. We established yeasts as whole-cell biocatalysts for the production of (+)-nootkatone from inexpensive carbon sources by introducing an optimized biosynthetic pathway including plant and yeast derived enzymes. Recently, our group has identified cytochrome P450-mediated hydroxylation of (+)-valencene as a major bottleneck in the biosynthesis of trans-nootkatol and (+)-nootkatone in *Pichia pastoris* or *Saccharomyces cerevisiae*. An extensive screening for effectors of CYP450 activity revealed the positive impact of two yeast genes, i.e. ICE2 and RAD52 on trans-nootkatol/(+)-nootkatone production. Remarkably, a very similar, positive impact was observed on two further cytochrome P450 enzymes. Thus, we have identified novel and generally applicable positive effectors of membrane-attached cytochrome P450 enzymes for biocatalytic conversion, e.g. terpenoid biosynthesis.

[P 017] Effects of Drying Methods on the Composition of Volatile Compounds in Fruits and Vegetables

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Aroma and taste of foods are the special mixture of different metabolites. Aroma, derived from unique combinations of volatile components, is essential for determining the quality of dried foods. Aroma profile of foods may be affected by loss, destruction, change or improvement of unexpected flavors during drying processes.
The Maillard reaction and autoxidation are the main chemical reactions responsible for the formation of new compounds during drying. These reactions have considerable effects on the flavor of dried fruit and vegetables. Maillard reaction derived compounds are classified in three groups which are sugar dehydration/fragmentation products (furans, pyrones, cyclopentenes, carbonyl compounds and acids), amino acid degradation products (aldehydes, sulphur compounds and nitrogen compounds) and volatiles produced by further interactions (pyrroles, pyridines, pyrazines, imidazoles, oxazoles, thiazoles and thiophene). Some of the flavor compounds (aldehydes and esters) formed through enzymatic oxidation of lipids and enzymatic biosynthesis of alcohols and acids.
Concentration of volatile compounds and activity of volatile forming enzymes are affected by drying methods and conditions. Besides that, loss of the precursors may also cause the loss of volatile compounds after drying. Conventional drying techniques adversely affect color aroma and flavor due to increased temperature and long exposure to heat and oxygen. On account of the negative effects of conventional drying processes, freeze drying and vacuum drying have been alternatively used in recent years. In spite of being expensive and time consuming, these technologies preserve flavor better than conventional drying. This review highlights the effects of drying methods on the volatile compounds of fruits and vegetables.

Key words: Volatile compounds, aroma, flavor, drying methods, fruit and vegetables

[P 018] In Vivo Flavor Release From Foods

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Perception of the flavor of foods is a complex process that involves mostly the senses of smell and taste, and this may be changed when food is consumed. The variation in physical properties of food leads to change the perception of flavor and texture in the oral cavity. The flavor sensations are identified by temperature, muscle actions in the mouth/throat during chewing and swallowing, food surface that exposed to saliva and air, dissolution of taste compounds in saliva and the release of volatiles in the mouth space. Moreover, saliva characteristics and mastication patterns may show difference between men and women or young and elderly people that contribute to differences in flavor release and perception.
The quality of food is comprised of many factors such as appearance, color, texture, flavor, and nutritional value. Flavor is one of the most important quality features. There are hundreds of volatile compounds present in trace amounts in foods and they can be detected by human olfaction. There are many studies monitored the online flavor release in several fresh foods (strawberry, tomato, apple and garlic) and processed foods (coffee, wine, cereal bars, bread, yogurt and cheese) with different analytical methods. In this review, in vivo flavor release from several foods is discussed.

Key Words: in vivo, flavor release, saliva

[P 019] Wine aroma persistence during wine intake is affected by differences in human oral physiology and on wine matrix composition

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Recent studies have shown that representative wine aroma compounds can be adsorbed into the oral cavity following in-mouth wine exposure (Esteban-Fernandez et al., 2016), therefore affecting their mass transfer to the exhalation flows and likely the duration of aroma persistence after wine intake. Besides the physico-chemical nature of the aroma compounds, others factors related to the oral physiology (saliva composition, flow, enzymatic activity) and wine matrix composition (ethanol, polyphenols, etc) might also have a large impact on the adsorption/desorption mechanisms that take place on the oral and pharyngeal mucosa affecting the availability of odorant molecules for the olfactory receptors and ultimately, wine aroma perception.Therefore, the objective of this work was to gain an understanding of the role of oral physiology and wine matrix compositional factors (ethanol and polyphenols) on wine aroma persistence. To do so, a wide array of -*in vivo* analytical techniques (intra-oral SPME, spit off odorant measurement analysis), -*ex vivo* studies (Static-SPME-HS analysis using oral epithelial cells, saliva, and wine matrix compounds), enzymatic measurements (saliva esterase activity after the consumption of different model wines) and sensory approaches using trained panelists (descriptive and temporal sensory analysis) were employed.Following this multi-approach study we found large inter-individual differences on the aroma release behavior among participants, which might be linked to differences in saliva composition. Among them, esterase activity was very variable among individuals, although it always increased after wine consumption. We also found a large wine matrix effect on intra-oral release. In general, polyphenols decreased wine aroma release, while ethanol increased it. Descriptive sensory analysis also showed a relation between the impact of some wine matrix components (polyphenols) and typical wine aroma descriptors. Therefore, this work has provided relevant information on the oral and wine compositional factors that influence wine aroma release and aroma persistence which might help in understanding wine aroma perception during wine consumption.

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Key words: wine aroma persistence, oral physiology, wine matrix, *in vivo* aroma release, descriptive and temporal sensory analysis

[P 020] Unexpected pungent effects from aldol products of hydroxymethylfurfural

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Chemestetic effects occur rather frequently when eating food. Hotness from eating peppers due to the presence of capsaicin and cooling from mint due to menthol are the most common examples.Tingling aspects from spilanthol, zingerone and polygodial are also known.
Unexpectedly we found that certain aldol condensation products of hydroxymethylfurfural generated a pungent effect as well.Their chemical structure is quite different from known pungent compounds [1-2].In the poster the synthesis and characterization of the molecules will be discussed.
Moreover, chemical structures will be compared with similar molecules in the same series that did not have these taste effects. Regretfully the molecules also had a clear bitter taste preventing commercial use of these molecules.

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[P 021] Aroma-active compounds in canned tuna fish by aroma extract dilution analysis

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The odor compounds from two types of canned tuna fish (albacore and skipjack) were studied using gas chromatography/olfactometry-mass spectrometry (GC/O-MS). Aroma extract dilution analysis (AEDA) showed that canned tuna odor was mainly contributed by aldehydes, ketones, sulfur compounds and fatty acids although the individual compound and level varied between the two species. On the basis of flavor dilution (FD) values, the potential important aroma compounds were 2,3-pentanedione, 2-methylthiophene, (Z)-4-heptenal, 1-octen-3-one, 2-methyl-3-furanthiol, 1-acetyl-1-pyrroline, ethyl thioacetate, dimethyl trisulfide, nonanal, 2-furfurythiol, acetic acid, methional, propanoic acid, (E,Z)-2,6-nonadienal, butanoic acid, isovaleric acid, 2-thiophenecarboxaldehyde, methionol, 5-ethylfurfural, (E,Z)-2,4-decadienal, (E,E)-2,4-decadienal, hexanoic acid, 2-acetylpyrrole, 4-hydroxy-2,5-dimethyl-3(2H)-furanone, octanoic acid, 2,6-dimethyloxyphenol. Most of these compounds were identified in both skipjack and albacore species, but their levels were different between the two types of samples. The saturated and unsaturated aldehydes could be from lipid autoxidation as well as thermal oxidation during canning process. The sulfur-containing compounds could be generated during cooking via Maillard reactions.

[P 022] Formation of volatile compounds and carotenoids degradation products in red pepper fermented by Lactobacillus parabuchneri

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Red pepper (*Casicum annuum* L) has been used as one of key ingredients of some fermented foods including *Gochujang* (fermented red pepper paste) and kimchi in Korea, mainly due to its hot and spicy sensation. During fermentation with microorganisms, some non-volatile components can be changed and degraded, leading to the formation of various volatile compounds, affecting the quality of foods. In this study, volatile compounds, including carotenoids degradation products, in fermented red pepper samples inoculated with *Lactobacillus parabuchneri* were investigated by gas chromatography-mass spectrometry (GC-MS) combined by stir bar sorptive extraction (SBSE) method. In addition, high performance liquid chromatography (HPLC) was employed for the analysis of carotenoids (carotene and neoxanthin). A total of 95 volatile compounds were identified in red pepper fermented by *L. parabuchneri*. Some carotenoids degradation products, such as ionone, cyclocitral, and damascenone, showed significant increase according to fermentation periods. In particular, the content of damascenone, which could be formed from neoxanthin degradation, was gradually increased during fermentation, although it was not detected in 0 day samples. In addition, partial least squares discriminant analysis (PLS-DA) was utilized to discriminate fermented red pepper samples according to fermentation periods. The application of PLS-DA to data of the volatile profiles revealed that the red pepper samples fermented by *L. parabuchneri* could be distinguished according to fermentation time. The contents of some alcohols, benzene and its derivatives, esters, hydrocarbons, lactones, pyrazines, and terpenes were increased in red pepper samples inoculated with *L. parabuchneri*, while those of aldehydes, sulfur-containing compounds, and ketones were decreased according to fermentation periods.

[P 023] Extrusion on aroma compounds in brown and polished rice

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Mechanic extrusion on aroma compounds in brown and polished rice was studied by gas chromatography-olfactometry (GC-O). Aroma compounds were isolated using solvent extraction followed by solvent-assisted flavor evaporation. Aroma extract dilution analysis (AEDA) was performed on both brown rice and polished rice before and after the extrusion process. A total of 71 odorants were identified. On the basis of flavor dilution (FD) values, the most important aroma compounds in extruded rice could be hexanal, heptanal, 2-acetylpyrroline, 1-octen-3-ol, octanal, (E)-2-octenal, nananal, and decanal. 4-Mercapto-4-methylpentan-2-one was also identified as potentially important aroma compound in extruded rice. The aroma compounds were similar in all rice samples but FD values were different. The FD values of 2-acetylpyrroline, 1-octen-3-ol in brown rice were much higher than in polished rice. Extrusion process greatly increased the FD values of most aroma compounds, particularly aldehydes in brown rice.

[P 024] Citral-like Thiophenes in Chicken Thigh Meat

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The isomers of 3,7-dimethyl-2,6-octadienal, more commonly known together as citral, are two of the most notable natural compounds in the flavor and fragrance industry. However, both isomers are inherently unstable, limiting its potential use in various applications. To identify molecules in nature that can impart the fresh lemon character of citral while demonstrating stability under acidic and thermal conditions has been a major challenge and goal for the flavor and fragrance industry. In the study of chicken thigh meat, several alkyl thiophenecarbaldehydes were identified by gas chromatography-mass spectrometry and gas chromatography-olfactometry that provided a similar citral-like aroma. The potential mechanism of formation in chicken is discussed. Furthermore, in order to explore the organoleptic properties of this structural backbone, a total of thirty-five thiophenecarbaldehyde derivatives were synthesized or purchased for evaluation by odor and taste. Certain organoleptic trends were observed as the length of the alkyl or alkenyl chain increased or when the chain was moved to different positions on the thiophene backbone. Several alkyl thiophenecarbaldehydes were tested in high acid stability trials (4 °C vs 38 °C) and outperformed citral both in terms of maintaining freshness over time and minimizing off-notes. Additional measurements were completed to calculate the odor thresholds for a select group of thiophenecarbaldehydes, which were found to be between 4.7 - 215.0 ng/L in air.

[P 025] Aroma profiles and proximate composition of Roselle seeds: Effects of different origin and different sample preparation methods

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Roselle (*Hibiscus sabdariffa* L.) is ranked among the most highly traded commercial and medicinal plants worldwide due to its phytochemicals and antioxidants capacity, high content of anthocyanin and vitamin C, and is also used as natural food coloring. Normally, in food industry only Roselle calyces are processed to produce various food products; the seeds are removed and disposed as a by-product. However, Roselle seeds are reported to be edible (Wilson and Menzel, 1964). To our knowlwedge, the study of Roselle seeds is limited and there is no aroma profile of Roselle seeds being reported. Therefore, this study addresses the influence of different origin on proximate analysis of Roselle seeds and different sample preparation methods on the aroma profiles of Roselle seeds. For both analyses, samples were collected from China and Malaysia. In the aroma analysis, samples were prepared by two different procedures (ground dry; ground and then mixed with water), which were hypothesized to potentially result in different aroma profiles. Aroma profiles were obtained through dynamic headspace sampling-GC-MS. Results showed that different sample preparation of Roselle seeds affects the amounts of aroma compound recovered. A total of 61 compounds were identified including alcohols (18), terpenes (15), aldehydes (13), ketones (9), furans (2), phenols (2), ester (1) and lactone (1). The major volatile compounds (by peak size; 2-methylpropanal, 2-methylbutanal, 3-methylbutanal, alpha-phellandrene, hexanal, 2-methyl-1-propanol, sabinene, 4-methyl-hexanone, beta-phellandrene, isoamylalcohol, 1-pentanol, 2-pentylfuran, para-cymene, 1-hexanol, 2-ethyl-5-methylphenol) were found in all different Roselle seeds samples in varying levels. Results from proximate analysis showed that Roselle seeds contain high total dietary fiber (49.8 to 54.6%), protein (21.3 to 23.6%) and lipid (11.8 to 18.1%).

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[P 026] Effects of Sodium Chloride, Potassium Chloride and Calcium Chloride on the Flavor Formation during Heating of Wheat Flour-Glucose Model System

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Metal cations interact with sugars and amino acids in a food system resulting in changes during Maillard (MR) and caramelization reactions. Degradation of sugars is accelerated in the presence of metal cations and 5-hydroxymethyl-2-furfural and 2-furfural are formed in higher concentrations as main products. On the contrary, the reactions of amino acids may be inhibited in the presence of metal cation, as evidenced by the mitigation of acrylamide formation from asparagine in the presence of calcium salts during MR. The aim of this study was to investigate the alterations in flavor profile of Maillard reaction model systems composed of wheat flour and glucose in the presence of NaCl, KCl, $CaCl_2$.Model doughs were prepared (wheat flour, glucose, water, and salt) and freeze-dried prior to dry heating at elevated temperatures, simulating the drying conditions on the surface of bakery product during thermal treatment. The ground dried mixtures (0.5 g) were transferred to tubes (with PTFE sealed screw caps) and heated at 180 °C for 5 min in an oil bath. Heated mixtures were analyzed by HS-SPME-GC/MS by adding 1 mL saturated NaCl.Addition of NaCl and KCl had no effect on the concentrations of the pyrazines, however a significant reduction was observed in the presence of $CaCl_2$. The effect of the salts on the formation of Strecker aldehydes varied across the amino acid precursor. In the presence of NaCl and KCl 2-methylpropanal, 2-methylbutanal and 3-methylbutanal concentrations increased while in the presence of $CaCl_2$ they decreased. On the other hand, all salts increased the level of methional and had no effect on phenylacetaldehyde. The most remarkable increases were observed in the concentrations of 2-methylfuran, 2-acetylfuran, 2-furfural and furanmethanol in the presence of $CaCl_2$. Results indicated that sodium and potassium have similar effects on the formation of the volatiles and therefore NaCl replacement by using KCl can be achieved without affecting thermal flavor formation. On the other hand, calcium as a divalent cation significantly reduces the volatile formation during MR and remarkably increases caramelization. Detailed studies on the reactants and products will be further investigated to understand mechanism of the alterations.

[P 027] An assessment of the effect of cinnamon spice on cocoa nibs (Theobroma cacao L.) - An approach to change flavor in stored roasted cocoa nibs

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The final flavour of fermented and dried cocoa has the potential to be manipulated at every stage of processing. The objective of this experiment was to determine whether the intrinsic flavour of 100g batches of roasted cocoa nibs could be altered to have a favorable cocoa cinnamon flavour by exposure of nibs to cinnamon sticks. Nibs were surrounded with cinnamon bark sticks at different concentration levels of 2g (2%), 10g (10%) and 25g (25%) per 100 g and stored either under aerated storage containers or in vacuum sealed storage bags. The time of exposure was also altered by sampling batches at five time intervals or infusion days, day 3, 7, 14, 28, 56. The treatments were arranged in factorial structure and replicated twice. A trained sensory panel was used to test the samples via descriptive sensory evaluation on a 10-point hedonic scale with an overall score and uniqueness evaluation of each sample. The 'Spice' flavour note, which was identified as a distinctively cinnamon note by the panelists, showed a significant ($P < 0.001$) interaction between concentration and storage condition, with the 'Spice' flavour note increasing in a much more pronounced way over concentrations in the vacuum treatment compared to the aerated storage. Infusion treatments with vacuum storage consistently showed higher mean spice flavour scores and increased significantly with storage time ($P < 0.01$) with no interaction of exposure time with either concentration of storage treatment. 'Floral woodsy' flavour note showed a significant ($P < 0.01$) interaction between concentration and storage treatment. Vacuum storage treatment at 25% concentration had higher mean scores for floral woodsy flavor note. The 'Uniqueness' of a sample, as identified by the panelists, also showed a significant interaction ($P < 0.001$) between concentration and treatment. The 25% concentration with vacuum storage gave the best uniqueness scores. The overall desirability score was significantly ($P < 0.01$) affected by concentration and was significant at 25% concentration. The outcome of the research indicated that the 25% infusions and vacuum treatment give or created a novel favourable and unique liquor (product) that is infused with cinnamon that has market potential for small to medium size chocolate makers and chefs.

Key words: cocoa nibs, flavor infusion, spice, vacuum storage

[P 028] Impact of Water-Soluble Precursors Leaching from Green Beans on Aroma Generation during Coffee Roasting

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Coffee is one of the most important international trade products. The two primary species of coffee dominating the world markets are Arabica and Robusta, which account for 61% and 38% of coffee production worldwide. Arabica, perceived with a smooth, and rich flavour is usually more desirable than Robusta that is concerned with a strongly muddy odour. Previous studies have attempted to improve Robusta coffee quality steaming or pre-soaking in water to removes substance responsible for the muddy odour (Becker et al., 1991; Izumitani & Yajima, 1992). However, several important flavour precursors, such as sucrose, protein, caffeine, trigonelline and chlorogenic acid are water-soluble and could be leached into the soaking water resulting in changes in the aroma generated during roasting. Therefore, the objective of this study is to investigate the loss of water-soluble aroma precursors pre-soaking of green beans, and the resulting impact on aroma generation during coffee roasting. Green Robusta coffee beans from the same origin were soaked in water with different time-temperature profiles. Samples were subjected to normal roasting (200 °C for 20 min) and then ground to a standardised particle size. Aroma compounds generated during roasting were evaluated by headspace analysis using Solid Phase Micro Extraction - Gas Chromatograph Mass Spectrometer. Water-soluble precursors such as sucrose, caffeine, trigonelline, chlorogenic acid, total water-soluble protein and minerals were detected in the soaking water by High-Performance Liquid Chromatography, BCA Protein Assay Kit and Inductively Coupled Plasma Mass Spectrometry. The results illustrated a significant impact of soaking time-temperature profile on the yield of water-soluble precursors in the soaking water. The loss of these precursors significantly affected aroma formation during roasting and resulted in a decreased level of furans, heterocyclic N containing compounds, ketones, organic acids, and sulfur-containing compounds ($P > 0.05$). However, the total yield of water-soluble precursors showed no significant impact on the level of pyrazines formation ($P > 0.05$). The results suggested that losses of water-soluble precursors could modify the total aroma formed during roasting as well as distort the final aroma profile.

[P 029] Revisiting the role of glycosidic aroma precursors on wine aroma: effects of microorganisms and of slow hydrolytical processes

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Grapes are determinant for the quality of the final wine since they not only provide a specific profile of nutrients which strongly determines the production of secondary metabolites by yeast, but they provide precursors of key aroma components. Glycosidic precursors were the first category of aroma precursors discovered and for long it has been known that they constitute the main source of relevant wine aroma molecules such as linalool, b-damascenone, b-ionone and some volatile phenols or vanillin derivatives. They are also main sources of some potential off-flavours such as 1,1,6-trimethyl-1,2-dihydronaphthalene (TDN) and may be also precursors of furaneol or of the ethyl esters of C6-branched acids.
In spite of their known importance and of the interest that their presence aroused in the 80's and 90's, the complexity of their genesis has made that its role in wine aroma genesis is not completely understood. Particularly relevant are the gaps in our knowledge in regards to the mass balance of the different precursors during fermentation and to the role that the remaining precursors play in sustaining wine aroma during aging. Difficulties arise because many aglycones undergo different chemical rearrangements to produce the aroma molecule. In order to better understand the role of yeast and of aging two large fractions of precursors from highest quality Riesling and Garnacha grapes were obtained by SPE, and used to prepare model musts. The musts have been fermented by different yeasts and resulting wines have been subject to accelerated aging in strict anoxic conditions. Analytical controls have been included all throughout the process in order to ensure an efficient control of the mass balance.
Results show that aromas formed from different grape varieties and, in combination with different microorganisms, lead to a high aroma diversity. Besides, this study has allowed to differentiate the aroma formation influenced by enzymatic or hydrolytic activity, as well as their evolution during bottle aging, enlightening about principal formation mechanism and the fate of these aromas during the shelf-life of wines.

[P 030] Organoleptic properties of dark chocolates investigated by direct-injection mass spectrometry (PTR-ToF-MS) and GC-Olfactometry

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Dark chocolates develop several organoleptic characteristics depending on cocoa origin, cocoa variety and fabrication process. These parameters influence the chemical composition of the chocolates, and particularly the qualitative and quantitative content in volatile organic compounds (VOCs) responsible for their aroma. Sensory evaluation is able to discriminate chocolates according to their organoleptic properties. A preliminary sensory study conducted on a set of 192 dark chocolates varying in terms of cocoa origin and variety allowed their classification into four distinct sensory categories. The first objective of this work was to check that this sensorial differentiation can be confirmed mainly based on VOCs composition. For this, a direct-injection mass spectrometry method using Proton Transfer Reaction Mass Spectrometry (PTR-MS) was used. The second objective was to identify the key odorants responsible for chocolates differentiation. Therefore, a GC-MS identification of targeted aroma compounds selected after GC-O analyses of extracts representative of each subset of chocolates was undertaken.

VOCs emitted from the samples were analyzed by dynamic headspace coupled to a PTR-Time of Flight (ToF)-MS instrument. The analyses of 1g of chocolate mixed with 1mL of artificial saliva in 20mL vials were performed in triplicate under stirring at 36.2°C after 2 hours equilibration time. The average areas under the curves obtained for the 2mn release of 314 significant ions present in the mass spectra were used to perform unsupervised multivariate data analyses. The produced 'chemical maps' showed that the headspace PTR-MS analyses of the chocolates allowed retrieving the classification of the 192 samples into the four sensory categories previously determined. Twelve samples (3x4) belonging to the four categories were selected and extracted using SAFE. The extracts were submitted to GC-O using a FFAP column and the detection frequency method. The odour events generated by a panel of 10 assessors were grouped into olfactive areas (OAs). On average 50 OAs were found in the extracts and the most frequent associated olfactory descriptors were floral, metal, sugary, cotton candy and peanuts. A correspondence analysis (CA) conducted on the complete set of GC-O data allowed to distinguish samples and their characteristic OAs that were further identified using GC-MS.

[P 031] Elucidation of the pattern of volatile compounds responsible of the odor profile in a fermented meat product (chorizo) during ripening time.

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Chorizo is a fermented meat product that undergoes many biochemical reactions during its processing, generating both volatile and non-volatile compounds, such as amino acids, aldehydes, organic acids and alcohols that are responsible of the characteristic odor and flavor profiles of chorizo. Odor perception is highly relevant on the overall acceptance in many types of foods because we commonly decide to ingest any product after smelling it through the orthonasal route. An odor is the result of more than a hundred volatile molecules that bind with specific receptors on the olfactory epithelium generating a pattern that elicits an electrical signal, which is transmitted to the brain developing an 'odor image'. This, for example, is what we could name herbal odor. Few investigations have focused on the patterns of volatile compounds that generate the principal odor in a product. The aim of this work was to elucidate the volatile compounds pattern that generated the principal odors (vinegar, fermented, rancid, pork meat, and pepper) in homemade chorizo during ripening time (0, 5, 12, 19, 26 and 33 days) using multivariate statistical analyses. Sensory analysis was performed by a panel specially trained for chorizo smell, while volatile compounds were extracted by SPME technique and analyzed by Gas Chromatography. Linear correlations between each odor and volatile compounds were determined as Pearson's coefficients; afterwards, Principal Component Analysis was applied to explore the inter-relationship between variables. A total of 144 volatile compounds were identified during the ripening time. The odor recognition pattern of vinegar was formed by 13 volatile compounds; butanal, propanal, dimethylamine, ethanol, heptanal, heptanoic acid, ethyl octanoate, phthalic anhydride, 2-metyl propanal, 2,3-butanediol, acetic acid and phenol. The pattern for fermented had 13 compounds; undecane, pentanal, propanoic acid, hexanal, ethyl octanoate, ethyl decanoate, 2-methyl-1-butanol, benzaldehyde, acetic acid, diallyl sulphide, 2,3-butanediol, 2-nonenal and isocaryophillene The pattern for rancid odor involved 26 volatile compounds, some of them were 4-Hexen-1-ol, 1-hexanol, 1-octen-3-ol, pentane, 2-pentanone, 1-pentanol, hexanal, hexanoic acid, 2-octenal, 2-octanone, benzenacetaldehyde, benzaldehyde and others. The pork meat and pepper odors were linked to 32 and 6 volatile compounds, respectively.

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[P 032] Influence of salt reduction on flavour release in ready-to-eat meal

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Salt reduction in food is becoming a major concern for public authorities since a high sodium diet leads to harmful effects on health. As ready-to-eat meals are one of the main sources of sodium, industrials are largely encouraged to reduce it in their formulation. However, salt is a well-known flavour enhancer and a reduction of its amount could modify the release of the volatile compounds and thus flavour perception. The aim of the KIDYSALT project* is to study the impact of salt reduction on food properties and to formulate salt reduced food with satisfying organoleptic qualities.
A recipe of pasta with chicken and cheese sauce with four levels of salt (control = 0.8g salt/100g food, -20%, -30%, -40%) was studied. Volatile organic compounds (VOC) were extracted by HS-SPME and analysed by GC-FID-MS. ANOVA followed by LSD test were performed on semi-quantification results (a=5%). The same samples were analysed by sensory analysis. A ranking test was performed with a trained panel (21 judges) on 11 attributes (odour, texture, flavour). Friedman test was performed on these data (a=5%).
Sensory analysis showed that salt reduction had no impact on the texture and odour but modified the perception of the aroma and taste. The flavour descriptors 'savoury', 'chicken', 'pepper' and 'salty' significantly decreased with salt reduction. The modifications perceived in sensory analysis could be explained by the chromatographic profile of the products. The impact of salt on the release of the VOC is known as the 'salting out' effect, and seems to be different depending on their chemical class. The main variations were observed on the amount of terpenes which decreases with salt reduction. The presence of terpenes, known as high odour-active compounds, could be related to the use of pepper and nutmeg in the recipe and possibly explained the decrease of the 'savoury' and 'pepper' flavours.
Solutions to compensate the aromatic loss due to salt reduction have to be reached by industrials in order to produce nutritionally improved food products with satisfying organoleptic qualities. The use of herbs and spices, rich in terpenes, may be a natural way to compensate salt reduction.

*Program founded by the County councils of Pays de la Loire

[P 033] Apple Flavour Characterisation from Skin to Flesh - On Basis of the Old Apple Variety 'Ilzer Rose'

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Apple cultivation has a long tradition in Austria, especially in Styria. About 25% of Styrian apples are grown in so-called meadow orchards. The traditional meadow orchards are a specific type of landscape since hundreds of years and have an enormous number of old apple varieties. Even though these varieties have been cultivated in this region for many decades, the flavour properties are not described. For most varieties, a molecular characterisation of the flavour compounds is lacking.

The old apple variety 'Ilzer Rose' is one of these old varieties which have been described especially from this region near the village Ilz (Austria) since about 1900. The rather small, intense-red apples with white flesh possess a very pleasant, intense fruity and slightly rose-like flavour. The aim of the study is to characterize the flavour of the old apple variety 'Ilzer Rose', but also to identify the main volatile compounds of the intact apples, as well as skin, flesh, and a mixture of the latter two. The formation of flavour compounds is dependent on enzyme activity of the fruits, but also on the conditions used during fruit processing. To be able to focus on primary flavour compounds, apple enzymes have to be inactivated before the investigations.

For the flavour characterisation, two different complementary approaches were used: (i) complete sensory characterisation with the use of an expert panel of the intact as well as of the sliced apples after enzyme inactivation, and (ii) identification of the volatile compounds by using GC-MS and comprehensive GC-MS (GC x GC-MS) after headspace SPME. The enormous capacity regarding separation as well as sensitivity of comprehensive GC x GC-MS allows deep insight into the flavour of this old apple variety.

[P 034] Analytical mapping of a Swiss Gruyère Cheese to highlight the distribution of aroma compounds using HS-ITEX-GC-MS-PFPD

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The evolution of aroma compounds in cheese depend on numerous factors such as the intrinsic raw milk flora, the bacterial cultures used for its manufacture, ripening conditions, and the texture of the cheese. In addition, it is well known that the distribution of aroma compounds in cheese is not homogenous. In order to understand which parameters influence the complex equilibrium of aromas in a large-scale food matrix such as an entire Gruyere cheese loaf, we generated a mapping of relevant aroma compound groups. These results contribute, for example, to the improvement of specific bacteria cultures for cheese production.
In the present work we studied 40 selected volatile aroma compounds in a 32 kg commercial Gruyère cheese loaf made from raw milk. For the analyses, one-half of the loaf was divided into a total of 258 equivalent pieces, taken over 5 levels from the bottom to the top rind, smear included. Each piece was extracted and analyzed by Headspace - In -Tube Extraction - Gas Chromatography - Mass spectrometry / Pulsed Flame Photometric Detector (HS-ITEX-GC-MS/PFPD). The target molecules were classified into six chemical families. Data was processed statistically to visualize the distribution of the aroma compounds within the cheese loaf. Additionally, a trained sensory panel evaluated the samples.
A clearly inhomogeneous distribution of aroma compounds was found within the Gruyère cheese. The associated variation in aroma perception was confirmed by the sensory tests. The sulphur compounds and pyrazines are more abundant in the cheese rind and migrate only a few centimetres in direction of the centre. In contrast, the intensity of carboxylic compounds is higher in the centre of the cheese. It is assumed that the observed aroma distribution is generated through chemical oxidation reactions near the rind and enzymatic, anaerobic reactions in the center, respectively. These results deliver insights into the complex distribution of aroma compounds in a cheese loaf. As a consequence, valuable knowledge for improved development and an adapted use of specific bacterial cultures for cheese production is provided. In addition, procedures of cheese sampling for analytical studies can be improved based on these findings.

[P 035] Aronia melanocarpa - the Styrian 'Super-Berry' A Flavour Characterization of Black Chokeberry NFC Juice

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Recently, the black chokeberry (*Aronia melanocarpa*) has gained new popularity. Traditionally cultivated in Eastern European countries and used as domestic remedy in these regions, black chokeberries have recently been incorporated into the group of 'superfoods'. Its superfood status is based on the very high antioxidative capacities due to the enormous concentrations of polyphenols (i.e. anthocyanins and proanthocyanindins, flavonols as well as phenolic acids). Several papers have proved the health benefits of aronia showing positive impact on blood pressure values, cholesterol- and triglycerids concentrations, anti-inflammatory effects, anti-tumor activity and as well as the exhibition of immunomodulatory activity in breast cancer patients.
In contrast to the health impact of aronia berries, little is known about the flavour properties of aronia products. Aronia juice represents a fruit juice that shows significantly different flavour properties in comparison to commonly consumed juice types. Besides a very complex odour, the taste and trigeminal sensations seem to be more important than for other juices. In this study, we aimed to reach a characterization of the flavour properties of aronia NFC juice with focus on the volatile compounds. Juices from one cultivar only (cultivar *Nero*) were obtained from various farmers from different cultivation sites in this region. Prior to our investigations, the juices had been evaluated in course of a local juice competition which made it possible to include high quality juices only. Headspace SPME was used for the subsequent analysis of the volatile compounds by using GC-MS, comprehensive GC x GC-MS and GC olfactometry. Sensory evaluation was applied by the use of (quantitative) descriptive analysis and projective mapping. The results show that - even though we tried to keep the external parameters as constant as possible - the flavour properties as well as the concentrations of the volatile compounds of the juices varied to a great extent. In this paper we demonstrate the correlation of several compounds with high odour impact with the overall flavour of the juices. As our producers would like to offer a superfood to their customers that does not only show health benefit, but that also gives pleasure upon consumption, these results serve as a broad basis for further investigations to improve the sensory properties of domestic aronia juice.

[P 036] Impact of media compositions on microbial-mediated volatile organic compounds released profile: Case study of a food spoilage bacterium in a model system

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The present study used proton transfer reaction mass spectrometry (PTR-MS), complemented with GC-MS for identification purposes, to investigate temporal changes in the volatile organic compound (VOC) release profile of a food spoilage *Pseudomonas* species. Due to the complexity of food matrices and therefore the difficultly to relate characteristic volatile biomarkers to specific carbon and/or protein sources, a simplified model system was designed to mimic a typical food spoilage scenario under controlled conditions. The food system consisted of Vogel's broth, supplemented with glucose (0.5 or 1%) and/or protein (egg white powder at 0 or 2%) with an inoculated *Pseudomonas fluorescence* bacterium cultivated at 25 °C. The level of glucose and/or egg white protein influenced the VOCs release profile, particularly for alcohols, esters, aldehydes, ketones and S-derivatives. Protein supplementation had the largest effect on the separation of the samples on PC1 and PC3 (42% of the variance) with lesser effects due to glucose supplementation and length of incubation time.. Separation of m/z on PC1 plot with 35% of variance were due to the presence of compounds such as alcohols (ethanol, 2 methyl-1-propanol, 3-methyl-1-butanol), sulphur derivatives (methanethiol), 2-methyl butanoic acid, ketones (3-hydroxy-2-butanone, 2-nonanone) and esters (methylacetate, ethyl acetate). The glucose content (0.5 or 1%) had a more limited effect on the VOC release profile, mainly impacting on the signal intensity of individual compounds, such as m/z 89 (3-methyl-1-butanol). In contrast, the presence of egg white protein enhanced production of volatiles such as m/z 75 (2-methyl-1-propanol) and m/z 63 (dimethyl sulphide) regardless of glucose level present in the medium. The present study highlighted how variations in growth phase and media composition can have a dramatic impact on the VOC release profile (fingerprint) from a food spoilage microorganism.

[P 037] On-line coffee flavour formation analysis using PTR-ToF-MS during roasting under different atmospheres

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Roasting is accepted as contributing most significantly to coffee aroma. During roasting the green coffee beans are transformed both physically as well as chemically into the consumer product. Thermally induced chemical pathways include the Maillard reaction, which is known to contribute a plethora of volatile organic compounds (VOCs). Some of these volatiles will be trapped within the coffee matrix and contribute to the coffees characteristic aroma. These reactions occur within the roaster that is constantly evacuated with air in order to facilitate dehydration of the beans. While the evacuation of the roasting chamber with air is routinely carried out, the importance of this oxidative atmosphere and its influence on aroma formation pathways has yet to be elucidated.
Using on-line proton transfer time-of-flight mass spectrometry (PTR-ToF-MS) the present study investigates the influence of gas composition, air versus nitrogen, on the exhaust gas VOC profile. Roasting was conducted by introducing the gas, either air or nitrogen, into an electrically heated reaction vessel, which mimicked temperature profiles encountered within a coffee roaster. Roasting was completed within 20 min reaching a temperature of 190 °C inside the roasting chamber.
The resulting dynamic PTR-ToF-MS time-intensity profiles yielded 141 mass peaks in total. When examining the area under the PTR-ToF-MS time-intensity curves five of the mass peaks were higher when roasting under nitrogen, while 26 mass peaks were higher when roasting in air. Signal intensity of protonated hydrogen sulphide was found to be higher when roasted under nitrogen, whereas intensities of seven mass peaks (CH_2OH^+, CH_2NO^+, $C_4H_6H^+$, $C_5H_6H^+$, $C_7H_6OH^+$, $C_9H_{12}O_2H^+$) were higher for 30 % of the roasting duration when coffee was roasted under air. Gas chromatography mass spectrometry analysis of the roasted product confirmed that methanethiol content was present at a higher concentration in coffee samples roasted under nitrogen, whereas in coffee sample roasted under oxidative conditions dimethyl disulphide was present at a higher concentrations. Conversely, to the coffee roasted in air, coffee roasted under nitrogen had an unpleasant smell and lacked the distinctive coffee aroma.

[P 038] Characterization of the Key Aroma Compounds in Two Types of Keemun Tea

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Due to the floral, sweet and slightly smoky odor notes, fine Keemun tea is one of the most famous Chinese black teas highly appreciated by consumers. In this study, we investigated two different types of Keemun tea differing in raw material and manufacturing process, namely '*gongfu*' type and '*mingyou*' type Keemun tea. Application of an aroma extract dilution analysis on the volatile isolated fractions of Keemun tea infusions resulted in the identification of 30 odorants in the flavor dilution (FD) factor range of 64-1024. Geraniol, 4-hydroxy-2,5-dimethyl-3(2*H*)-furanone and coumarin showed the highest FD factor followed by methional, 2-phenylethanol, phenylacetic acid, and 3-methyl-2,4-nonanedione. These odorants were identified in both Keemun teas. Quantitation of 38 odorants by means of stable isotope dilution assays (SIDA) and calculation of odor activity values (OAV) yielded 27 key odorants with an OAV > 1. The obtained quantitative data enabled the preparation of aroma recombinants of both types of Keemun tea. Comparative aroma profile analyses between recombinants and respective types of Keemun tea showed excellent similarity of the overall aromas and validated these volatiles as the key components creating the unique odor profile of Keemun tea.

[P 039] Age-related changes in oral physiology and their significance in aroma release and perception

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Introduction: With aging comes many physiological changes including those in the oral and nasal cavity, such as reduced salivary flow, respiratory changes and impaired dental status and function [Vandenberghe-Descamps, 2016., Duizer, 2015., Coffey, 2012]. These changes may impact on aroma release and subsequently the perception and enjoyment of foods, leading to a risk of undernutrition.
Aim: This review aims to summarise current literature on how oral and nasal physiology is affected by both aging; with a focus on the changes which are significant in aroma release and perception.
Method: The main databases searched were Scopus and Web of Science using specific keywords; some examples being 'aging', 'oral', 'nasal', 'saliva', 'respiration', 'oral processing' and 'dentition'. References within selected papers were also investigated.
Results: Papers were selected by their relevance to the research question. The most significant physiological changes, with relevance to aroma release and perception, will be presented.
Conclusions: This research is novel and is the first stage in understanding how aroma release is affected by aging. With the worldwide projected increase in the older population, the economic and social burden of undernutrition is expected to be severe. Tackling this issue is of interest to both clinical practice and industry as there is potential for successful new products to be developed which meet the needs and desires of this specific, increasing population.

[P 040] Sensory and physicochemical quality attributes of honeys from native plants: a sensometric approach

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In order to determine the botanical origin of honeys, it must be evaluated the sensory characteristics, physicochemical properties, and results obtained from pollen analysis. Overall, these investigations provide results that are valid but not confirmatory. However, the aroma profile is one of the most typical features of honeys for both organoleptic quality and authenticity. By the high number of volatile components, the aroma profile represents a 'fingerprint' of a honey, which could be used to determine its origin. Aroma compounds are present in honey at very low concentrations as complex mixtures of volatile components of different functionality and relatively low molecular weight. The aroma of honey has several functions, not only conveying its essential character and providing variety and interest to its consuming, but also alerting us about deteriorating. Since GC-MS combines high separation efficiency and sensitivity and provides qualitative and quantitative data for the compounds involved, it is usually the technique of choice for their determination. But, GC-O is essential in determining which aroma compounds are likely to contribute to the aroma of a foodIn this study, we propose a sensomics approach to interpretate a combination of GC-MS and olfactometry results in order to stablish the main determinants of the differences, and preferences, in the flavor profiles of less known monofloral honeys selected as test model. Besides, using examples of identified off-flavors, it will be shown, how close odorant concentrations may determine liking and disliking of the honeys studied. Monofloral honeys from aromatic native plants of Uruguay were studied and the data processed using multivariate statistical approaches.

[P 041] 9-decen-2-one biosynthesis by Aspergillus oryzae

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ANTILLONE TM (9-decen-2-one) is a methyl ketone with olfactory and taste properties that may be used in flavourings and fragrances applications.
Bioconversion of undecylenic acid to 9-decen-2-one represents an attractive opportunity for synthesizing a bio-based product, that can be label 'natural' according to current food regulations. In this work, the possibility of producing ANTILLONE TM with a high yield was investigated by using cells of Aspergillus oryzae strain. Process parameters were optimized both for the biomass production phase and the bioconversion phase using food-grade undecylenic acid as substrate. Under optimized conditions, 9-decen-2-one production up to 14,8 g/L was achieved.
Flavour properties of ANTILLONE TM were evaluated in various applications and the molecule was described as powerful and fruity, instantly recognizable as pineapple. It can easily replace allyl hexanoate.

[P 042] Effect of degree of milling on the taste characteristics of pigmented rice wine

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Pigmented rice wine (PRW) is produced domestically from whole grain rice in some Asian countries, especially China. In contrast to Sake, a pale/colourless beverage that is prepared from rice which has been milled to remove the bran, PRW is brewed from rice which has not had the bran removed. Although the antioxidant properties have been investigated in PRW much less is known in terms of its characteristic flavour which, unlike Sake, has a distinctive savoury taste and smoky aroma. The hypothesis of this study is that the bran fraction of the pigmented rice not only generates a higher antioxidant activity than Sake, but is also responsible for the development of the characteristic taste and aroma. For this study, pigmented rice was subjected to a different degree of milling (whole grain, 30%, 50% and 65%), brewed with an optimized brewing process (2 days for saccharification, 9 days for fermentation at 30°C) and pasteurised at 70°C for 10 min. The ethanol content, as well as compounds contributing to taste including sugars, organic acids, free amino acids, cyclic dipeptides (diketopiperazines (DKPs)), gamma-glutamyl peptides and also phenolic compounds were characterised in these PRW samples.
The degree of milling did not affect significantly ($p > 0.05$) the ethanol content of the PRW samples (11.6-12.3 %). Aspartic acid and glutamic acid were the predominant amino acids found in all wine samples, especially wine brewed from unmilled pigmented rice. The glutamic acid was present at concentrations above the reported threshold and is likely to contribute to the umami taste in PRW. Three DKPs (cyclo(pro-val), cyclo(Ile-pro) and cyclo(leu-pro)) which are known to impart bitter/astringent or metallic tastes to wine, beer, beef and coffee, were identified in all samples, and they were highest in wine brewed from unmilled pigmented rice ($p > 0.05$). Cyclo(Ile-pro) and cyclo(leu-pro) were present in the unmilled pigmented rice wine at concentrations higher than their reported threshold and are likely to contribute to the bitter taste. In addition, this study will report the presence of other unique taste-related compounds responsible for the astringency notes and kokumi taste in PRW.

[P 043] Optimisation and characterisation of the chocolate aroma developed during fermentation and roasting of jackfruit seeds

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The flesh of the jackfruit (*Artocarpus heterophyllus* Lam.) is popular in tropical countries where it grows in abundance in the wild. The seeds, which are usually discarded, account for 15-18% of the weight of the fruit and are an under-utilised waste stream which could be exploited by local communities in Brazil. In this paper, we show that when jackfruit seeds are fermented and roasted using a process similar to that used for cocoa beans, a distinctive chocolate aroma develops. Various novel applications are currently being developed for its use as a partial substitute for cocoa powder in cakes, cappuccino and cosmetics.
The development of the desirable chocolate aroma is very dependent on the post-harvest treatment, and the subsequent drying and roasting processes. Response surface methodology was used to compare fermentation and acidification steps prior to roasting, and to identify optimum roasting conditions to maximise the chocolate aroma of the roasted seeds. Twenty-seven different roasted jackfruit seed powders were assessed for 'chocolate aroma' by a sensory panel (n=162) using ranking tests. Moisture, colour and pH were monitored for comparison with cocoa powder and other substitutes such as carob and cupuaç.
The best products were selected for volatile analysis, before and after roasting, using either SPME/GC-MS or SPE/GC-MS, and compared to a commercial cocoa powder. The volatile profile will be discussed in relation to the precursors present. GC-Olfactometry of the SPME extracts revealed 59 odour-active regions, 29 of which were in common with those reported to have high flavour dilution factors in cocoa or chocolate extracts. These included 3-methyl-butanal, phenylacetaldehyde, trimethylpyrazine, 2,3-diethyl-5-methylpyrazine and 2-phenethyl acetate which are amongst those most often cited. Many of the other aroma regions were described as cardboard/earthy/typical jackfruit aroma and were attributed to methylpropyl- and methylbutyl-substituted pyrazines and pyrroles which were not found in the cocoa extract by GC-O. Identification of these pyrazines was by comparison with authentic standards where possible or with those previously synthesised in our laboratory. Those previously unreported were generated in glucose/glycine model systems heated with valine, leucine or isoleucine. Quantitative comparison of selected compounds was carried out by stable isotope dilution analysis.

[P 044] Investigating the phytochemical, flavour and sensory attributes of mature and microgreen coriander (Coriandrum sativum).

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The term 'microgreen' is generally used to describe young (7 - 14 days) stem and leaves of growing plants. In recent times, microgreens have been the subject of much interest due to their higher concentrations of nutritive and bioactive compounds in comparison to their mature plant counterparts. However, there is currently little information available in relation to the flavour and sensory attributes of microgreen species, which may ultimately prove important in determining consumer acceptance. In this study, the flavour profile and sensory attributes of mature and microgreen coriander (*Coriandrum sativum*) were investigated, while the total phenolic, carotenoid and chlorophyll contents were also measured.
A total of 49 volatile compounds were identified in mature and microgreen coriander using SPME-GC-MS, where terpenes (36% and 75%) were the main aromatic compounds present. Elevated concentrations ($>$ 10-fold) of linalool and pinene, the major flavour and aroma compounds associated with coriander, were observed in microgreen samples in comparison to mature ones. Descriptive evaluation showed that microgreen coriander was rated as more intense for both bitterness and sweetness ($P < 0.05$). Microgreen extracts were shown to contain significantly higher ($P < 0.05$) levels of phenolics in comparison to mature extracts, while no significant difference was observed in either carotenoid or chlorophyll content.
The present study showed that there are significant differences between microgreen and mature plants in both their nutritional and organoleptic properties. The knowledge of these differences is important for consumer acceptance of microgreens as a product and for incorporation of these plants into food matrices.

[P 045] Research on the aroma characteristics and impacts of the nonvolatile matrix composition on the aroma release of Vidal icewine based on sensomics

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The key aroma compounds of Chinese Vidal icewine were characterized by means of gas chromatography-olfactometry (GC-O) coupled with mass spectrometry (MS) on polar and non-polar columns. Solvent-relative extraction (solid-phase extraction, SPE) was selected as a suitable method for icewine. The impacts of icewine non-volatile matrix on important aroma compounds were studied, further.Their flavor dilution (FD) factors were determined by aroma extract dilution analysis (AEDA). A total of 59 odor-active aroma compounds in three ranks of Vidal icewines were identified, and 28 odorants (FD $>$ 9) were further quantitated for aroma reconstitution and omission tests. γ-Damascenone showed the highest FD value of 2187 in all icewines. Methional and furaneol were first observed as important odorants in Vidal icewine. Aroma recombination experiments revealed a good similarity containing the 28 important aromas. Omission tests corroborated the significant contribution of γ-damascenone, and the entire group of esters. Besides, 4-hydroxy-2,5-dimethyl-3(2H)-furanone (furaneol) and 3-(methylthio)-1-propanal (methional) also had significant effects on icewine character, especially on apricot, caramel, and tropical fruit characteristics. By instrumental analysis and sensory evaluation, the impacts of icewine non-volatile system on 4 kinds of important aroma compounds aroma were explored. The results showed that ethanol, fructose and (-)-epigallocatechin (EGC) had different impacts on headspace concentration and intensity of aroma compounds.

[P 046] Identification and quantification of aroma-active compounds during soy sauce fermentation process

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Soy sauce, a traditional fermented soybean product, is widely used as flavoring in Asian cuisine, and its popularity in the Western countries is growing up due to its characteristic flavor. High-salt liquid-state fermentation soy sauce (HLFSS) is considered as the traditional Chinese-type soy sauce and its flavor quality is generally higher than others. HLFSS production contains two fermentation stages: *koji* fermentation stage (solid-state fermentation) and *moromi* fermentation stage (liquid-state fermentation). The typical HLFSS production has a long *moromi* fermentation period (90-180 days) and the high brine solution concentrations (17-20% NaCl). However, the odorant profile evolution during two-stage fermentation process of HLFSS are not fully described.

Therefore, the aim of the present work was to determine the formation of key odorants in HLFSS during the fermentation processus. To do that, first a comparison of the usefulness of three extraction methods (HS-SPME, SDE, and LLE) for isolation of aroma-active compounds by using sensory evaluation, gas chromatography-mass spectrometry/olfactometry (GC-MS/O) and aroma extract diluted analysis (AEDA), was carried out. A total of 61 aroma-active compounds were identified in soy sauce, among which 38, 41 and 40 aroma-active compounds were detected by using HS-SPME, SDE, and LLE, respectively. The volatiles with caramel-like, roast, fruity and malty notes were the major aromas in soy sauce. The most intense aroma-active components in HLFSS were: 2-phenylethanol, 3-methylbutanal, 2-methylbutanal, 2-methyl-1-butanol, 3-methyl-1-butanol, ethyl 2-methylpropanoate, 3-(methylthio)propanal, phenylacetaldhyde, maltol, HEMF (2 isomers), sotolone, HDMF and 2-methoxyphenol. Sensory evaluation results showed that the smells of three different extractions were remarkably different. It appeared that both SPME and LLE methods should be used for the fully characterization of odor-active compounds in soy sauce because of their high representativities of the global aroma of original soy sauce. Secondly, by using these two methods, the changes of important odorants during *koji* and *moromi* fermentation processes were monitored and quantitated. The results showed that most of the key aroma-active compounds were already present in the *koji* stage.

[P 047] Quantitation of the newly evidenced glutathione S-conjugates in dual-purpose hop varieties. Efficiency of chemical and biochemical pathways to release free thiols through the brewing process.

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As in other food matrices such as grape, onion and bell pepper, many odorant thiol precursors occur in hop. The occurrence of cysteine S-conjugates has been demonstrated. In plants, cysteine-S-conjugates derive from their glutathione S-conjugate equivalent, which are involved in detoxification [1-2]. Since the grapefruit-like 3-sulfanyl-4-methylpentan-1-ol (3S4MPol) and 3-sulfanylhexan-1-ol (3SHol) were found in monovarietal dry-hopped beers at concentrations much higher than expected on the basis of the free thiol content in hop and their cysteinylated precursors, S-glutathione precursors were investigated in three dual-purpose hop cultivars (Amarillo, Hallertau Blanc and Mosaic). Their chemical syntheses have been adapted from Roland *et al.* (2010) [3]. The occurrence of S-3-(1-hydroxyhexyl)glutathione (G-3SHol) and S-3-(4-methyl-1- hydroxypentyl)glutathione (G-3S4MPol) was confirmed in those three cultivars, at levels well above those reported for their cysteinylated counterparts [4].
The aim of the present work was to assess the linked-potential in other dual-purpose hop cultivars, namely Citra and Sorachi Ace. The extraction pathway of glutathione adducts, as described by Kankolongo *et al.,* was used. HPLC-ESI(+)MS/MS allowed us to quantify G-3SHol (70 and 64 mg/kg in Citra and Sorachi Ace respectively), whereas G-3S4MPol was not detected. In order to understand how free thiols can be released through the brewing process, various chemicals, enzymes and yeast strains have been compared in their efficiency to degrade glutathione adducts.

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[P 048] Tracking of hop-derived compounds in beer during fermentation with PTR-TOF-MS

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The craft beer market is experiencing a rapid increase in growth. To help brewers optimise hop character, and to make beer with distinctive hop profiles, a better understanding of the role that yeast play in the development of hop character is required. Beyond anecdotal evidence, a paucity of published data exists on the interactions between hop varieties and different yeasts and the resulting effect on beer flavour. In the current study, proton transfer reaction-time of flight-mass spectrometry (PTR-TOF-MS) was used as a novel, direct and real-time analytical method to monitor small-scale fermentations carried out in 20 mL vials (3 mL sample volume) at 20 °C with repeated measurements of the headspace VOCs every six hours for four days. A design matrix of two yeast strains (California Ale and Edinburgh Scottish Ale) and two New Zealand aroma hop varieties (Motueka and Nelson Sauvin), together with their respective no addition controls, were used to investigate yeast-hop interactions. VOCs that showed evidence of hop-yeast interactions were identified. Differentiation between isomeric compounds was achieved through separation with fastGC and identification of compounds was supported by GC-MS and scientific literature.
The results highlighted the advantages of using online analytical measurements, such as PTR-TOF-MS, to understand temporal changes that occurred in VOCs during fermentation. For example masses such as ms145.121 (2-nonanol, or ethyl hexanoate), ms105.068 (pentanethiol, or 3-methyl-1-butanethiol) and ms173.153 (isoamyl isovalerate, or octyl acetate) initially increased during the fermentation process and then decreased towards its end due to competing reactions. Distinct differences were observed in the VOCs profile of the different beers based on combinations of yeast strain and hop type; e.g. samples with Motueka and California Ale were associated with higher levels of ms75.077 (2-methyl-1-propanol), while samples with Motueka and Scottish Ale had higher concentrations of ms137.132 (pinene, or myrcene) and ms89.057 (3-methyl-1-butanol).
A better understanding of how hop-derived compounds in beer are influenced during fermentation by yeast will improve our understanding of the generation of the hop aroma of beer and will give insight on how to achieve a desired hop character by selecting yeast strains and modifying fermentation parameters.

[P 049] Reaction pathways of alpha-diketones in model systems and real foods

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Numerous studies have been conducted to better understand the generation of the buttery smelling 2,3-butanedione from reducing sugars. The majority of these studies were carried out in model systems and permitted to propose several reaction pathways. The use of labelled precursors and the introduction of the so called Carbon Module Labelling (CAMOLA) technique has allowed gaining a more precise insight into the formation pathways, but also estimating their relative importance [1]. The reaction mechanisms were shown to be strongly affected by reaction conditions such as moisture, temperature, pH and type of amino acid [1-4]. Similarly to 2,3-butanedione, the generation of 2,3-pentanedione was also shown to proceed by several mechanisms, i.e. from intact skeleton, by recombination of C4/C1 or C3/C2 sugar fragments, and by alanine mediated chain elongation of methylglyoxal [3-5]. However, the impact or reaction conditions on the importance of the individual pathways contributing to 2,3-pentanedione is much less understood as compared to 2,3-butanedione.
The aim of this study was to gain additional knowledge regarding the impact of reaction conditions on the formation of both a-diketones in model systems containing glucose and amino acids and to compare the results with those obtained for extruded cereals, wafers and roasted coffee.

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[P 050] Unravelling the effects of interindividual variability of human saliva (flow and composition) on aroma compounds

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In the last 20 years a lot of research has been devoted towards the understanding of the intra-oral release of aroma compounds, and particularly about the role of saliva on this process [1]. During eating, aroma compounds are released from the food matrix and dissolved in saliva, where they can be submitted to different effects (e.g. retention, salting-out, hydrolysis) due to enzymes, proteins and/or salts. These effects might determine the rate and the type of aroma compounds available to reach the sensory receptors. In spite of the well-known variability of saliva among individuals [2], most of the studies on this topic have been carried out with artificial salivas or pools of human saliva, which cannot reflect this variability, in particular in specific populations such as elderly.
Therefore the main objective of this work has been to elucidate the role of human saliva on aroma compounds taking into account interindividual variability and matrix effects.
For this work, a wide variety of experimental approaches have been used. *Ex vivo* methodologies adapted to the use of small volumes of saliva have been developed to explore the effect of saliva on 17 aroma compounds. HS-GC analyses have shown that carbonyl compounds are more affected than alcohols by saliva composition (protein content and total antioxidant capacity (TAC)). HS-SPME-GC/MS and LLE-GC/MS results allowed identifying new products from the reduction of the affected compounds (e.g. aldehydes to alcohols and diketones to hydroxyketones) suggesting a role of oxido-reductases. In a further experiment, the *ex vivo* methodologies were tested on salivas from older individuals (n=30) presenting a low or normal salivary flow and on 3 aroma compounds. Interestingly, TAC explained also significantly the differences observed on aroma release between the two groups (ethyl hexanoate $p=0.010$; octanal $p=0.008$ and 2-nonanone $p < 0.001$). Finally, *in vivo* studies using PTR-ToF-MS have allowed to assess the role interindividual variability of saliva (flow and composition) in older individuals (n=80) in a closer consumption situation (on line monitoring and presence of matrix components).

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[P 051] New comprehensive procedure for enhanced data analysis and interpretation of Real-Time Measurements: A unique feature for real time flavour generation.

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Real-time measurements of low-abundance aroma compounds in breath from release during food consumption are already feasible due to progress in analytical technologies, such as PTR-ToF-MS. Nevertheless, the information content of real-time measurements is not fully exploited, due to the limited number of suitable data handling methods for, namely, in-vivo measurements [1]. Other software tools have been reported, but not focusing on food systems [2, 3]. This study developed a data scientific procedure to enhance flavor data analysis and interpretation from real-time studies, during food processing and consumption. The developed software addresses challenges such as mass calibration, variable number reduction and extraction of relevant masses. The developed features include 1) data projection, 2) establishment of a threshold for peak apex extraction, 3) visualization of sample expression for a specific mass, 4) application of co-clustering and principal component analysis for sample clustering exploration. These were validated for real time flavor generation in a dynamic study designed to evaluate different parameters in the formation of phenylacetaldehyde in model systems. Sequential additions of metals, glucose, gallic acid as well as sulphur dioxide have been tested. As way of example, it was observed in real time that different reaction rates for phenylacetaldehyde formation occured when metals were added in the end or in the beginning of the experiment. The developed software showed a considerable increase in efficiency of data treatment mainly in the extraction of candidate masses, capable to be contextualized for both flavor release and flavor generation as function of process conditions.

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[P 052] Advances in understanding unpleasant herbaceous character of red wines

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Sometimes red wines have unpleasant herbaceous and/or vegetative aromas, which may cause consumers rejection. In some cases these odors appear in wines make with grapes known for their pyrazine character, for example Cabernet Sauvignon, however vegetative notes appear in other varieties, which are appreciate for their fruitiness. These attributes could be associated with a lack of ripeness of grapes. Until now, previous studies about herbaceous character [1] of wines report that responsible compounds could be: aldehydes and alcohols, alkylmethoxypyrazines and selected sulfur compounds; in contrast there are wines with unpleasant vegetative notes which do not have high concentration of compounds mentioned before.
The objective of the present work is elucidate sensory equilibria responsible for unpleasant herbaceous notes in red wines. Fifteen oenologist were invited to participate in a sensory analysis of 15 different wines. Panelists were asked to orthonasally and retronasally smell each sample and to rate the intensity of herbaceous note of wines, and other attributes which were found in wines too. Six wines were selected with herbaceous characteristics and one which had not off-odour (reference). One of the herbaceous wine and the reference were fractionated using reverse phase, then fractions were submitted to sensory analysis by 'sorting task' method. The chosen fractions and wines were analyzed by Gas Chromatography-Olfactometry (GC-O), quantitative analysis of major aroma compounds (GC-FID) and minor and trace aroma compounds (GC-MS) was carried out too.
Aldehydes, methoxypyrazines, 3-mercaptohexanol or (Z)-1,5-octadien-3-one were detected when wines were analyzed by GCO. A wine with odor described as geranium was also analyzed and 3-ethoxy-3,5-hexadiene was identified, although its origin could be exogenous [2]. Quantitative analysis revealed a higher concentration of isoamyl alcohol and methionol in vegetative wines than in reference wine. An addition test of isoamyl alcohol in two different wines supported the hypothesis of its importance on the vegetative nuances of some wines. Several causes could be responsible for unpleasant herbaceous notes as a higher concentration of fusel alcohols or presence of exogenous compounds.
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[P 053] Volatile composition change of strawberry after several processing

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Strawberry is the 6^{th} most eaten fresh fruit after banana, apple, orange, grape and watermelon. The United States is the world's largest producer of strawberry. The next highest producing countries are Turkey, Spain, Egypt, Korea, Mexico, and Poland. Strawberry is one of the most economically important fruit in the food industry, because it is used as an ingredient in jam, jelly, yogurt, several milk based products, ice cream, syrup, fruit juice, tea, and other processed foods. Strawberry is rich in phytochemicals such as phenolic acid, ellagic acid, anthocyanins, catechins, quercetin and kaempferol which are important compounds for human health. Strawberry also has unique fresh and fruity flavor with contribution of more than 360 volatile compounds which widely studied by many researchers. Characteristic of strawberry aroma is complex mixture of furanones, esters, aldehydes, acids, alcohols, and sulphur compounds. Besides, strawberry aroma is highly changed during processing. Jam making and fruit juice processing, which are important to preserve strawberry for long time, requires heat treatment. Actually, fresh characteristic of strawberry volatiles is mostly replaced in processed strawberry by certain heat-induced volatile compounds, such as isobutyraldehyde, furan, furfural and dimethyl sulphide. Even these compounds are important flavor source of most heat processed foods; some of them are also known as carcinogenic so their control is necessary. In this review, change of volatile compounds of strawberry after several processes (heating, blanching, osmotic dehydration, high hydrostatic pressure, pulsed electric field, etc.) is summarized.

Key words: strawberry, volatile compounds, phytochemicals, food processing

[P 054] (Un)targeted analysis to unravel critical interactions between sugars and phenolics in Strecker aldehydes formation in beverages.

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The knowledge of the chemical processes occurring during wine aging that result in a specific chemical/sensory profile remains limited. This lack of knowledge and understanding significantly limits the ability to improve product quality and consistency. For that reason, unravelling the chemical changes occurring during aging that are responsible for wine flavour, constitutes a critical task when one attempts to address issues related with authenticity and sensory quality.
The interaction between phenolics oxidation and Maillard reaction in the formation of sensory active substances, such as Strecker aldehydes, has been reported recently for wine model conditions (1). In order to gather more information to rank oxidation and Maillard reaction regarding phenylacetaldehyde formation, the interaction between sugars and phenolic compounds were further studied. Three solutions have been prepared: (a) glucose and phenylalanine, (b) gallic acid and phenylalanine, (c) gallic acid, glucose and phenylalanine. The chemical supervision of the dominant mechanisms was obtained by quantifying reaction intermediaries such as: Amadori compound, 3-deoxyglucosone, dicarbonyls, o-quinones as well as hydroxyalkylsulphonic acids by LC-ESI-UHR-QqTOF-MS. It was observed that phenylacetaldehyde formation was 4 times higher in the solution B when compared with C. The presence of glucose in system C decreased by half the amount of *o*-quinone and showed as a result a lower concentration of phenylacetaldehyde. This is in line with previous results (1), where for the first time, it was reported that when glucose, gallic acid and phenylalanine are combined, the rate of formation of phenylacetaldehyde decreases when compared with the model solutions where glucose is absence. The same behaviour was observed for the phenolic *o*-quinone, a crucial substrate for the formation of aldehydes in wine. On the other hand, the presence of sugar together with the gallic acid increased the formation of the Amadori compound an intermediate of Maillard reaction. Finally, an untargeted analysis has been performed to better contextualize the observed behaviour. This work brings new insights into the role of glucose in managing the beverages shelf-life in particular wine.

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[P 055] Identification of Nonvolatile Creaminess Compounds in Dairy Products

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Creaminess is a distinct and desirable attribute of food, frequently identified by consumers as an important indicator of quality in dairy products. In the current project, the contribution of nonvolatile small molecular weight compounds to the overall mouthfeel of dairy products was investigated. An extraction protocol was developed and optimized to isolate the compounds of interest from heavy whipping cream. Food grade extracts were profiled for mouthfeel-active compounds utilizing multidimensional HPLC sensory-guided fractionation techniques based on descriptive analysis protocols developed using a 5-attribute lexicon (mouthfeel/thickness, astringency/drying, fatty texture, dairy mouthfeel, tingling/irritation). Five main compounds were identified by UPLC/MS/MS-ToF and NMR, which consisted of vitamin-related compounds, conjugated hippuric acids, and a conjugated sulfate compound. The compounds were quantified (LC/MS/MS) in milk and yogurt of ranging fat content. Sensory recombination studies using a 2-AFC test ($n = 20$) further confirmed the significant contribution of these compounds to the mouthfeel attributes of dairy products. These findings lend insight to a larger context for texture perception (mouthfeel) in dairy ingredients and products.

[P 056] Odor perception and matrix interactions of monoterpenes isomers in Pinot gris wine

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Monoterpenes are aromatic compounds that contribute to the characteristic aromas of white wines. Monoterpene isomers were identified and quantitated in 46 Pinot gris wines from different regions. The concentrations of the majority of isomers ranged from 0.17 μg L^{-1} to 46.46 μg L^{-1} and were under their known perception thresholds. An interest in the actual influence of these compounds on odor perception in Pinot gris was investigated, specifically since concentrations were found to be low. Ten profiles with different monoterpene isomer combinations were chosen based the monoterpene isomer composition of Pinot gris wines. Additionally the effect of the matrix on odor perception was investigated. Nine monoterpene isomers were chosen, including *S*-(-)-limonene, *R*-(+)-limonene, (2*S*,4*R*)-(-)-*cis*-rose oxide/ (2*R*,4*R*)-(-)-*trans*-rose oxide mixture, furanoid (2*R*,5*R*)-(+)-*trans*-linalool oxide/(2*R*,5*S*)-(-)-*cis*-linalool oxide/ (2*S*,5*S*)-(-)-*trans*-linalool oxide/(2*S*,5*R*)-(+)-*cis*-linalool oxide mixture, *R*-(-)-linalool, linalool, *S*-(-)-terpineol, *R*-(+)-terpineol, and *R*-(+)-citronellol. The effect of 10 monterpene isomer profiles in three different matrices: (1) 14% ethanol solution adjusted to pH 3.2 with tartaric acid, (2) de-aromatized Pinot gris wine (14% ethanol content) and (3) original Pinot gris wines (14% ethanol content) with measured non-detectable monoterpene enantiomers were investigated through triangle tests. Monoterpene isomers in five profiles were found to significantly impact odor perception in matrix 1, suggesting that synergy among isomers may occur in model solution. Odor perception of nine profiles changed when the monoterpene isomers were added to de-aromatized wine, showing that the odor perception was enhanced as isomers were in combination with other non-volatile compounds. However, odor perception was suppressed in original wine (matrix 3) as significant differences were only found in five profiles, showing that interactions between the isomers and other aroma components suppress perception. These results support the fact that the low impact compounds at sub-threshold concentrations, such as monoterpene isomers may act as impact odorants by interacting synergistically with other components to change the odor perception of the mixtures. The knowledge of these interactions will further help in the development of balanced and tasteful wines and wine products.

[P 057] Modification of bitterness and astringency in lingonberry products using cyclodextrins

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Bitterness and astringency are flavor characteristics of various polyphenol-rich foods, and these features are often perceived as negative by consumers. Although in some foods and beverages they may be considered as wanted characteristics, in many cases they are among the key factors limiting the consumption of the potentially healthy plant-based food. Lingonberries (*Vaccinium vitis-idaea*) are commonly found in Nordic forests and typically have notably sour, bitter and astringent flavor. The berries have high contents of various polyphenols, such as proanthocyanidins and flavonols, which may contribute to the flavor of the berry. Despite of being rather well-known and familiar to the Nordic consumers the berry is not equally well exploited. Methods are needed to modify the flavor of bitter and astringent foods, such lingonberry, without affecting their health-contributing properties. Application of various bitterness-blockers, such as cyclodextrins, that bind bitter compounds and thus prevent their access to the bitter receptors, may be considered as potential techniques to improve food flavors.

The aim of this study was to investigate the impact of cyclodextrins on the bitterness and astringency of lingonberry juices and in sweets produced from the juices. Cyclodextrin was added to the 100% juice, gelatin-treated juices (protein-binding polyphenols were removed) or juices with elevated pH. Juices (n=6) and sweets (n=6; made using pectins) were assessed by an untrained consumer panel (n=40) and a trained panel (n=15), respectively, under controlled sensory laboratory conditions.

Cyclodextrin additions alone did not have notable impact on the flavor, whereas combination of cyclodextrin in combination with gelatin or higher pH was more effective. In juices, both combinations decreased the bitterness more efficiently. In sweets, cyclodextrin together with gelatin treatment did not result in similar impact although the bitterness was somewhat lower. Compared with the flavor of lingonberry juices, making sweets from the juice reduced significantly the bitterness and astringency due to sugar addition and binding of polyphenols by the pectins. All in all, bitterness and astringency of lingonberry juices can be affected using cyclodextrins. However, the cyclodextrins alone may not be sufficient and combination with other treatments may be needed.

[P 058] Sensory-directed strategies for isolating compounds driving dryness and persistence in red wines

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It is widely accepted that astringency in wines is mainly driven by ethanol content, acidity levels and flavanol-derived compounds. Oligomers and polymers of those compounds, also called tannins, are able to either precipitate or form complexes with salivary proteins, leading to an absence of lubrication of the oral cavity, which is traditionally thought to elicit sensory astringency or dryness. The role of other polyphenolic compounds in astringency is not clear. Recently, it has been demonstrated that monomers of anthocyanins (malvidin-3-*O*-glucoside) are able to form complexes with proteins and thus suggested to be candidates to be involved in astringency formation [1]. Results presented in this work go further strongly suggesting that some anthocyanin derivatives are in fact the key elicitors of dryness and persistence of some red wines.

Three wines with different astringency levels were submitted to a fractionation method which provided 6 different odorless fractions per wine (F1.1, F1.2, F1.3, F2.1, F2.2 and F2.3) [2]. Interestingly, the in mouth sensory properties of one of the wines (mainly described as dry and persistent) were retained in fraction F1.3. This fraction contained exclusively anthocyanin-derived pigments and no presence of flavanol-derivatives has been detected.

Additional separation strategies have been further developed to isolate the compounds driving dryness and persistence in this particular fraction F1.3. The fraction was refractionated by SPE, using LRC-C18 resins, to obtain 4 different and simpler subfractions (F1.3 A, F1.3 B, F1.3 C and F1.3 D). The sensory similarity between these subfractions and the un-fractionated reference was assessed by a highly trained sensory panel. The chemical characterization of the subfractions retaining most sensory characteristics strongly suggest that a series of trimers of monomeric antocyanin are key elicitors of dryness and persistence in red wines.

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[P 059] Yoghurt fat levels determine synergy with natural occurring flavors

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Fermented milk products like yoghurt are consumed all over the world and there are many varieties available. Substantial studies on volatile flavor compounds-matrix interactions, flavor release mechanisms, and the synergistic effects of flavor compounds have been done; correlating these to the sensory properties of yoghurt. However, only limited research has been done on the natural occurring flavors and their effect on flavor and texture perception. The main natural occurring flavor components of yoghurt are: acetaldehyde, diacetyl, acetoin, acetone, 2,3-pentanedione, and 2-butanone [1, 2].
In order to fully elucidate the role of natural occurring aroma and flavor components, yoghurt was spiked with diacetyl and the effect on the sensory perception of adding this component was studied. Although the levels of diacetyl were on the lower end of the levels normally present in yoghurt, the effect of fat was of more importance to the creamy flavour than differences in diacetyl levels. As fat plays an important role in flavour perception, a thorough understanding of the role of fat in relation to the natural occurring flavor compounds was needed. Therefore diacetyl and acetaldehyde were spiked at three levels to no-fat yoghurt, semi skimmed yoghurt, and full fat yoghurt. These yoghurts were evaluated by Quantitative Descriptive Analysis (QDA) and headspace analysis was done with GC-MS. One of the main findings was that higher fat content is synergistic to the cream flavour of diacetyl, whereas the green flavour of acetaldehyde was more perceptible at a lower fat level. So, in contrast to what has been reported for milk [3], fat levels of yoghurt do influence the perception of acetaldehyde (and other volatiles). Therefore, this study strongly supports that the changes in natural flavor perception needs to be taken in to account when modifying the fat content of yoghurt.

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[P 060] Structure-odor relation in homologous series of dithio(hemi)acetals

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1,1-Dithio compounds have scarcely been reported in food so far. One of the rare exceptions is durian, the fruit of *Durio zibethinus*, a huge tree originating in the rainforests of tropical Southeast Asia. Durian fruits are infamous for their strong and penetrating odor which combines fruity notes with a pronounced oniony smell. Nevertheless, in countries like Thailand and Indonesia, durian consumption is extremely popular and durian is considered the 'king of fruits'.
When studying the key aroma compounds in durians [1, 2], we detected numerous odor-active 1,1-dithio compounds among which were 1,1-dithiols, dithiohemiacetals and dithioacetals, all of which were structurally derived from acetaldehyde and propanal on the one hand and hydrogen sulfide, methanethiol, ethanethiol, and propanethiol on the other hand, and exhibited sulfury and oniony odor characteristics. Among these, 1-(ethylsulfanyl)ethane-1-thiol contributed most to the overall aroma of durians [2].
The abundance of 1,1-dithio compounds in durians prompted us to have a closer look at the relation of their structure and their odor properties. Starting from ethane-1,1-dithiol, the structure was modified by formally adding alkyl groups of increasing length to the two sulfur atoms to yield 1-(methylsulfanyl)ethane-1-thiol, 1-(ethylsulfanyl)ethane-1-thiol, 1-(propylsulfanyl)ethane-1-thiol, 1,1-bis(methylsulfanyl)ethane, 1-(ethylsulfanyl)-1-(methylsulfanyl)ethane, 1-(methylsulfanyl)-1-(propylsulfanyl)ethane, 1,1-bis(ethylsulfanyl)ethane, 1-(ethylsulfanyl)-1-(propylsulfanyl)ethane, and 1,1-bis(propylsulfanyl)ethane. The compounds were synthesized and their odor thresholds in air were determined by GC-O [3]. Results indicated consistently lower odor thresholds for dithiohemiacetals than for dithioacetals. The most potent odorant in the series was 1-(ethylsulfanyl)ethane-1-thiol. Similar results were obtained for the homologous series starting from propane-1,1-dithiol.

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[P 061] Effect of carbonation level on the perception of sparkling wine

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From a sensory perspective, sparkling wines are highly complex products. Carbonation imparts characteristic mouthfeel effects that include tingling and other sensations, and may trigger gustatory, olfactory, trigeminal, and auditory perceptions as well. To investigate the effects of carbonation level on perception, McMahon et al (J Wine Res, in press, 2017) made eleven wines starting from the same base cuvee, resulting in 1 (still) base wine and 10 sparkling wines, each at a different carbonation level. Wine chemistry analysis confirmed differences amongst samples with respect to carbonation, and similarity in terms of sensory thresholds levels in recorded concentrations of sugars, titratable acid, pH, and ethanol. As reported McMahon et al (Food Qual Pref, 59, 14-26, 2017). Wines were evaluated according to a replicated experimental design by trained assessors via (i) sensory descriptive analysis (which provides static data on attribute intensities), and (ii) temporal check-all-that-apply (which provides dynamic data related to attribute applicability over time).

Correlation analysis as well as various multivariate statistical techniques were applied to investigate analytical-sensory correlations, e.g. partial least squares regression (PLSR). The relationship between carbonation level and mouthfeel sensations related to effervescence is big and obvious, but more subtle for taste and flavour attributes. Intensities of vanilla flavour, caramel flavour, and sweet taste were correlated. In contrast to other research, sourness did not increase with carbonation concentration. Although sourness intensities of the wines were not significantly different, increased carbonation concentration affected the *dynamics* of sourness perception. Specifically, increased carbonation delayed the onset (and extinction) of sourness perception. The sourness response temporal curve was right-shifted and damped. A potential explanation is that dynamic effects of carbonation draw attention away from sensations that arise in other sensory modalities, including gustation.

Findings are relevant to product developers working on carbonated products, and suggest potential for further research for systematically investigating how carbonation level interacts with other wine components at different concentrations to affect how products are perceived in mouth.

[P 062] Explaining fat sensitivity in cottage cheeses by aroma release and oral physiology parameters

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In the aim to increase sensory acceptability of low fat content foods, a better understanding of the physiological mechanisms involved in fat perception is needed. Fat perception is considered as a multimodal sensation in itself involving smell, taste and texture perception [1,2]. Moreover great inter-individual differences in fat sensitivity were observed in detection thresholds for fat in cottage cheeses [3]. The aim of this presentation is to determine on forty well characterized subjects the physiological parameters which better explain fat perception in cottage cheeses.
A panel of 40 subjects carried out a series of eight 2-AFC tests including a reference (0% or 3% fat respectively for absolute and difference thresholds) and a test sample with a higher amount of fat (up to 11% fat). An Ascending Hierarchical Classification evidenced three subsets of subjects with contrasting sensitivity profiles: high, medium and low absolute and difference thresholds [3]. These data are explained by other parameters measured on the same subjects. The release of 2 aroma compounds with fatty notes (pentan-2,3-dione and hexan-3,4-dione) was followed by PTR-MS while consuming a 1% fat content cottage cheese. Detection and recognition thresholds were determined for these 2 aroma compounds. Respiratory and salivary flows were measured together with saliva composition at rest, mouth coating and number of fungiform papillae. Subjects more sensitive to fat (low thresholds) are more sensitive to fatty aroma compounds, have a higher respiratory flow, a higher aroma release rate, which confirms the impact of olfaction. They also present a low salivary flow, high antioxidant activity, low lipolytic activity and low amount of free fatty acids in saliva, which suggests an impact of fat taste perception. They also present a greater amount of fungiform papillae and a low amount of product remaining in the mouth after swallowing, which is in favour of a textural modality. Altogether these results confirm that fat perception in real foods is a multimodal perception.

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[P 063] Neohesperidine Dihydrochalcone increases Stevia preference in young Piglets

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Stevia extracts (SE) are sweet-tasting compounds that could be used as sweeteners in pigs. Our objective was to determine if SE at different inclusion levels and their interaction with Neohesperidine dihydrochalcone (NHDC) may increase feed preference in weanling pigs. A total of 432 piglets (14 to 35 d post-weaning) were used. In Period 1, a basal diet + 4% of sucrose (R) was compared to 6 Treatment diets (basal diet + 4% of maltodextrin + x ppm SE; x= 0 (T1), 100 (T2), 200 (T3), 300 (T4), 400 (T5) and 500 (T6)). The two experimental diets (R and T1 to T6) were offered to pens of 3 piglets following a double-choice test (DCHT) protocol (n=12 for each comparison). Feed intake and preference for each diet were calculated. No differences were observed on the comparisons, but T2 (100ppm SE) showed a quantitative higher preference than R (56.0%) while higher levels depressed the preference with lower values than 42.8%. For Period 2 the R diet was compared to 5 different combinations of SE and NHDC (basal diet+4% Maltodextrin+150ppm SE+ x ppm NHDC; x= 0 (T1), 2 (T2), 3 (T3), 4 (T4) and 5 (T5)). Higher preferences ($P > 0.05$) for SE+NHDC over R were observed for T2 (65.0 %), T3 (74.4 %) and T4 (67.1 %) (150ppm SE + 2, 3 and 4 ppm NHDC, respectively), which suggest that NHDC can increase SE preference in pigs as compared to sucrose.

[P 064] Serial dilution sensory analysis applied to exploring sensory attributes for characterizing aroma notes of green tea and black tea

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Objectives: The AEDA has been widely used as a useful technique in flavour research. However, we do not feel each aroma component individually but instead sense a mixture of aroma chemicals simultaneously, where mutual interactions of components may take a place. The serial dilution sensory analysis (SDSA), where beverage being directly diluted and analyzed by descriptive sensory analysis, has given us some new information on the significance of aroma notes in liquid food. Although both green tea and black tea are produced from the same starting materials, young leaves of *Camellia sinensis L.*, their aroma notes are different each other. We attempted to explore sensory attributes playing key roles for characterizing aroma notes of green and black teas by applying SDSA and the following chemometrics analysis.
Methodology: Bottled green tea and black tea commercially distributed in Japan were diluted log linearly from 10 to 1000-fold and 10 to 10000-fold with purified water, respectively. The descriptive sensory analysis using attributes identified in preliminary sessions was applied for each dilution. The contribution of each attribute for the aroma notes of two teas was calculated as a regression coefficient in a PLSR model.
Results:For green tea, 27 attributes, 11 for aroma including the green tea note, 5 for taste, 4 for flavour, 4 for mouth feel and 3 for aftertaste were identified in all dilutions. For black tea, 14 for aroma including the black tea note, 5 for taste, 6 for flavour, 3 for mouth feel and 3 for aftertaste were recognized. Sensory scores in all attributes decreased exponentially according to dilutions. Therefore, proportions of scores for individual aroma attributes in each dilution were calculated based on their total. According to dilution, proportions of *green tea*, *roasted* and *sea breeze* decreased but those of *sweet*, *steamed* and *dusty* increased in green tea profiles. In black tea profiles, fractions of *sweet floral*, *smoky* besides *black tea* decreased but those of *sweet*, *dusty* and *cardboard* increased. Regression coefficients in highly predictive PLSR models suggested that *roasted*, *sea breeze* and *hay* associated with *green tea* but *sweet floral*, *dry leaves* and *smoky* related to *black tea*.

[P 065] The effect of plant variety and domestic cooking on flavour volatiles and their impact on sensory profile and consumer liking of cabbage.

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Several volatile compounds are produced upon cabbage tissue disruption. Some of these compounds are undesirable sulfur volatiles produced from enzymatic degradation of sulphur-containing amino acids, S-methylcysteine and its sulfoxide, by cysteine S-conjugate lyases. However, thermal processing has been reported to lead to denaturation of cysteine S-conjugate ?-lyases which can reduce the amount of sulfur volatiles produced. Isothiocyanates, which are hydrolysis products of glucosinolates found in cabbage, are also partly responsible for the characteristic flavour/aroma of cabbage, as well as its health promoting properties. Allyl isothiocyanate, produced from sinigrin hydrolysis, is considered one of the desirable flavour volatiles of cabbage. Despite its health benefits, cabbage consumption is low, commonly related to its bitter taste or pungent flavour. This study evaluates the impact of cabbage variety and domestic cooking on flavour volatile production and their impact on sensory profile and consumer liking.
Three varieties of red cabbage and of black kale were planted and harvested at commercial maturity following standard agricultural practices. Cabbages were prepared raw, steamed and stir-fried. Sensory profiling of the cabbage was carried out by a trained panel (n=11) using Quantitative Descriptive Analysis. Consumers (n=118) rated samples for liking and bitterness. For flavour volatile analysis, prepared sample (5g) was immediately blended and volatiles released into the headspace were captured and measured using SPME-GC/MS.
Cabbage type had an effect on the type of volatiles produced. Isothiocyanates were detected in red cabbage but undetected in black kale. The types and amount of flavour volatiles produced was affected by both cooking and cabbage variety. Cooking significantly reduced the amount of undesirable sulfides (dimethyl sulfide and trimethyl sulfide) produced. Raw cabbages were perceived to have more sulfurous flavour and aroma, which correlated negatively with consumer liking. Allyl isothiocyanate, found in red cabbage, was significantly higher in cooked cabbages and correlated positively with cooked and sweet aroma and consumer liking. Cooked kale correlated positively with dimethyl sulfide and consumer liking and negatively with other sulfides and sulfurous flavour.This study suggests that selection of cooking method can reduce the production of undesirable sulfide volatiles and thereby increasing consumer liking of cabbage.

[P 066] Elucidating the mechanisms of individual variation in fat perception and preference

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Fat can be perceived through mouthfeel, odour and taste; however the relative contributions of these to perception remains undefined. Fatty acids (FA) are the gustatory stimuli and individual sensitivity to fatty acids varies. The association between fatty acid sensitivity, fat intake and preference has been studied in model food systems, but limited studies associate this to fat perception in real foods.
This study examines this association and the effects of modalities on fat perception. Furthermore, the impacts of salivary lipase and CD36 genotypes, both known to influence individual variation in fat perception, were explored.
Two studies were conducted. In Study 1 (n=46), fat intensity was rated in milk/cream of five fat levels; under four conditions: mouthfeel-odour-masking, odour-masking, mouthfeel-masking and no-masking. FA sensitivity was measured by staircase-3-AFC using milk containing oleic acid (0.0088 %-0.89 % w/v). In Study 2 (n=85), 7 fat levels were rated and a 2-AFC-test used to confirm discrimination. Food preference and frequency questionnaires assessed food liking and intake. Masticated (15s at 1bite/s) and expectorated almonds were collected for free FA analysis, buccal swabs collected for CD36 genotype analysis. Free FA in almond was analysed.
Odour and mouthfeel enhanced fat perception ($p < 0.05$). High-fat-likers (HFLs, n=34) and dislikers (HFDs, n=51) were identified from the preference questionnaire. HFLs reported higher liking in 25 high-fat foods ($p < 0.05$) and higher fat intake ($p = 0.004$), but rated lower fat 'taste' intensity ($p < 0.0001$). HFLs/HFDs did not differ in overall intensity ratings, nor in FA threshold sensitivity.Oleic acid of total fat (OA%) in expectorated almonds varied between individuals, ranging from 0 % to 0.55 % w/w. Individuals with expectorated OA % above almond OA % were identified as OA-producers (n=25), others were OA-non-producers (n=60). These groups did not differ in their intensity ratings of fat in the milk / cream model. The results of CD36 will be discussed at the conference.
This study suggests that fat can be discriminated by taste. Individual preference to high-fat foods varies and it significantly relates to fat taste perception. The role of FA generation through oral processing on fat perception requires further investigation.

[P 067] Molecular and Cellular Mechanisms of the Pungent and Tingling Impression of Black Pepper (Piper nigrum L.)

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Besides its alluring aroma, the characteristic pungent and tingling orosensory impression is one of the key criteria used by spice traders to describe the quality of the world's most widely used spice, black pepper (*Piper nigrum* L.). Although the pungent impact of the amides present in *Piper nigrum* L. is known for many decades and, the well-known piperine has been demonstrated to be the quantitatively predominating amide present in black pepper corns, the data published on the sensory attributes of the purified individual amides and their contribution to the pungent and tingling effect of black pepper as well as their psycologically perception is rather fragmentary and sometimes even contradictory.
The objective of the present investigation was, therefore, to target the sensory active key molecules in black pepper corns by application of a SENSOMICS approach. Purification of the compounds perceived with the highest sensory impact, followed by LC-MS and 1D/2D-NMR experiments, as well as synthesis, led to the structure determination of 25 key pungent and tingling phytochemicals with recognition thresholds ranging from 3.0 to 1150.2 nmol/cm^2 for pungency and from 520.6 to 2162.1 nmol/cm^2 for the tingling orosensation. Their pungency is partially explained by the agonist activity of some of their active principles, especially piperine, on TRP channels [1, 2]. However, we found that piperine, as well as other pungent/tingling compounds, additionally possesses a marked effect on two-pore domain (KCNK, K2P) K^+ channels, which have been shown by Noël et al. [3] to 'fine-tune' the cellular response to stimuli that activate TRP channels. It is important to mention that our results do not exclude TRP channels as targets for chemosensates from black peppercorns, indeed both families of ion channels seem to play a complementary role, since neither of them alone suffice to fully explain the mechanism by which black pepper elicits its characteristic impression.

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[P 068] Temporal Effects in Odorant Mixtures

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In 1994, Laing found evidence for temporal processing of odor mixtures in humans. Using four different odorant pairs, he observed a latency ranging from 92 ms (Carvone-Limonene) to 580 ms (Carvone-Benzaldehyde). Twelve years later, Rinberg studied the speed-accuracy tradeoff in mice. He discovered that, depending on the task difficulty, the time required to reach the maximal accuracy can be up to 600 ms (harder tasks). In 2015, Resulaj demonstrate that mice processes odor information in 70-90 ms after odor inhalation proving that mice can make decisions surprisingly fast. As the temporal processing in olfaction still remains unclear, we have investigated the temporal effect of different pairs of odorants. Starting with the binary odorant mixtures at which subjects had equal probability to detect one compound or the other (Equal Odd Ratios). We prepared solutions of each component separately and puffed these separated solutions at different times between 0 to 200 ms (latency times) and different concentration ratios. The results indicate a linear relationship between latency and concentration ratios confounding the meaning of Laing's results.

[P 069] Real-time percept flavor balance derived from retronasal threshold and in vivo measurements of retronasal aroma release with PTR-MS

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Retronasal aroma is one of the most important factors for palatability of foods and drinks during consumption of them, is distinguished from orthonasal aroma inhaled from nostrils. Aroma extract dilution analysis (AEDA) or Odor Activity Value (OAV) is widely known method to determine a contribution value of each aroma compound in a food by sniffing via orthonasal route, but can indicate neither an odor profile during ingestion of the food nor time changes of the aroma compounds. A lot of studies conducted to measure *in vivo* aroma release with atmospheric pressure chemical ionization (APCI) or proton transfer reaction (PTR) mass spectrometry (MS), and referred to changes of aroma compounds concentration over time. However, few report referred to time changes of contribution of each aroma compound. In this study, we aimed to develop a method which shows time changes of aroma contribution during ingestion of foods and drinks.
First, behavior of retronasal aroma was directly analyzed by PTR-MS while subjects drank several water solutions contain aroma compounds. The behavior of each aroma compound was changed for AUC (area under curve in a plot concentrations vs time) of each breath. Because the behavior of AUC can be approximated as a power law function, AUC of an arbitrary breath can be calculated. Next, subjects evaluated an odor threshold value for each aroma compound by drinking aroma water solution. AUC of the 1st breath released from their nose was estimated, because AUC is approximately proportional to the concentration of each aroma compound in the water. This AUC of the 1st breath was defined as retronasal threshold. Finally, the value which divided AUC of retronasal aroma by retronasal threshold was calculated to each compound, and was defined as the contribution value of retronasal aroma perception (CRA).
Each CRA can be calculated by using correspondent decayed curve on each aroma compound in every breath. Thus, a balance of each CRA at an arbitrary breath permits prediction of odor profile at the moment. Sensory evaluation by trained panel supports this prediction.

[P 070] Perceptive Interactions in Red Wines: How Physico-Chemical Pre-Sensorial Effects May Affect Fruity Aromatic Expression?

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More than a thousand volatiles have been identified in wine. To be perceived, these aroma compounds need to be first volatilized from the matrix to the headspace in order to reach the olfactory epithelium. From a physico-chemical point of view, compounds release may be explained by its partition coefficient, which represents the ratio of aroma concentration between gas and liquid phase.
In red wine, a part, at least, of the fruity aroma is the consequence of perceptive interactions between various aromatic compounds thanks to synergistic effects [1, 2], as well as masking effects, thus modulating this fruity expression [3, 4]. Even if these effects have been clearly described, the levels where they occur have been poorly investigated [5].
This work propose to explore the pre-sensorial level, where the release of flavour-active compounds from the matrix take place, using multiple partition coefficients determination.For that, partition coefficients for 9 esters, representing the typical fruity aroma of red wines, were determined before and after the addition of various aroma compounds for which previous perceptive interactions have been highlighted [1-4].
Results showed, for the first time to our knowledge, that addition of some aroma compounds impacted the release of other volatiles from the matrix. This physico-chemical modulation were in agreement with sensory results. For instance, masking effects due to higher alcohols or lactic acid bacteria metabolites were correlated with a decrease of esters release, whereas synergistic effects due to hydroxylated esters were not linked to the modification of the volatilisation of other compounds, suggesting potential sensory effects on the olfactory receptors or at a central cognitive level.

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[P 071] Configural and elemental: odor or odorant processing?

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Deductive Tasting is a formal process used by Sommeliers to identify a wine: it's cultivar, region, vintage, quality, etc. The process of becoming a Master Sommelier involves a ritualistic sensory examination using touch, sight, taste, smell and the memory of hundreds of identical tastings of scores of wines over many years. This is the same process people on a smaller scale use every day to understand the flavor of food and drink. The question is: do humans use an elemental (analytical) process or a configural (synthetic) processes to decode the multiplicity of sensations our many sensors send to our cortex? Evidence that lobsters can do both configural and elemental processing choosing one or the other depending on the situation was documented by Livermore in 1997. Recently, evidence that humans use both configural and elemental processing in the same way sommeliers identify wine was demonstrated using sniff olfactometry of odorant mixtures.
Here subjects, during 70 ms puffs of headspaces above aqueous solutions, repeated 18 times, behaved stochastically. The probability they would choose one label in a binary forced choice was proportional to the ratio of the two components in the solution. However, the slopes of the logistic plots of the data depended on the identity of the odorants. This presentation will discuss the results of these and published experiments as they relate to odor image formation and the analytical process we use to identify the objects odor images represent.

[P 072] OR51E1 : Exploring the structure-activity relationship of agonists in multiple assays

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A total of 92 compounds have been tested for their ability to activate the olfactory receptor OR51E1 expressed in HEK293T cell using 2 different assays: CRELuc gene reporter and homogeneous time resolved fluorescence (HTRF). Activation of the endogenous beta$_2$ adrenergic receptor and forskolin have been performed for comparison and normalization (in the case of forskolin). Activation curves have been analyzed according to the Hill's equation allowing the calculation of EC_{50} values, E_{max}(maximal activation) and n_H (the Hill's coefficient). Hill's coefficients are close to unity and similar in both assays. EC_{50} values ranging from 10^{-3}M to 10^{-6}M in the 2 assays are highly correlated. The presence of a carboxylic function is mandatory for OR51E1 activation since substitution of that function by alcohol, aldehyde, or ester abolishes activation. EC_{50} values are modulated by the structure of the aliphatic moiety. Substitution or introduction of a double bound on the carbon adjacent to the carboxylic function increases EC_{50} values. At the opposite, increase chain length and introducing branching and/or double bound decreases EC_{50} values for compounds having 4 to 10 aliphatic carbon atoms. Cyclization of medium length analogs (4, 5, 6 ,7 ring system) further increase EC_{50} values with respect to the corresponding open analogs. While cyclohexyl analog leads to one of the most active compounds, its benzyl analog is inactive. Bridging the cyclohexyl analog further increases EC_{50} values. Altogether this results allows the characterization of a hydrophobic pocket contributing to the binding and activation of OR51E1.

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[P 073] Why does this wine smell like apricots?

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'Stone fruit' aroma attributes are important to many varieties and styles of white wine. However, the aroma compounds that give rise to the 'stone fruit' aroma attributes in wine are not well understood. To identify the aroma compounds responsible, this study focused on Viognier and Chardonnay wines from France and Australia with differing levels of 'stone fruit' character. The wines were characterised by sensory descriptive analysis and by comprehensive quantitative chemical analysis, targeting over 100 volatile aroma compounds using stable isotope dilution analysis, plus standard wine chemical parameters. The sensory data showed the set of wines had varied ratings of 'apricot' and 'peach' aroma attributes and the two attributes were not closely correlated. Subsequently, the sensory attribute ratings were related to the chemical composition data by partial least squares regression. Several aroma compounds were positively associated with the 'apricot' aroma attribute notable in some of the Viognier wines including: three aliphatic -lactones (nona, deca and (Z)-6-dodeceno); three monoterpenes (linalool, geraniol and nerol); and several aldehydes. 3-Mercaptohexyl acetate and *trans*-ethyl cinnamate were negatively correlated. 'Peach' aroma was associated with a range of fermentation-derived fatty acid ethyl and acetate esters.
Interestingly, some n-alkyl lactones, monoterpenes and aldehydes have been reported as important aroma compounds in stone fruits. In the wines studied, nonalactone and decalactone were present along with the previously little studied and potent (Z)-6-dodeceno-lactone but all were below their reported aroma detection threshold values. However, linalool and geraniol were above their aroma threshold values and, for the aldehydes, only (E)-2-nonenal was above. To establish if a combination of compounds produced the 'apricot' attribute, addition and omission sensory studies were conducted in a base model wine reconstitution, consisting of 55 aroma compounds and a range of common wine non-volatile compounds plus sulfur dioxide. These studies confirmed that the mixture of the three monoterpenes was the most important group to be added for the model to be perceived as having an 'apricot' attribute.

[P 074] Structure-odor relationship study of C-6 unsaturated acyclic monoterpene alcohols: a comparative approach

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Acyclic monoterpenes are a valuable class of compounds useful for the flavor and fragrance industries [1]. Among them are the C-6 unsaturated monoterpene alcohols, namely, linalool, geraniol, nerol and β-citronellol. These substances exhibit pleasant smell properties, are widely found in the essential oils of many plants and are pharmacologically and physiologically active. Thereby, it is interesting to note that linalool and geraniol, specifically, do not only activate the olfactory receptors, but also are shown to be anticancer agents [2, 3]. However, no detailed studies are at hand reporting which structural features are responsible for these prominent effects. In addition, systematic elucidation of the structural, analytical and human sensory characteristics of this substance group is very limited as most work, until today, focused just on the basic acyclic monoterpene compounds and not their metabolite derivatives. Although oxygenated derivatives of these monoterpenes have not yet been comprehensively investigated with regard to their physiological effects, our previous studies were able to show that some of these metabolites are odor active compounds [4, 5]. Thereby, starting from these monoterpene alcohols and their corresponding acetates, a series of oxygenated derivatives were synthesized and their olfactory properties were characterized within this study, yielding a total of 24 derivatives. Specifically, these compounds were tested for their odor qualities, relative odor thresholds (OTs) in air, and inter-individual variations in human sensory perception for each single substance. Finally, a comprehensive substance library was successfully established comprising the respective retention index data (RI values) as well as mass spectrometric and nuclear magnetic resonance data, to aid in future analytical studies on this sensorially fascinating substance class.

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[P 075] Biotransformation, transmission and excretion processes of garlic odorants in humans: impact on human milk, urine and exhaled breath

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Garlic (Allium sativum) is a well-known plant whose bulb is used as a popular food seasoning ingredient worldwide. As well as being savored for its characteristic aroma, garlic has also been associated with beneficial health properties, e.g., a reduction in blood pressure and an improvement in cholesterol levels. Garlic is therefore believed to have a protective effect against cardiovascular diseases. The specific compounds that are responsible for these beneficial effects have not been fully resolved to date, although saponins and flavonoids have been proposed as active compounds. Another garlic constituent that has been associated with positive health effects is allicin and its (unspecified) degradation products. Since odorants (as well as odorless volatiles) ingested with food can be strongly modified by biotransformation processes within the body, however, it is possible that not only the primary garlic constituents are responsible for the specific physiological properties, but also their metabolites.
Potential biotransformation processes were investigated by monitoring the influence of raw garlic consumption on the odorant and metabolite composition of human milk, urine and exhaled breath. Sample sets of these three bodily fluids were gathered, with one collected prior to garlic consumption and further sets subsequently sampled at regular intervals thereafter for each test subject. Milk and urine samples were analyzed both chemo-analytically using gas chromatography-mass spectrometry/olfactometry (GC-MS/O) and sensorially by a trained sensory panel. The analyses revealed three garlic-derived metabolites in human milk and urine, namely allyl methyl sulfide (AMS), allyl methyl sulfoxide (AMSO) and allyl methyl sulfone ($AMSO_2$). The excretion rates of the metabolites into the specific body fluids were strongly time-dependent and exhibited large inter-individual variations. Complementary analyses of exhaled breath were carried out using proton-transfer-reaction mass spectrometry (PTR-MS) via a buffered end-tidal sampler. Breath analyses revealed the presence of AMS and methanethiol in exhaled breath, albeit with highly varying post-consumption rates between individuals.
These findings indicate that the volatile fraction of raw garlic is strongly metabolized and that different garlic-derived metabolites are excreted via different metabolism pathways.

[P 076] Exploiting the gustometer for sensory testing: evaluation of sweetness.

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The gustometer is an instrument that can deliver samples in a controlled and pre-defined process for sensory tests. The aim of this study was to investigate the application potential of the gustometer and for this three different sensory tests were done. Main purpose was to check if the gustometer can get comparable results as traditional sensory methods and/or similar results to studies in literature in a faster and/or more practical manner.
The sucrose threshold was determined by both a traditional method and the gustometer method. From the outcome it can be concluded that the results of both tests were (a) within the range of sucrose thresholds found in literature and (b) that the gustometer can be used as a fast screening method to determine an indicative threshold level.
Sweetness evaluation of sugar mixtures was done based on traditional sensory tests. The sweetness intensity of eight sugar mixtures was evaluated by the sensory panel and converted to their perceived relative sweetness. A similar sensory test was conducted with the gustometer to compare the results with the traditional method. The general trend of the sweetness evaluation of the sugar mixtures was comparable between the two methods. However, the test using the gustometer was more flexible which has practical benefits for both the panelists as for the panel leader.
A pulsatile stimulation test was conducted comparing a pulsatile sample (pulsation includes 2.5 s 10% sucrose solution and 2.5 s water) to continuous samples of 5% and 6% sucrose solutions. The results showed that the pulsatile sample was evaluated significantly sweeter than the two continuous samples during the delivery of the sample.
Overall, the gustometer is an interesting additional tool in sensory testing (and therefore flavour research) and it can be used to speed up sensory testing and/or to increase throughput.

[P 077] Flavor peptides of Takifugu obscurus and Takifugu rubripes from China

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Takifugu is very popular among consumers for its delicious taste, and taste-active peptides are the important compounds contributed to its palatable taste. In this study, cultured *Takifugu obscurus* and *Takifugu rubripes* under different treatment including chilling, heat processing and enzyme are used as samples. Separation and purification technology including membrane separation, gel filtration chromatography and semi-preparative reversed-phase high performance liquid chromatography were used to pure oligopeptides from Takifugu. Mass spectrometry, protein N-terminal sequencing techniques, taste dilution analysis, the group deduction and sensory evaluation combined with electronic tongue techniques are used to identify these specific taste-active peptides. The total 11 flavor peptides were identified. The results showed that the range of amino acid number is 4-8, and these amino acids mostly composed by hydrophobic and hydrophilic ones. These peptides most contained basic amino acids like Arg and Lys, acidic amino acid like Glu and hydrophilic amino acid like Tyr. The effect of different processing on Takifugu was analyzed by comparing the structure, taste characteristics and changing trend to make sure the effects of endogenous enzymes, exogenous enzymes and heat processing on taste. This study would provide theoretical basis and technical support for revealing the flavor of Takifugu, the processing and utilization of Takifugu and the development of similar flavoring.

[P 078] The role of the salivary proteome in salt sensitivity

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Taste preferences and a growing demand for aliments with nutritional as well as health benefits determine consumers acceptability of food products to a significant extent. Understanding individual subjects taste sensitivity and the mechanisms involved in peri-receptor events taking place in the oral cavity would open new avenues for the reformulation of food products. Salivary proteins are believed to interact with key food taste molecules like sodium chloride and, by doing so, seem to impact taste receptor activation. Therefore, the present study set a particular focus on the salivary proteome level before and upon chemosensory stimulation.
35 Healthy panellists were screened in their full detection functions for sodium chloride and classified according to their sensitivity. Highly sensitive and non-sensitive panellists were challenged with a series of salt stimuli and saliva collected. Time-dependent changes in the salivary proteome were further analysed by tryptic in-solution digestion and nano-LC-MS/MS. The application of the iTRAQ labelling technique further allowed to relatively quantify identified proteins which were either modulated upon tastant challenge or differentially expressed between sensitivity groups. Surprisingly, dynamics upon stimulation and differential proteome pattern between sensitivity groups seemed to be two largely independent conditions. Tastant stimulation resulted in the release of proteins exhibiting antimicrobial and anti-inflammatory activities whereas sensitivity relied on the panellists initial conditions. In this context, key proteins were taken for gene ontology enrichment analysis and revealed augmented endopeptidase activity for sensitive subjects. Non-sensitive subjects, in contrast, were high abundant in proteins showing endopeptidase inhibitor activity. In order to cross-validate previous results and further predict individual panellists sensitivity, a large-scale screening was implemented and a method for targeted protein quantitation by means of stable-isotope incorporation developed. 20 healthy panellists were then classified according to their sensitivity, saliva samples were collected and analysed. Interestingly, a serine-type endopeptidase was found for the first time to exhibit a salt enhancing effect assigned to an *in-vivo* generation of salt-modulating peptides.

[P 079] Aroma compounds of wild edible Finnish mushrooms measured with gas chromatography-olfactometry

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Finnish wild edible mushrooms have an annual harvest of over one billion kilograms, but only a fraction of this harvest is utilized as food. There is anecdotal evidence of the highly varying odour profiles of edible mushroom species in guidebooks, but scientific examination of these differences is still scarce. Volatile compounds of Finnish mushrooms were analysed 40 years ago without focusing on orthonasally active aroma compounds. Thus, there is a need for re-evaluation of aroma compounds in Finnish mushrooms. The aim of this study was to characterize the aroma compounds of two Finnish wild mushroom species with trained assessors.

The mushroom samples (*Lactarius camphoratus* and *Cantharellus cibarius*) were processed with sous vide cooking, frozen at -20 °C, and the frozen batches were pooled and divided into aliquots. Volatile compounds were extracted from sample headspace using solid phase micro extraction (SPME) with a 1 cm StableFlex divinylbenzene/carboxen/polydimethyl siloxane fibre. The assessors (n=15) were trained to describe the aroma properties of various compounds over three sessions; twice using sniffing bottles and once by the gas chromatograph to familiarize them with the method. The evaluations were done with the detection frequency method. Each assessor took part in 1-2 sessions, resulting in 12 analyses from individual assessors for each mushroom species. Compounds were identified based on reference compounds, mass spectral library (Wiley 275) and retention indices on two columns. Aromagrams were built from individual responses and compared to FID chromatograms.

The resulting aromagrams and compound identifications display that 1-octen-3-ol, butanal and hexanal seem to be common aroma compounds for the studied wild mushrooms and that they form the general aroma of mushrooms. However, the aroma profiles of the studied mushrooms are otherwise distinct and it seems that each species creates their distinct aroma with a unique combination of odorants. For example, *C. cibarius* had unique peaks described as cucumber, citrus and plastic that were absent in *L. camphoratus*.

[P 080] Comparison of the Sensory Properties of Six Rice Varieties, Focusing on the Role of the Popcorn-like Aroma Compound 2-Acetyl-1-pyrroline

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2-Acetyl-1-pyrroline (2-AP) has been widely reported as being a key contributor to the popcorn-like odour of fragrant rice. In order to understand more about the contribution of 2-AP to the aroma of fragrant rice and to highlight the sensory differences between fragrant and non-fragrant rice, a vocabulary was developed to describe the sensory properties of boiled rice. Six different boiled rice samples (three varieties of fragrant rice (Basmati, Jasmine and Sintanur) and three varieties of non-fragrant rice - American long-grain, Arirang and Ciherang) were profiled by 13 trained panellists, focusing on popcorn-like flavour and aroma. It was clear from the results obtained that many of the panellists could not distinguish fragrant and non-fragrant rice on the basis of popcorn-like aroma and flavour. However, fragrant rice possessed more popcorn-like aroma and flavour than non-fragrant rice ($p = 0.016$ and 0.026, respectively). When ranking tests were carried out on the six boiled rice samples by trained panellists, focusing on popcorn aroma and popcorn flavour, a significant difference was observed for popcorn flavour ($p = 0.031$).
2-AP was extracted from the six boiled rice samples by headspace solid-phase microextraction and was quantified by gas chromatography-mass spectrometry (GC-MS). 2-AP was quantified in fragrant rice samples (38 μg/kg in Jasmine rice, 24 μg/kg in Sintanur rice and 20 μg/kg in Basmati rice) and was absent from non-fragrant varieties. Correlation was found between 2-AP concentration and popcorn flavour from both profiling ($p = 0.037$, $r^2 = 0.702$) and ranking ($p = 0.002$, $r^2 = 0.928$) results. However, it could be concluded that assessors have difficulty in distinguishing fragrant and non-fragrant rice on the basis of popcorn-like aroma and flavour.

[P 081] Influence of aroma precursors on human-sensed truffle flavour

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Truffles (*Tuber spp.*) are belowground forming fungi that establish symbiosis with trees and shrubs.
Their fruiting bodies are considered luxury food items due to their enticing aromas, specific components of which might be derived from amino acid catabolism through the Ehrlich pathway. Using a collection of mycelial strains belonging to the white truffle *Tuber borchii*, we employed ^{13}C-labeled amino acids to proof the existence of the Ehrlich pathway in truffles. We also explored through sensory and volatile profiling techniques how natural variability in the Ehrlich pathway could be used for identifying strains that produced the best flavors. Our results confirm the existence of the Ehrlich pathway in truffles for leucine, isoleucine, methionine and phenylalanine. Quantitative differences in volatile profiles among strains could be observed upon feeding amino acids. For example, the concentration of specific volatiles (i.e. sulfur, aromatic) varied by up of 128 times among strains. Triangle tests and descriptive sensory analysis illustrated that this natural variability in the Ehrlich pathway could be used to select strains with the most 'sulfurous' or 'floral' notes. Overall our results highlight the influence of the genetic background on flavor formation in truffles and illustrate how aroma precursors influence human-sensed truffle flavor.

[P 082] Comparison of the key aroma compounds in a bottom-fermented German lager beer and an Irish Guinness beer

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To elucidate aroma differences in several famous national and international beer brands on a molecular basis, investigations were initiated in our group to find out the reason for the differences in the aroma profiles. Results of a study aimed at unravelling the aroma compounds of Guinness eliciting a very smoky aroma, and a bottom-fermented German lager beer by application of the Sensomics concept will be shown.
The aroma profiles of both beers obtained by quantitative descriptive analysis differed clearly from each other. In Guinness 44 key odorants were identified on the basis of the application of an aroma extract dilution analysis and finally quantitated by stable isotope dilution assays. The highest odour activity values (OAVs; ratio of concentration to odour threshold) among the odorants with OAVs 1 were calculated for ethyl butanoate (fruity), 2- and 3-methyl-1-butanol (malty), 2,3-butandione (buttery), and ethyl 4-methylpentanoate (fruity). In the German lager beer in particular ethyl butanoate (fruity), β-damascenone (cooked apple-like), 3-methyl-2-butene-1-thiol (beer-like), 2- and 3-methyl-1-butanol (malty), and 2-phenylethanol (flowery) showed the highest odour activities. Generalist aroma compounds occurring in similar concentrations in both beers and specialist aroma compounds mainly occurring in one beer will be discussed and correlated to the aroma profiles.

[P 083] Discovering Aroma patterns in food products using Latent Dirichlet Allocation and Jensen Shannon divergence

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Gas chromatography-olfactometry (GC-O) is used to judge the sensory relevance of the volatiles present in foods. In particular, Aroma Extract Dilution Analysis (AEDA) evaluates the odour activities of the volatiles by sniffing the effluent of a series of dilutions of the original aroma extract. The result is expressed as the flavor dilution (FD) factor that corresponds to the maximum dilution value detected. Compounds with the highest FD are assumed to be most likely contributing to the overall aroma of the sample. Because AEDA is a time-consuming technique, most of previous studies merely report the analysis of 1-3 samples. However, when multiple samples are analysed, the interpretation of AEDA results become challenging because the data set is fairly high-dimensional but sparse and it is difficult to conclude similarity among samples. A common approach in situations like this is to map the data into an adequate lower dimensional sub space where the comparison and clustering is done. When the data is normally distributed, this is often done with Principal Components Analysis. This is not the case for FD values, because the data are discrete. In this paper, a new methodology to interpret AEDA results from multiple samples is presented. Latent Dirichlet Allocation (LDA) was developed in the context of text analysis by Blei *et al.* (2003) as a means of dimensionality reduction and has been successfully applied for the interpretation of AEDA results. Furthermore, Jensen Shannon divergence measure was a useful tool to compare the distribution of volatile compounds with similar descriptions ('berries', 'cheese' or 'fruits') among different samples.

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[P 084] Route cause analysis of an off smell detected in a powdered ingredient packed in 25 kg paper bags

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A customer complained about a strange smell in product that was packed into 25 kg paper bags containing a powder ingredient. Various 25 kg bags, that did contain powder showing either no or a very clear off flavour, were sensory evaluated. The smell or off flavour of the powders was described as woody/coffee grounds. It was also shown that in an aqueous solution the off smell cannot be perceived anymore.
Based on this observation it was decided to analyse the volatile component composition of the powders as such by using GC/MS-SPME. This analysis showed that bags containing the off smell showed the presence of alpha-terpineol.
A route-cause-analysis was started and showed that the typical off smell was also detected in the warehouse were the bags were stored. It was also observed that the bags were placed on wooden pallets.
Sensory analysis showed that bags that had been in direct contact with the wooden pallet contained the typical off smell in a high intensity. GC/MS-SPME analysis of the powders showed the highest peak intensities for alpha terpineol in samples that were in direct contact with the wooden pallets. Analysis of the wooden pallets itself showed the presence of alpha terpineol in very high peak intensities.
The results showed that the off smell of the powder packed in bags was caused by contamination of volatile components present in wooden pallets. Measures were taken to avoid contamination of such bags by using plastic pallets that both do not generate or transfer such an off smell.

[P 086] Searching for Tuber Melanosporum naturally generated volatiles as markers to determine authenticity of black truffle infused vegetable oils

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The great popularity of black truffles and its derivatives resides mainly in its volatile aromatic fractions which contribute to their characteristic aroma. Some culinary preparations are made with this fungus, especially black truffle infused oils. The adulteration of these products must be controlled due to the high economic cost of natural black truffles. In this study the volatile profile from some Tuber Melanosporum truffles, a black truffle infused oil prepared in the lab, and black truffle infused oils commercially available were exhaustively characterized by headspace solid-phase microextraction (HS-SPME) with PDMS and PDMS/carboxen /DVB fibers, followed by gas chromatography-mass spectrometry (GC-MS) analysis using methylsilicone and wax capillary columns. In order to confirm the black truffle infused oils authenticity some naturally generated volatiles in the black truffle but not present in vegetable oils were selected as markers. Profile differences with other varieties of truffles or with commercial truffle flavorings were remarked. Complementary, to determine differences in the aroma of the black truffles and authentic black truffle infused oils with flavored products a statistically calculated descriptive sensory analysis was also performed.

[P 087] Odor qualities and odor thresholds of halogenated, alkylated, alkenylated and methoxylated guaiacol-derived odorants

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Guaiacol-derived odorants are commonly found in nature. Guaiacols are produced by various plants and are widely used in food and perfume industry. They are employed, inter alia, as antiseptic and anesthetic agents [1,2]. Guaiacol derivatives have been found in smoked foods like smoked ham [3], in wheat beers [4]and brandy amongst a series of other foods. Halogenated guaiacols are, however, up to now mainly found in nature due to human intervention. Halogenated guaiacols are for example present in waste water of pulp mills and therefore responsible for some off-odors in fish [5,6]. However, comprehensive data on sensory characteristics of guaiacol derivatives and the impact of halogenation have not been reported until now.

In the present study, we compare the odor qualities and odor thresholds of guaiacols with different structural moieties with special focus on the impact of halogenation on their sensory properties. Thereby, a series of substances, which were not commercially available, was synthesized. In total, 40 compounds were systematically analyzed regarding their retention indices, odor qualities and odor thresholds. 17 of these compounds were synthesized for this purpose. Odor qualities of alkylated, alkenylated and methoxylated guaiacols were mainly smoky, clove-like and vanilla-like. Halogenated derivatives also exhibited smoky, sweet and vanilla-like odors, but also medicinal and plaster-like smells. Odor thresholds in air were very low, namely between 0.00018 and 111 ng/L for all compounds. Huge inter-individual differences were found for odor thresholds, whereas the perceived odor qualities were quite comparable between different individuals. The analytical and sensory data library created in this study will aid future analytical discovery of this interesting substance class. Parts of this work will also be published in [7,8].

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[P 088] Characterisation of the key aroma compounds in alcohol free beer by aroma extract dilution analysis

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Alcohol-free beer (AFB) consumption has increased over the last years, mainly associated with strict drink driving legislation, medical recommendation or religious grounds [1], but also with an increasing health awareness. However, the low alcohol content in AFBs (below 0.05% alcohol by volume in EU countries) is not the only difference when compared to regular Lager beers. The pleasant fruity flavour of Lager beers is one of the most appreciated features of these beverages, whereas AFBs exhibit a flavour reminiscent of wort [2]. Even though several studies have been carried out to characterise the key odourants in different alcoholic beers, such as pale Lager, dark Lager and wheat beers [3], there are no similar works for AFB. Hence, the aim of this research is to identify the compounds contributing to the characteristic aroma of AFB, as well as to determine their contribution to the main aroma by means of the Sensomics approach. In this work, the volatile fraction of the AFB was isolated using solvent assisted flavour extraction (SAFE) and split into both basic/neutral and acidic fractions [4]. Twenty-two odour regions showed high FD factor after AEDA experiments, among which the most potent were 5-ethyl-3-hydroxy-4-methyl-2(5*H*)-furanone, 3-(methylthio)-propanal, 2,3-butanedione, 4-vinylphenol and 2-methoxy-4-methylphenol. 2-Methylpropanal, 2-methylbutanal, 3-methylbutanal and 3-methyl-1-butanethiol an exhibited potent odour regions on further HS-SPME-GC-O experiments. The Strecker aldehydes have already been described as contributors to the worty flavour [5]. None of the esters typically found in regular lager beer (such as ethyl hexanoate, 3-methylbutyl acetate or ethyl acetate) were identified by GC-O, explaining the lack of fruitiness of AFB. We conclude that the absence of odour activity from fruity esters and the potency of Strecker aldehydes play a crucial role in the different aroma of AFB and its predominant worty nuance.

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[P 089] Studies on off flavours in lamb

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Across Europe, there is a move to produce lamb meat from entire males rather than castrates for welfare reasons. However, the meat industry in Ireland perceives that ram lamb has a less desirable flavour than castrates and females. A considerable amount of research has been conducted on off-flavours in sheep meat and this has identified a number of compounds which can contribute to the characteristic flavour of lamb and/or off-flavours. These include medium chain branched fatty acids, skatole and indole.
A trial was conducted on 144 lambs to determine the role of gender (entire male or castrate), breed (Suffolk Cross and Blackface x Swaledale) and finishing diet (concentrate, grass or clover silage, grazed grass, rape or turnip) on the incidence and cause of off-flavours in ram lambs. Lambs were slaughtered at between 8-10 months old and the loin subjected to sensory profiling and volatile analysis by headspace concentration and GC-MS-O. Branch chain fatty acids were determined in adipose tissue by GC-MS analysis of the methyl ester, after preparation by saponification, derivatisation and extraction.
The results show that there were effects of breed and diet on flavour, but fewer effects of gender. However, sensory evaluation showed that there were some off-flavours to which some panellists were sensitive and some were not. Those panellists exhibiting sensitivity reported elevated scores for off-flavours in the same animals. These off-flavours occurred sporadically in both ram lambs and castrates. The incidence of off-flavours was affected by diet. The links between these occurrences, odours detected by GC-O and concentrations of off-flavours compounds is presented.

[P 090] Application of hydratases for flavour and fragrance synthesis

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Hydratases catalyze the addition of water to the carbon-carbon double bond of a large diversity of substrates. Thereby, they provide access to secondary and tertiary alcohols in a highly regio- and enantiospecific reaction. Many of the resulting products are highly sought-after molecules for various industries or serve as building blocks for the production of both fine and bulk chemicals. These include, among others, additives for food and cosmetics industries. Promising enzymes for the production of value-added flavours and fragrances from inexpensive raw material such as plant oils are monoterpene hydratases and fatty acid hydratases. Whereas monoterpene hydratases catalyze the generation of chiral monoterpenoid alcohols from monoterpenes, fatty acid hydratases add water to the *cis* double bond of unsaturated fatty acids to yield the respective hydroxy fatty acids. Hydroxy fatty acid products can be further converted into different lactons exhibiting characteristic, pleasant smells by microbial reactions. Application of hydratases for flavour and fragrance production offers notable advantages compared to chemical synthesis or natural extraction from fruits, such as environmentally friendly production conditions, consistent product quality and overall lower costs. However, the applicability of hydratases on an industrial scale is currently limited, primarily by either a narrow substrate scope or low activity. In order to explore the potential of hydratases for sustainable flavour and fragrance synthesis, we have characterized promising representatives of monoterpene and fatty acid hydratases upon heterologous expression in *E. coli*: The linalool (de) hydratase from *Castelaniella defragrans* (LDI) and the oleate hydratase from *Elizabethkingia meningoseptica* (OhyA). Whereas LDI is a periplasmic, co-factor free homopentameric enzyme, OhyA is a homodimer with a non-covalently linked flavin co-factor. Upon reduction of the co-factor to $FADH_2$, the turnover rate of the hydration reaction by OhyA is enhanced by roughly one order of magnitude. We have identified E122 and Y241 as essential amino acids and have proposed the first reaction mechanism on the molecular level for this enzyme family. Based on the conservation of catalytically important residues in different classes of hydratases, our findings are paving the way to develop this enzyme class for industrial applications.

[P 091] Comparison of key aroma compounds in industrially manufactured and traditionally prepared meat bouillons

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Nowadays, there is a big consumer demand for organic, natural products without further additives. Therefore, already a broad range of 'all-natural' meat bouillons is on the market. Sensory evaluation showed that most of these industrially manufactured bouillons have a very different flavour compared to traditionally prepared ones.
Aroma compounds of traditionally prepared chicken [1, 2] and beef bouillons [1, 2, 3] have been well studied, but there is no data available regarding the difference in aroma compared to commercial products.
In order to gain insight into the molecular basis responsible for this aroma difference, traditionally prepared and commercially available products were screened for aroma compounds. In the present study extraction was performed by SPME and/or liquid extraction followed by solvent assisted flavour evaporation. Odour-active compounds were characterized by applying gas chromatography-olfactometry. Aroma compounds were identified and some of the key marker compounds quantitated. The role of some process parameters, e.g. pressure and temperature, was evaluated in model studies to get a deeper insight into formation mechanisms of these compounds.
The paper will give an overview of the major findings illustrating how key marker compounds influence the overall aroma of meat bouillons.

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[P 092] Malolactic fermentation of sea buckthorn (Hippophaë rhamnoides L.) berry juice with Lactobacillus plantarum: impact on sugars, sugars alcohols, and organic acids

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Sea buckthorn (*Hippophaë rhamnoides* L.) berries contain versatile combination of chemical compounds having health promoting features such water-soluble vitamins (C, B1, and B2), fat-soluble vitamins (A, K, and E), fatty acids, flavonoids, and plant sterols. However, the sour, bitter and astringent taste characteristics limit its regular consumption. The main chemical factors related to the sourness of sea buckthorn are the high concentrations of malic and quinic acids. Additionally, strong sourness intensifies the perception of astringency. Currently, malolactic fermentation is used commonly to decrease acidity in wines, as in this microbial process dicarboxylic malic acid is converted into carbon dioxide and monocarboxylic lactic acid. Therefore, in this study, we investigated potential to use *Lactobacillus plantarum* as a novel malolactic fermentation organism in sea buckthorn juice for decreasing concentrations of malic and quinic acids, ultimately leading to a juice with less sour and astringent traits.
Juices was extracted from Estonian sea buckthorn (subspecies *mongolica*) berries with hydraulic pressing, and the juice diluted to 1:1 with distilled water. Diluted juices were pasteurized in 85 °C for 5 min. Fermentations were performed with four different strains of *Lactobacillus plantarum*. An over-night growth of un-adapted cells was collected, washed, and inoculated ($\sim 10^8$ CFU/ml) to the juice samples with no additional nutrients. Samples were fermented in 30 °C for 72 hours.Conversion of malic acid (initial level of 11 g/L) into lactic acid was most effective with strain DSM 10492 (100 %), followed by DSM 100813 (31.4 %) and DSM 20174 (28.7 %). Additionally, a small but significant decrease in quinic acid content was measured from samples fermented with DSM 10492. No significant changes were detected in the concentrations of glucose, ethyl-glucose, fructose, L-quebrachitol, and methyl-*myo*-inositol after pasteurization or fermentation. This work shows that malolactic fermentation with *L. plantarum* could be used to decrease acidity of sea buckthorn juice without affecting its sugar content.

[P 093] Analysis of the aroma profile of cypress spurge (Euphorbia cyparissias) when infected by rust fungi (Uromyces pisi agg.)

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Cypress spurge (Euphorbia cyparissias), a herbaceous plant 15 - 50 cm in height, is common throughout Europe. The plants' flowers are intense yellow and excrete a honey-like smelling nectar, which attracts especially bees [1]. E. cyparissias is often infected by rust fungi, like Uromyces pisi aggregate. The anamorphic form leads to formation of pseudoblues which are yellow-orange colored by pycnidia and acecia, consisting only of a shoot with leaves. Infected shoots usually do not come into flower. In addition, the rust fungus releases an intensely smelling secretion to attract insects. These insects play an important role in the fertilization of the rust fungus: the spores get distributed and the spread of the fungus is secured [1][2].E. cyparissias plants were collected in the Rhine-Main area. The infected plants showed an intense smell which was significantly different from the odor of not infected plants. After DNA extraction a phylogenetic family tree for the investigated plants was generated. In parallel, the flavor compounds emitted by the plants were extracted by means of headspace solid phase microextraction (HS-SPME), separated by gas chromatography and were analyzed with mass spectrometry and olfactometry (HS SPME-GC-MS/MS-O).

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[P 094] Impact of enzyme treatment on flavour of aronia juice

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Aronia (*Aronia mitschurinii*), also called chokeberry, is a deciduous shrub that originates from the eastern part of North America. Berries are rich in polyphenols and sorbitol, and low in organic acids. Due to the strong and mostly unfamiliar orosensory properties of the berry, chokeberries are usually used in blended juices. The aim of this work was to analyze smell and taste of aronia juices prepared from berries grown in South-West of Finland.
Aronia juices were pressed from crushed berries without (I) and with (II) pectinolytic enzyme treatment applying incubation for 5h at 50°C. Samples were studied using projective mapping by volunteer participants (n = 32) in controlled sensory laboratory environment (ISO 8589). Pure juices were diluted with water (carbon-filtrated) 1:2 before sensory evaluation. Moreover, qualitative descriptive analysis (n = 7) was applied to describe the sensory properties of juices. In addition, a gas chromatography analysis of sugar and acid contents in juices was carried out.
Our results showed a clear impact of enzyme treatment on smell and taste of aronia juices. Juice w/ enzyme was described as 'unpleasant' with descriptions such as 'almond', 'nutty', 'oat', 'stale' and 'astringent'. In both juices main sugars were glucose, sorbitol and fructose, and main acids were malic and quinic acid. This study shows that although enzyme treatment will contribute to yield of pressed juice, it also creates specific flavours to aronia juices, which are in many cases undesired and unpleasant to consumers.

Keywords: chokeberry, aronia, sensory evaluation, sugars and acids, GC

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[P 095] Validity of marker compounds for authenticity control - Case Study: Methylcinnamate

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There is a global trend towards natural food solutions. Hence the industry is looking for ways to increase their portfolio of natural aroma compounds. Good examples are the esters of cinnamic acid, which are widely used for fragrance compositions including soaps and cosmetics as well as for the creation of flavors for beverages, baked goods, dairy products and convenience food. Especially the methylester of cinnamic acid is widely used due to its sweet, aromatic and balsamic notes combined with a fruity odor. Methylcinnamate occurs naturally in a variety of plants, including fruits like strawberry and some culinary spices, such as thyme and basil. However, the isolation from these species is not economically feasible. Alternative sources for natural methylcinnamate are essential oils of rhizomes of various *Alpinia* species, e.g. *A. malaccensis* (from Malaysia) containing approximately 78 % of this aroma compound. Another alternative would be the esterification of widely available natural cinnamic acid with methanol form natural sources under conditions permitted by corresponding national or international laws. Natural aroma compounds are mostly more expensive than their synthetic equivalents and are therefore prone to adulteration. Several sophisticated methods have been developed to identify adulterated material, e.g. isotopic ratio mass spectrometry or SNIF-NMR. As these methods are not always conclusive, the presence of trace components is often considered as an additional marker for adulteration. Within this study we investigate the relevance of methyl 3-methoxy-3-phenyl-propanoate which is currently discussed, as a marker for possible adulteration of methylcinnamate, and shed light on its formation regarding different preparation methods or extraction protocols.

[P 096] Mapping the Origin of Cajuput Essential Oil to Its Compatibility as Cajuputs®Candy Functional Flavor

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Cajuput oil is one of non-timber forest products which recently has been successfully utilized as a functional flavor in functional candy namely Cajuputs. However, the quality of cajuput essential oil which is distilled from *Melaleuca cajuputi* leaf and small stem would be influenced by geographical origins. To obtain any physical or chemical characteristic markers to the sensory compatibility of the essential oil as targeted flavor is a challenge. A total of 11 samples representing different geographic areas in Indonesian plantations were analyzed based on physicochemical and sensory properties. The physical properties such as specific gravity, refractive index, optical rotation and solubility in ethanol 80% were examined. The cineol content and the volatiles profiles of its samples were also analyzed by GC-MS. Hedonic sensory test and Quantitative Descriptive Analysis (QDA) method have been conducted to evaluate the sensory quality. Principal Component Analysis (PCA) was applied for oil origin mapping based on their volatiles composition. Partial Least Squares (PLS) was used to study the correlation between volatile compound and aroma characteristics. The result showed that cajuput essential oil from Ponorogo and Pasuruan potentially had a good compatibility as a Cajuputs®candy flavor with the best acceptance rate in terms of taste, aroma and overall; even they exceeded the reference values. The result showed that the compatibility of sensory quality can be mapped through the physic-chemical attributes.

Keywords: cajuput essential oils, mapping origin, flavor compatibility, physical properties, hedonic test, QDA

[P 097] Parameters impacting flavour profile and shelf-life of dairy ingredients

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Dairy ingredients are key to many snacking and confectionary products delivering flavour and texture functionalities. It is therefore important for the industry to be able to evaluate the dairy raw materials based on parameters which impact product quality. Both the actual flavour profile of dairy ingredients as well as the shelf-life will influence the selection of dairy ingredients for specific applications and therefore need to be characterised with relevant analytical and/or sensory measurements. It is well known that the drying technology which is used to transform the wet dairy ingredient into a dry system has an influence on the resulting flavour profile and shelf-life. Spray drying is the most widely used technology in the dairy industry due to its favourable processing costs. However, it can result in changes to the initial flavour profile and have detrimental effect on shelf-life if not carefully managed. Another important aspect is to understand and predict the final flavour profile and shelf-life of products containing dairy ingredients as well as whether the incorporation of dairy ingredients into products such as chocolate, caramel, and biscuit can delay undesirable reaction which could occur during the shelf-life of dairy ingredients.
This poster will provide a summary of existing knowledge including the impact of drying technology of typical dairy systems on loss of flavour compounds, generation of off-notes and generation of precursors for oxidation, the comparison between different technologies such as spray drying and freeze drying, hypotheses on potential mechanisms behind the differences, and relevant measurements to characterise the dairy flavour profile and shelf-life. The poster will also provide results from a new shelf-life study of dairy ingredients.

[P 098] Identification of orange juice and peel molasses non-volatiles with sweet and bitter modulating sensory effect

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Huanglongbing (HLB) or Citrus Greening disease threatens the Florida orange juice industry because fruit from infected trees exhibit delayed maturity and varying degrees of off-flavor described as bitter-harsh, metallic and sour, as well as less juicy and fruity. In this study we hypothesized that identifications of compounds from orange with sweet optimizing and bitter mitigating sensory effects may help breeders and juice producers to improve fruit and juice quality.
To locate single compounds or groups of chromatographically isolated compound fractions with the desired sensory activities, a method was developed to quantitatively profile the descriptors sweetness, sourness, bitterness, astringency, and after-taste or after-mouth sensations in pasteurized orange juice. A -5 to +5 scale was adopted and an HLB-affected orange juice, anchored at the value of 0, was used as reference sample to assess sensory differences. Taste guided fractionation of orange peel molasses and orange juice by fast centrifugal partition chromatography, with subsequent sensory evaluations and chemical composition studies, revealed significant taste modulating effects of two fractions generally containing hydroxycinnamates, flavone-di-*C*-glycosides and flavonols at 120 ppm. Tasting commercially available individual compounds showed that a much lower concentration (10-20 ppm) was sufficient for the taste modulating effect. These compounds/fractions resulted in a reduction of bitterness, astringency and after-taste perceptions, whereas sweetness was often increased and sourness decreased. Panelists described the samples as having a 'rounded' taste rather than 'harsh', as is often associated with HLB-affected juice. This taste modulating effect was found to be concentration dependent, highlighting the complexity of using natural products and importance of dosage optimization. Fractions containing flavones, coumarins and hydroxycinnamic acids, on the other hand, were found to exacerbate HLB off-flavor by increasing bitterness and/or sourness, astringency and undesirable after-taste while reducing sweetness.
Based on the described results, strategies for the development of specific technologies and dedicated flavor systems for the management of off-flavor are discussed.

[P 099] Influence of protective inert gas atmospheres on the aroma stability of orange juice with pulp

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The complex profile of volatile fraction of defrosted raw orange juice - immediately 'slightly' pasteurized was studied in context of different inert gases applications in production process. For comparison, effects of three diverse processing atmospheres - conventional air, nitrogen and carbon dioxide - to individual volatiles was investigated during four months-long shelf-life of juice over two production years. The study demonstrated use of headspace-solid phase microextraction (HS-SPME) with gas chromatography-mass spectrometry (GC-MS), and in parallel, with gas chromatography coupled to the flame ionisation detection and simultaneous human olfaction (GC-FID/O) to the complex characterisation of the total aroma of orange juice originated from Costa Rica. Gained results showed that inert processing atmospheres can partly preserve the aroma profile of the orange juice. The best results were obtained with nitrogen atmosphere. The effect of carbon dioxide application was comparable with nitrogen one, but its acceptability by consumers has to be considered because of the sparkling character of final products. None of two investigated inert atmospheres was able to avoid all changes in the composition of volatiles during storage. However, GC-FID/O analyses proved that these changes were not significant sensorially and they did not lead to the worsening of organoleptic properties of analysed juices. On the contrary, negative sensory changes in flavour were observed for juices processed in air atmosphere within the storage period. Most of the changes arose after the second month of storage. GC/FID-O analyses revealed that mostly generation of certain aldehydes, mainly hexanal, nonanal and perillaldehyde could be principally responsible for the off-flavour phenomenon occurred in longer-stored orange juice. Concerning the observed changes in odour intensities of these aldehydes, they can explain worsening of the organoleptic properties of juice processed in conventional atmosphere that occurred during storage. There was noticed increase in bitter and waxy odour and taste, as well as appearing of considerable astringent taste of juice, certain loss of freshness and fruity sweetness, and undesirable colour changes.

Acknowledgement: This contribution is the result of the project APVV-15-0023 'Quality and authenticity of fruit juices - study of relationships between the origin of feedstock, processing technology and quality of fruit juices'.

[P 100] Identification of a mold-like off-flavour in Original Taco Spice Mix

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The aim of the present study was to identify the compounds and mechanism responsible for the mold-like off-flavor in a batch of commercial 'Original Taco Spice Mix'. Sensory analysis confirmed an off-odor in comparison with the non-contaminated batches. Gas chromatography (time-of- flight) mass-spectrometry (GC/MS(tof)) and gas-chromatography-olfactometry (GC-O) analysis led to conclusion that differences between the reference and the lesser quality spice mix is due to the difference in dried oregano used as an ingredient. Apparently, smaller amount of *thymol* and larger quantities of *camphor, borneol, terpineol* and *bornyl acetate* in oregano leads to a different odor perception and volatile balance. Latter compounds give a moldy, camphoraceous, herbal and leafy note to the oregano as well as to the taco spice mix and the lack of *thymol* reduces the typical thyme-like note. The oregano used in the spice mix was most probably from other subspecies with different essential oil composition and therefore sensory properties. Additionally, a fingerprinting method was developed based on *front-face* fluorescence spectroscopy (FFFS) and principle component analysis (PCA), which can be used in oregano quality control. The new method differentiated the low quality oregano from reference products with the highest probability.

[P 101] Characterization of Odorants in Wood

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Wood is a material humans come into contact with every day, e.g., in the form of furniture and building materials, products of daily use, or secondary products that are derived from wood such as paper and cardboard. Whereas general emissions of volatile organic compounds from wood are well known, only limited information is available on the odour-active substances. The present study therefore aimed at specifically elucidating the odorous constituents of wood.

Previous investigations have predominantly focused on odorants in wood from wooden barrels that are used for wines and spirits, and their impact on the filling goods. Apart from that, information about odorous substances in untreated wood is rare.

To gain an overview of the odour-active constituents in wood, different wood species were investigated.

Targeted odorant analysis requires specialized techniques combining modern odorant analytical tools with human-sensory evaluation. Following this concept, the odour profiles of the wood samples were first evaluated by human sensory analysis. The odorants were then characterized by gas chromatography-olfactometry (GC-O) and ranked according to their odour potency via aroma extract dilution analysis (AEDA). Using this approach, more than 60 odorous substances were detected and the most potent odorants were identified by gas chromatography-mass spectrometry/olfactometry (GC-MS) and two-dimensional gas chromatography-mass spectrometry/olfactometry (2D-GC-MS/O).

The identified odorants belong to a variety of substance classes that exhibit a great diversity in odour character. Some of the substances are known constituents in wood whereas others were identified for the first time in wood or even for the first time as being odour-active.

The successful identification of potent odorants in wood is a first important step towards the understanding of the molecular basis of the odour profile of a commonly-used material in daily life.

[P 102] Odor-active compounds in inflatable beach toys

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Inflatable beach toys such as beach balls and pool floats are typically manufactured from polyvinyl chloride (PVC). Particularly when new, these PVC toys often exhibit an intense and characteristic 'plastic-like' odor, the molecular background of which has not been fully elucidated yet.
Within the current study, PVC beach balls from different manufacturers and sources were orthonasally evaluated by a trained test panel. One sample showing the characteristic odor in high intensity was selected for further investigation. The beach ball volatiles were isolated by solvent extraction and solvent-assisted flavor evaporation (SAFE) [1] and subjected to gas chromatography-olfactometry (GC-O) and aroma extract dilution analysis (AEDA) [2]. In total, 38 odor-active compounds were detected, among which 14 compounds showed a solvent-like, plastic-like or pungent smell. FD factors covered a range of 1 to 4096. Structure assignments of the odor-active compounds were accomplished by comparing their odor quality, their retention indices on two GC columns of different polarity (DB-5, FFAP), and their mass spectra as recorded by gas chromatography-mass spectrometry with the respective data obtained from the parallel analysis of authentic reference compounds.
Among the most potent odorants present in the PVC beach ball were 2-ethylhexanal, 2-ethylhexyl 4-methylbenzoate, 2-ethylhexan-1-ol, and 2-ethylhexanoic acid, all of which were most likely derived from the decomposition of di(2-ethylhexyl) terephthalate (DEHT) used as plasticizer. Plastic-like smelling 2-ethylhexyl 4-methylbenzoate was found for the first time in PVC.

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[P 103] Malodourous emissions of wood pellets during storage

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In recent years a significant increase in the demand of wood pellets has been observed. Besides beneficial characteristics for the combustion process, e.g. wood pellets exhibit a high energy density, the customer also expects an inherent wood pellet flavour of the product.
During storage of pellets, various compounds like e.g. carbon monoxide (CO), carbon dioxide (CO_2) and unpleasant volatile organic compounds (VOCs) could be formed. Research on this so-called off-gassing phenomenon is focusing on the one hand on the identification and characterisation of these unpleasant odoractive VOCs and on the other hand on the toxic atmosphere caused by formation of CO and depletion of oxygen (O_2). However, both effects have in common that they cause insecurity and complaints by the end-user. The research project 'SMELL' study on malodourous emissions from wood pellets' was aimed at the development of possibilities for reduction of the off-gassing phenomenon.
The formation pathways of these unpleasant odoractive VOCs and CO could not be explained completely, but one reason for the release of emissions is the degradation of naturally wood components like resins or fatty acids. Also the microbial spoilage of raw material during storage could be another way for the formation of VOCs (especially aldehydes and acids) and CO.
It could be shown that the higher the concentration of unsaturated fatty and resin acids in the raw material the more VOCs could be detected. So the formation of unpleasant VOCs and partially CO could originate by the autooxidation of unsaturated fatty acids during production of wood pellets. Therefore the addition of antioxidative acting substances to the pelletizing process was investigated for the reduction of undesirable emissions.

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[P 104] Describing the smell of wet cat food using a common sensory language

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Meal time is increasingly considered by pet owners as a privileged moment to create emotional bonds with their animal. To make meal time a shared enjoyable moment, pet food manufacturers not only need to satisfy pets appetite, they also need to satisfy pet owner expectations towards food. For instance, pet food cosmetic and sensory properties such as appearance and smell highly contribute to its acceptance by the pet owner. These factors play an important role in the act of repurchase of the pet food product.
Only a few research studies have used human sensory analysis to describe the smell of wet petfood. The purpose of this study was to characterize the smell of different wet cat foods available on the European market using Petscript, a sensory language specifically developed for this type of product.First, a full set of olfactory descriptors was generated by a human expert panel in order to have a common sensory language to describe the odor profile of wet pet food. Then, several products were selected to offer a representative picture of the market. All these products were assessed via a Rate All That Apply (RATA) method in association with a free description to have an exhaustive odor characterization.
The products were then positioned on a map according to their olfactory profile.
The Petscript sensory language was successfully used to build the olfactory space for wet cat food. The results highlighted the existence of clusters of products showing similar odor profile. The Petscript language can be used to support petfooders strategy by positioning their products in the landscape, and helping them to reach a specific target or to differentiate from the other products on the market.The next challenge would be to couple these descriptive sensory results with studies on preferences to enable an identification of appreciated smell profiles by pet owners.

[P 105] Comparison of Different Analytical Methods for the Quantification of Odor-active Haloanisols in Food Contact Materials

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2,4,6-Trichloroanisol (2,4,6-TCA) the major compound responsible for cork taint in wine belongs to haloanisoles, which are formed by microorganisms, primarily fungi [1]. They can contribute to off flavour in food and food contact material at low concentrations. There are significant differences in the sensory thresholds of different polybrominated and polychlorinated anisoles. In parallel to the determination of the odor threshold concentration (OTC's) by our trained expert panel in different matrices we developed and compared different analytical methods which are able to reach detection limits within the sensitivity of the human nose.
Due to the fact that 2,4,6-TCA and 2,4,6-Tribromoansiole (2,4,6-TBA) exhibit extremely low threshold concentration in the low pg/L range in water the applied methods need highly sensitive and selective detection systems.
Based on headspace solid phase microextraction methods (HS-SPME), the applicability of several one and two dimensional separation systems with mass selective detection will be compared.
For the comparison of the methods we used real world samples (food packaging material based on recycled card board). Methods were validated for LOD and LOQ using quadrupole mass filters with electron impact ionization (EI), negative chemical ionization (NCI) and tandem mass spectrometry (MS/MS), respectively. In addition, the influence on the increase in selectivity and sensitivity using comprehensive GCxGC was evaluated.

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[P 106] Emissions of compost bedded pack barn for cattle

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The compost bedded pack barn is an animal-friendly housing system for cattle. It consists of a large, open resting area, usually bedded with sawdust. The most critical success factor for managing a compost bedded pack barn (CDB) is providing a comfortable, dry resting surface for cows at all times.
Within the project 'Assessment of compost dairy bedded-back barns with regard of compost quality, odour and greenhouse gas emissions' emission measurements (NH_3 and CO_2) of 23 CDB were executed and samples for the analysis of odouractive volatile organic compounds (VOCs) and chemical parameters (e.g. pH value, dry matter, C/N ratio) were taken. In addition, an extensive microbiological screening was carried out with special attention to harmful bacteria. The samples were picked from the compost manure mattress during three different seasons (summer / autumn / winter). Furthermore, various basic data were collected by questionnaire in order to determine the analytical results and the operational management better.
In CDB mainly sawdust is used for bedding. Sawdust got more and more expensive in the last years, but has a good absorptivity as well as a structural stability and a good decomposition under aerobic conditions. Spelt husk are very well suited to improve the composting process (temperature increase), which may be particularly important under wet and cold weather conditions as well as in wintertime.
Concerning the assessment of emissions in CDB no correlations between ammonia and odouractive VOCs could be determined. In comparison with the ammonia emissions analysed on the bedding surface only 1/4 of the analysed CDBs rates above the concentrations derived from stables cubicles, whereas the majority shows ammonia data below or in this concentration range. The results of the analysis of the odouractive VOCs show considerably lower concentrations than stables cubicles.

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[P 107] Investigation of odor-active compounds in grapefruit (Citrus paradisi)

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The odor-active compounds in grapefruit juice have been investigated for several decades by many researchers. So far, over 320 volatile compounds including intense odorants such as 1-*p*-menthene-8-thiol and 4-mercapto-4-methylpentan-2-one were identified [1]. However, there should be room to find some other unidentified odor-active components in grapefruit juice. The aim of this study is to unveil new odor contributors in grapefruit juice.
The odor-active compounds of grapefruit essence oil obtained by distillation of grapefruit juice were investigated by AEDA technique. As a result, 15 odor-active compounds showed high FD factors in the range of 64-1024. Among them, we focused on a 'woody' odor because of few reports about 'woody' note in grapefruit, so far.
Recently, we have developed a GC omission test method using a preparative capillary GC for comparison of odor characteristics between an original sample and a sample omitted target component(s) [2]. Thanks to this method, two materials with and without components eluted in a certain GC retention time range can be prepared. Through the sensory evaluation of them, the odor contribution of omitted components is elucidated.
The GC omission test was applied in order to elucidate the effect of the target 'woody' odorant. Consequently, the omitted sample was described to be 'less juiciness' compared with the original one by trained panels.Subsequently, a multi-dimensional GC/MS-Olfactometry (MDGC/MS-O) analysis revealed that the woody odorant was mustakone, a sesquiterpene ketone. It was found that mustakone presented in grapefruit juice in concentration of a few mg/kg. To reveal the enantiomeric distribution of mustakone in grapefruit, each enantiomer were obtained by oxidation of (+) and alpha-copaene, respectively [3]. As a result of an enantioselective MDGC/MS analysis, mustakone were in a ratio of 8.5% for (+)-isomer and 91.5% for -one. To confirm the effect of mustakone for grapefruit odor, a mixture of both synthesized enantiomers in the resulted enantiomeric ratio was added to the omitted sample prepared by the GC omission test, followed by sensory test. The result indicated addition of appropriate quantities of mustakone to the omitted sample enriched natural juicy aroma note like the original essence oil.

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[P 108] Combining on-line analysis of volatiles with data visualisation for rapid answers in commercial flavour research

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Outsourcing of flavour analyses by large and small companies has become commonplace in the last decade as witnessed by the increasing number of companies offering conventional or niche services. Clients of these companies frequently need rapid answers to flavour problems and, often, it is not quite clear what the exact problem is or where the problem lies. Preliminary screening of samples can help understand the scale and extent of the problem in a short period of time and develop a more focused analytical approach. While the conventional chromatographic techniques are the gold standard in flavour analyses, they are relatively slow as the chromatography step is the key rate-limiter.
We report an alternative approach using on-line headspace analysis using the MSNose system, which provides rapid analysis, coupled with a data visualisation and data processing platform, which can handle the multi-factor nature of the data. A coffee supplier provided eight samples (with different origins and colours) and asked us to identify differences in the odour profiles and which compounds were involved. Direct sampling of the headspace into the MSNose system in triplicate produced ion traces within 2 h and the data was loaded into a data visualisation programme and plotted in 3D; X axis coffee sample, Y axis m/z value, Z axis ion abundance. Using colour coding and different shapes for the data points, the country of origin and the sample colour values were also built into the plot. The presentation will demonstrate how these visualisation packages can be used for rapid data interpretation, using visual and statistical methods. Ions can be analysed singly (e.g. to determine variation across samples) or together to identify correlations or trends. The mixture of text and numerical data can be filtered to test potential hypotheses to explain the differences. The presentation will demonstrate how visualisation of the data can be used, not only to help the analyst in their interpretation of the data but also to show the client in a clear way where the potential causes of the flavour problems are and what the next steps should be.

[P 109] Rapid analysis of important taste active components in chocolate by ultra high performance liquid chromatography coupled with high resolution mass spectrometry (UHPLC-QToF-MS)

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Chocolate is appreciated by consumers around the globe due to its unique organoleptic properties. The combination of desirable textural features and a boost of flavours when melting in the mouth made chocolate become one of the most beloved treats in the human diet. Several decades of research have focussed on deciphering the flavour active components in cocoa and chocolate and deepening the understanding of their origin [1]. In particular the role of cocoa derived aroma active components and their fate during roasting has been studied in detail [2].
The most important taste active components in cocoa nibs have been investigated using molecular sensory science concepts [3]. The calculation of dose over threshold (DoT) values revealed that in particular alkaloids and diketopiperazines contribute to the bitter taste of cocoa, while flavan-3-ols, procyanidins and *N*-phenylpropanoyl-L-amino acids are among the compound classes responsible for the astringency of cocoa [3]. The role of individual tastants in chocolate samples remains less understood and the fast and reliable identification and quantification of these tastants represents a gap.
The present study illustrates a rapid approach to qualify and quantify taste active compounds in chocolate matrices. After direct extraction with aqueous, acidified methanol the samples were analysed by UHPLC-QToF-MS. The approach allowed the (semi)-quantification of a series of taste actives within a single injection, while the high resolution of the mass analyser allowed a high confidence in their identification. The calculated DoT values for key chocolate taste compounds allowed a deeper understanding of the orosensory properties of chocolate and created a link with human-sensory investigations. The outcomes of this study illustrate the benefit of UHPLC in combination with high resolution mass spectrometry to identify and quantify key tastants in chocolate samples, while requiring minimal sample preparation.

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[P 110] Evaluation and optimization of sample preparation techniques towards the differentiation - origin of Chinese green tea

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Green tea provide a very light flavoured beverage. Consequently, the concentration of aroma compounds is significantly lower than in black tea. Green tea is the most consumed beverage in China, therefor variations in levels of the potent odorants are crucial to the characteristic aroma of green tea.
In this study, aroma profiles of 18 green tea samples from Guizhou, a well known province for high quality green tea, were investigated and compared to teas from other Chinese regions. Several preparation techniques like Static (SH) and Dynamic Headspace (DHS), Solid-phase Mircroextraction (SPME), Stir-bar Sorptive Extraction (SBSE) and Solvent Assisted Flavour Evaporation (SAFE) were performed in order to compare their efficiency and applicability. All methods were coupled with gas chromatography and mass spectrometry (GC-MS).
Headspace-SPME proved to be the most efficient method overall regarding robustness, selectivity, reproducibility and practical performance. The optimization of this technique conveyed further aspects. Here, it was observed that high extraction temperatures lead to a decrease of extracted very volatile substances. Moreover, a formation of volatiles caused by incubation temperatures of 40-80°C was not detected and was thus negligible. Furthermore, it was possible to increase the selectivity for certain compounds when using different SPME fibers.
Finally, it was possible to distinguish different tea samples from various origins by HS-SPME. In addition to that, statistical analysis like discriminant analysis (PLS-DA) enables a classification of all samples into their provinces.
This poster will sum up the comparison between the mentioned preparation techniques and present HS-SPME as a potential method for green tea analysis also concerning authenticity.

[P 111] On-line high-throughput analysis of the volatilome of microorganisms that have agroindustrial relevance

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Yeast and bacterial species are widely used for leavening, brewing, wine making or dairy fermentations and play a key role in producing the characteristic sensory profile and perceived quality of these products through the volatile organic compounds (VOCs) they generate. These VOCs synthetized by microorganisms as secondary metabolites, not only impart important sensory notes but also have important technological functions. As such, an on-line and non-invasive screening of the microorganism volatilome is of high importance to better understand and control these processes and support innovation in this traditional sector by unlocking the flavor generation process.
This contribution describes our activities investigating the potential of using Proton-Transfer-Reaction Time-of-Flight Mass Spectrometry (PTR-ToF-MS) coupled with multipurpose head-space automated sampling (MHSA) to enable the efficient monitoring of agroindustry-relevant microbiological processes: dough leavening, lactic acid fermentation, brewing and wine making. This experimental setup also enabled the measurement of VOCs produced by yeast grown on solid medium.
Automation of the analytical process as provided by MHSA guaranteed reproducibility over the whole microorganism life cycle, the accurate control of process parameters (temperature and sampling times). Analysis could be completed as frequently as every second but typically the headspace of each sample was measured for one minute while displacing the headspace with zero air or pure nitrogen. In addition, the fermentation processes can automatically be monitored for several hours in the case of dough leavening and lactic acid fermentations or days for alcoholic fermentations or yeast colonies grown on a solid medium. The set-up allows the monitoring of 128 samples at the same time.
To deal with data matrices containing several hundred of mass peaks for each measurement multivariate data analysis is needed to provide the general overview of biological processes and phenotypic variability among different microbial strains. Observations of single VOC emission curves allow the opportunity to study known metabolic pathways and unravel unknown ones.
In general, PTR-ToF-MS coupled to MHSA allows insight into the dynamic nature of the microorganism volatilome and, consequently, on flavor.

[P 112] Conventional SPME vs dynamic headspace with sorbent tubes to explore breast milk volatile fraction

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Headspace composition of biological matrices contains many volatiles, carrying multiple interests or significances. Besides the odorant aspect of certain compounds, volatiles can vehicle biological information (food safety-status, health- or reproductive-status of congeners). Volatile content analysis of biological substrates by gas-chromatography (GC), prior requires an extraction by a technique that do not distort its original profile. Biological samples can be synthetized in small quantities and volumes available for analysis can be limited. Hence, a suitable extraction technique should be representative of the sample, workable on small-scale samples and able to concentrate molecules. Headspace extraction methods using sorptive phases were widely developed. Because of its simple procedure and great aroma representativeness, solid phase micro-extraction (SPME) is regularly used. However, the little amount of sorbent on fibers limits its use for analysis of samples with weak headspace concentration. Dynamic headspace (DHS) methods demonstrate enrichment capabilities through the constant displacement of headspace equilibrium although, implementation of this technique can be complex.

The objective of this work was to evaluate the capability of DHS associated to sorbent tubes for the exploration of breast milk headspace and to compare it with SPME.

Volatile fraction of pooled breast milks was extracted by SPME with a Car/PDMS fiber or by DHS associated to Tenax or Bio-monitoring sorbent tubes. Extracts were analyzed by GC coupled to Mass spectrometry and Flame Ionization Detector. Performance of extractions were compared on the basis of quantitative and qualitative chromatograms investigation and regarding physico-chemical properties of compounds detected.

Both techniques enable to detect compounds from a large range of chemical families but DHS associated to sorbent tubes enables to detect greater number of compounds than SPME. Moreover, DHS displays a greater concentration potential, up to a factor of 15 for some compounds. The two sorbents tested in DHS exhibit equivalent extraction capabilities regarding all criteria.

In conclusion, despite a challenging implementation, DHS with sorbent tubes is a better option than SPME with Car/PDMS fiber to investigate volatile fraction of small-scale or little concentrated samples like breast milk. Widely used, Tenax will be preferred to Bio-monitoring sorbent to enhance comparison of results with current literature.

[P 113] Characterization of volatile key compounds in different strawberry cultivars: complementarity of SPME & SBSE techniques and comparison with DHS technique.

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For the last twenty years, SPME or SBSE have been currently used for the qualitative characterization of volatile compounds profiles of numerous food matrices.
Each of them shows advantages and disadvantages from a qualitative or a quantitative point of view. The current work proposes to use these two techniques for their complementarity in term of extraction efficacy for polar and non-polar compounds, from very volatile to semi-volatile compounds. SPME is used in the headspace for its high sensitivity for very volatile to volatile compounds extraction, even if some limits for quantification are well known. In parallel, SBSE allows to extract and quantify volatile to semi-volatile compounds, even at traces level, directly by immersion in the food matrices.
This complementarity is strengthened by the choice of chromatographic column polarity combined with each specific extraction technique.
This study shows how qualitative results obtained both by SPME and SBSE techniques are very useful to highlight overall aromatic profiles of strawberries, and discriminate several cultivars according to aromatic key-compounds. As only aromatic tendencies are evaluated using SPME/SBSE combinations, a quantitative method need to be implemented to assess the real aromatic impact using OAV approach.
To establish a quantifying method of these main strawberries key-compounds, a conventional DHS-GC-MS method is tested to evaluate its efficacy regarding qualitative overall profile of strawberries.

[P 114] Real-Time Flavour Release by PTR-TOFMS: Recent Applications and Latest Developments

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Proton-transfer-reaction mass spectrometry (PTR-MS) has undisputedly contributed to a wealth of knowledge on the kinetics and mechanisms of flavour release since the inception of the technique a little over two decades ago. Since the early, pioneering studies exploring its utility in diverse flavour release applications, technological advances and the development of peripheral equipment have resulted in a reliable, robust system for rapid monitoring of volatiles down to ultra-trace levels and with high precision. In particular, the transition from a quadrupole-based mass analyser (PTR-QMS) to a time-of-flight mass spectrometer (PTR-TOFMS) offers yet faster analyses of complex (flavour) samples with a high resolution, allowing for the discrimination of isobaric compounds. The recent implementation of a selectable gas chromatographic pre-separation column (in the form of a fastGC) enables flavour compounds with identical elemental compositions, i.e., isomers, to be distinguished from one another. Thus, in combination, this system offers unsurpassable insights into flavour release, both *in vivo* and *in vitro*.
In the past, published PTR-MS data have typically relied on calculations of gas-phase compound concentrations based on ion kinetic theory, but such conversions inherently suffer from inaccuracies in proton transfer reaction rates (either theoretically or experimentally derived) and from ionisation efficiency nuances arising from variations in sample gas composition (humidity, CO_2 content, etc.), as well as uncertainties in branching ratios of target compounds upon ionisation. The recent introduction of a calibration system for use with bespoke liquid standards (liquid calibration unit, LCU) is an indispensible tool for data quality assurance by allowing calibration and simultaneous fragmentation assessment of target aroma compounds.
This lecture will focus on the most recent developments of PTR-MS for real-time flavour analysis, will demonstrate the calibration of aroma compounds using the LCU, and will offer example applications on cocoa roasting and flavour profiles of milk undergoing photooxidation, as well as recent uses of PTR-TOFMS in non-flavour/food applications.

[P 115] Predicting fishy off-flavor and identifying lipid oxidation compounds in dairy powders using SPME-GC-MS and machine learning

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The correlation between solid phase micro-extraction gas chromatography / mass spectrometry (SPME-GC/MS) data and sensory fishiness data of dairy powders fortified with long-chain polyunsaturated fatty acids and iron has been studied. A machine learning approach for the prediction of fishiness off-flavor from raw CG/MS data is presented and its potential to determine key marker compounds. To find peak correspondence and to correct retention time shifts, peaks of the GC/MS raw data of different samples were aligned on a peak matching graph using dynamic programming. Sensory modeling and prediction was done without prior peak identification in the mass spectral library. A classifier was trained using the Random Forest model to compare the fishiness between two samples on the basis of the instrumental data. Prediction of the sensory data is done by applying this classifier to compare a new sample to every training sample, following a voting mechanism. Predictions of fishines perception obtained by the presented approach showed good accuracy, in particular when compared with regression based modelling, both in leave-one-out evaluation and on a separate powder sample test set. 10 aroma components and process markers (methyl and ethyl-ketones, lipid derived aldehydes & acids as well as one unsaturated alcohol and alkylfuran furan) were identified by Random Forest to significantly correlate with fishiness perception. These molecules are mostly secondary lipidoxidation products.
It will be shown how machine learning techniques can be used to bridge between different types of data obtained upon the analysis of food. Although the present study was limited to fishiness perception of LC-PUFA and iron fortified dairy powders, a similar approach will be employed for other types of data and product categories.

[P 116] Characterization of particularities in the male-female volatile metabolism of plants: role in Baccharis tridentata adaptation and potential applications

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Volatile metabolites analysis remains as an important step for understanding plant metabolism and for prospecting the flora in the looking for new aromatic resources. Modern analysis approach is focusing in technological gas chromatography improvements besides to in a more careful sampling process of the plants. In dioecious species, female/male metabolic differences are poorly understood and it must be of relevance if the economic exploitation of such resources is the objective. Baccharis tridentata Vahl is an aromatic and ornamental shrub native from Southern Cone of Americas, previously identified by us as for a relative-high content of bornyl acetate in its volatile profile. In this work, We have analyzed (qualitatively and quantitatively) the essential oil composition of the flowering aerial parts of both male and female plants separately by GC-MS, GC-FID (internal standard) and CPGC-MS (modified cyclodextrin) reporting enantiomeric distribution of monoterpenes hydrocarbons as a genuineness criteria. The results confirmed high qualitative similarities between both genders oils but quantitative differences for the main components: pinene (794 $\pm$ 40 vs. 1173 $\pm$ 40 mg/mL female/male, respectively), pinene (287 $\pm$ 14 vs. 362 $\pm$ 18), limonene (204 $\pm$ 10 vs. 273 $\pm$ 14) and bornyl acetate (69 $\pm$ 3 vs. 60 $\pm$ 3). Despite this, no high differences were found in semi-quantification by GC-MS area percentage normalization, highlighting the importance of GC-FID internal standard quantification for accuracy in volatile compounds analysis, mainly if ecological or biological roles want to be associated to the composition. Regarding to the analysis by CPGC-MS of monoterpene hydrocarbons, both sexes presented both enantiomers in the same ratio, which is differential to values reported in literature for related plants. However, natural bornyl acetate (isolated from B. tridentata essential oil) demonstrated a 100% of enantiomeric excess of the levogyre enantiomer, a fact which has chemotaxonomic relevance. The quantitative differences in the volatile profiles could be of chemical ecology interest and additional studies are needed to gain a complete picture of differential gender metabolism in B. tridentata Vahl.

[P 117] Continuous monitoring of volatiles produced by Streptomyces grown on oatmeal agar by headspace extraction and GCMS

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The bacterial volatile organic compounds (VOCs) are known to play significant role in inter and intraspecies interaction of an ecosystem along with flavor attribution to food products. *Streptomyces* is one of major group of organisms that produces geosmin and 2-Methylisoborneol well known off-flavor compounds in drinking water and aquaculture systems. Apart from geosmin and 2MIB, *Streptomyces* produces a wide range of secondary volatile metabolite with potential clinical and industrial applications. The production of bacterial volatiles is majorly influenced by culture conditions; culture condition affects metabolism of organism and thus the metabolite production. It has been well established to measure VOCs from liquid cultures with existing tools. However it is a challenge to capture and measure VOCs from bacteria typically grown on solid media, and such limitations could bias the measured VOCs profiles from bacteria. The present study intended establish a method that can suit measuring volatiles produced by *Streptomyces sp 2R*, an off-flavor producing organism isolated from a Danish aquaculture system. A special approach used in the study where by *Streptomyces* was grown on oatmeal agar in a large headspace flask attached with Tennax trap. Volatiles produced by *Streptomyces* were monitored for 5 days by the collection of headspace onto a Tennax trap with a nitrogen flush for every 24 hrs followed by GCMS analysis. The obtained VOC profile of *Streptomyces sp 2R* shows the presence of geosmin and 2MIB along with several other terpenes. We also intend to establish relation between volatile profiles with increased biomass of *Streptomyces* over a period of time.

[P 118] Human Perception and Instrumentation of Aroma

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Sensorial characteristics, such as flavor and texture, are important for making food more pleasurable, since the quality and consumer acceptance of food product is determined largely by these characteristics. Perception of flavor is a mixture of sensory responses in the mouth and nose. Flavor is associated with basic tastes (sweetness. sourness, saltiness, bitterness and umami), mouthfeel and aroma. Aroma is perceived when the volatile food components reach to olfactory receptors in the nasal cavity. The stimulus for this sensation can be orthonasal or retronasal. Retronasal olfaction is the perception of odors emanating from the oral cavity during eating and drinking, as opposed to orthonasal olfaction, which occurs during sniffing. Without aroma, it is very difficult to identify the flavor of a food product. Sensory analyses are generally preferred during a new product formulation. This process may vary over time, number of subjects and panelists attitudes. Cheaper and faster instrumental techniques are being developed to minimize evaluation errors and examine what happens during food consumption by simulating the mouth in connection with temperature, chewing and salivary environment. The chemical composition of an aroma can be analyzed by gas chromatography and mass spectrometry (GC-MS), proton transfer reaction mass spectrometry (PTR-MS), atmospheric pressure chemical ionization mass spectrometry (APCI-MS) and selected ion flow tube mass spectrometry (SIFT-MS). Moreover, electronic nose and tongue available to identify simple or complex aroma close to human sense even they cannot substitute real human perception during eating. The most adequate way to measure the release of volatile compounds during eating is to monitor the breath air close to the olfactory receptors in the nose space. The aim of this review is to explain chemistry of human perception on flavor and investigate instrumental progress on aroma analyses.

Key words: aroma, human perception, electronic nose

[P 119] InnOscent chromatographic system: An innovative device to revisit aroma analysis and recombination perspectives

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Food aroma is a major criterion in consumers appreciation prompting food producers and processors to regard it as a perennial issue. However, comprehension of aroma is still an ongoing scientific challenge. An aromatic balance results from a complex mix of volatile compounds. All do not contribute equally to the aroma due mainly to their respective concentrations, detection thresholds, interactions with the matrix and emergence of complex aroma-aroma interactions. Gas chromatography coupled to olfactometry (GC-O) is a both analytical and sensory technique used to identify odor-active compounds and estimate their individual odorant potential; nevertheless, there is a gap between this individual characterization and the effective contribution to the food aroma. Thus, investigation of many aroma products turns to models reconstituted with chemicals, generally based on odorant activity values, and contribution of compounds are evaluated by omission experiments. While functioning, this approach is time-consuming and requires compounds to be identified, quantified, and commercially available.
The aim of this work was to develop a device that overcome constraints of conventional approaches to go further in aroma analysis. The innovative configuration of the present system not only permits to realize classical GC analysis coupled with multiple detectors but also incorporates multiple preparative fraction collection possibilities.Assessment of the system capabilities was both conducted on model solutions and real wine aroma. For demonstration purpose, analysis of a wine was performed by GC coupled to mass spectrometry and dual olfactometric-port with an 8 judges-panel. Then, compounds selected on the basis of GC-O results, were directly recovered, giving an overview of the recombination potentialities. These fractions were sensorially evaluated to determine the actual contribution of compounds to the wine aroma.Thirty-three odorants were significantly detected. Evaluation of the recombined extracts demonstrates that the mixture of all these odorants, mimics the original wine aroma. Moreover, a mixture of the 14 most perceived odorants is sufficient to mimic this aroma.
The findings of this study illustrate the relevance of the system to realize a comprehensive aroma exploration using a single disposal. While freeing from chemicals, it becomes possible to evaluate the contribution of any compound to an overall aroma.

[P 120] Identification of Thiols in Yellow Onion (Allium cepa L.) Using Solvent Vented Large Volume Injection GC-MS

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The onion plant has been cultivated over the last thousands of years. It is one of the most widely used and versatile vegetables globally used in cooking. Whether sautéed, baked, fried, boiled, or raw, yellow onions provide savory profiles for many different culinary applications. Yellow onions can contribute pungent, sulfury notes that characterize savory dishes. The intense flavor of Allium species develops enzymatically. Analysis of the volatile molecules in onion oil has been extensively reported in literature, whereas analysis of the fresh juice is less common. Fresh onion juice contains highly odorous sulfur compounds which are often reactive, thermally instable thiols that occur in extremely low concentrations. This makes analysis of samples challenging. Hot injection conditions have been criticized in the literature, as providing an erroneous picture of the compositon of these plants[1-3]. Cool on-column injection has become the favored technique for Allium analysis by gas chromatography. Traditional on-column injection however limits the amount of sample which can be loaded, and also deposits any non-volatile material present in the extract onto the column. Goal of this work was to find and identify novel thiol compounds which contribute to the aroma of fresh onion. In this study, yellow onion juice was solvent extracted, followed by thiol enrichment using a mercuric agarose gel column. Chromatographic analysis utilized larger volume solvent elimination injection GC-MS combined with GC-Olfactometry (GC-O). From the analyses conducted, various sulfur compounds were identified, some of which for the first time in nature, and their synthesis and sensory properties were reported. We propose a possible pathway of formation for each of these novel compounds.

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[P 121] The Odor Activity Value of Aroma-active Esters - An Appropriate Means to Assess the Aroma Quality of Apple Juices

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Aroma quality of apple juice from concentrate is dependent on an appropriate re-aromatization. Nevertheless, until now, there is no working concept available to evaluate the aroma quality of apple juices by means of analytical parameters. Already proposed concepts focused only on the concentration of esters, important odorants for the aroma of apples and apple juices, to rate the aroma quality. However, without consideration of the different odor thresholds of the esters no satisfying results for a practical application of the concept was reached. In order to develop an analytical evaluation of the aroma quality of apple juices based on odor activity values (OAV), odor-active compounds were characterized in apple juices by means of the Sensomics concept including gas chromatography-olfactometry. Following this approach, six esters with high odor activity were determined. Furthermore, less-odor-active esters were identified by GCxGC-TOFMS. In total 29 esters were found and 17 were selected for quantitation. The concentrations of these esters were determined in 23 industrial produced apple juices using a fast, multicomponent stable isotope dilution assay (SIDA), based on headspace-solid phase micro extraction (HS-SPME) in combination with GCxGC-TOFMS and OAVs were calculated. The newly developed method enabled a high throughput of samples due to the absence of any sample work-up.
Ethyl 2-methylbutanoate, ethyl butanoate, methyl 2-methylbutanoate, 2-methylbutyl acetate, butyl acetate, hexyl acetate, ethyl 2-methylpropanoate, propyl 2-methylbutanoate, ethyl propanoate and ethyl hexanoate revealed OAVs higher than one. Furthermore, limits were determined for every ester, representing a good aroma quality, when scored for all esters. In addition, to evaluate additive effects of esters on the overall aroma, sensory experiments were carried out ruling out some esters as markers for the juice quality.

[P 122] Selected Ion Flow Tube Mass Spectrometry (SIFT-MS) for real time flavour analysis; sampling possibilities and automation

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Selected Ion Flow Tube Mass Spectrometry (SIFT-MS) is an analysis technique that offers real-time, targeted measurement of volatile and semi-volatile compounds without the need for chromatographic separation. The choice of eight reagent ions provides unique selectivity and enables separation of some isobaric compounds through ion chemistry reactions.One of the key considerations with any real time technique, particularly when looking at flavour release is the sample introduction. The automation of sampling ensures reproducible analysis and enables a true comparison of different samples. SIFT-MS provides rapid, highly sensitive static or dynamic headspace analysis of aroma compounds without preconcentration and discrimination. It offers simple, non-destructive sample analysis.Through good experimental design, it can provide rapid chemical analysis that better correlates with human aroma perception. As well as providing objective, real-time aroma analysis it can be used to probe enzymatic, roasting or other processes and to study flavour release over time for comparison of technologies such as encapsulation.
Real-time analysis, coupled with high sensitivity and robustness to water vapor, also enables flavour release to be monitored in vivo and retronasal and mouth sampling are readily accommodated.
This presentation will give an overview of the underlying science that gives Syft Technologies' Voice200ultra SIFT-MS its selectivity and sensitivity. It will also outline the pioneering work that has been done by Anatune in automation of sample introduction using the GERSTEL MPS platform. Example applications from work that has been performed in the Anatune lab in Cambridge will be presented.

[P 123] WheelOscent : Presentation of an innovative olfactometry-dedicated software using intuitive aroma wheel interface

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Olfactometry is a valuable methodology commonly used to investigate odorant active compounds in complex food aroma profiles [1]. Considering the number of studies using this technique, little is done to improve olfactometric data acquisition, although it is essential for quality outcomes. Efforts were mainly done to automate recording of moment and duration of perception but intensity and description of perception are still often communicate orally, which disrupt rhythm of judge's breathing during analysis. Solutions that integrate intensity and description parameters recording, result in a multiple steps acquisition procedure, scarcely compatible with the transience of the perceptions evaluated during olfactometry.
The objective of this work was to develop a new software better adapted to olfactometric process, both to improve the user task and to overcome constraints and bias of existing systems. More specifically the software, coded with Java technologies, implements 3 innovative components:
a data acquisition interface, for judge users, based on aroma wheels which permits judges to characterize all parameters related to odors perceived, easily in a single and intuitive move,
a data store, which stores the collected data into adapted representation describing aroma wheels, experiments, products, judges, and aromagrams,
a data analysis interface, for analyst users, which provides an easy and direct analysis of data displayed into interactive and graphical visualization, resulting from several processing such as data aggregation over judges, molecule identification, aromagrams comparison over products or judges.
Assessment of the software was performed on food products with complex aroma [2]. Providing a good usability for judges, this software enables a precise aromatic characterization that allows to point out special characteristics of products with close and complicated aroma. This disposal is now used for wine analysis, where judges take advantage of the wheel aroma presentation, currently use for wine sensory characterization. This consistent presentation of olfactometric and conventional sensory descriptors facilitate chemometric approaches that attempt to determine contribution of compounds to a global aroma and apprehend existing interactions.

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[P 124] Optimization of Aroma Dilution Analyses by means of Stir Bar Sorptive Extraction for the Identification of Potent Aroma Compounds in Submerged Basidiomycete Cultures

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Aroma extract dilution analysis (AEDA) is a well-established method for the identification of key aroma compounds in food matrices. AEDA relies on liquid/liquid extraction (LLE) with organic solvents for the preparation of the aroma extracts and is often used in combination with solvent assisted flavour evaporation (SAFE). Therefore, sample preparation for AEDA is usually a very time-consuming technique and discrimination of highly volatile compounds due to LLE might occur. A recently established alternative for the determination of flavour dilution (FD) factors is the aroma dilution analysis by means of headspace solid phase microextraction (ADA-HS-SPME). The idea of ADA is to dilute the sample after thermodesorption (TD) within the gas chromatography-olfactometry (GC-O) system via adjustment of the split ratio. This technique is more reliable than simple dilution of the aqueous samples prior TD, because it eliminates possible matrix effects due to alteration of the sample composition. Recently, this approach was transferred to direct immersion stir bar sorptive extraction (ADA-DI-SBSE) and validated for a range of FD factors from 8 - 128. ADA-DI-SBSE was shown to be especially useful for liquid samples like submerged basidiomycete cultures, as it allowed to identify significantly more compounds compared to ADA-HS-SPME.
The objective of the present work was to further optimize ADA-DI-SBSE and thus to extend the range of applicable FD factors. For this purpose, the split vent flow rates of the thermal desorption unit (TDU) as well as of the cooled injection system (CIS) were varied in order to achieve an extended linear dilution range. The validation was performed with a defined mixture of various aroma compounds to cover broad spans of polarity and volatility. The applied split ratios were plotted against the measured peak areas of the compounds in binary logarithmic scaling, and linear regression analysis was performed. The obtained regression coefficients and the slopes of the regression curves indicated the reliability of this method. In order to demonstrate the applicability, the developed ADA-DI-SBSE method was tested with a submerged basidiomycete culture. The obtained results were compared to AEDA after LLE of the same sample.

[P 125] Is Sensomics a Perfect Approach to Odour Analysis or Can Improvements be Made?

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Sensomics, developed by the Technical University of Munich, is the best approach to identify the key odorants in foods, with over 100 publications determining key odorants in over 200 different foods [1]. But is Sensomics the perfect approach, or are improvements needed? Here, meta-analysis of the Sensomics data is carried out, proposing two areas where improvements can be achieved: (i) prioritisation of odorants using Gas Chromatography - Olfactometry (GC-O); (ii) sensory comparison of the final odour simulation to the original material using Flavour Profiling®.

Sensomics uses the GC-O methodology of Aroma Extract Dilution Analysis (AEDA) to identify odorants and prioritise them for quantitation. The quantitated results are then used to calculate odour activity value (OAV); an odorant's amount divided by its odour threshold. OAV is used to express an odorant's importance to a food's odour. However, meta-analysis of data comparing GC-O results to OAV shows direct correlation is poor, with $R^2 < 20\%$. Using statistical modelling, correlation can be improved (R^2ca. 40%) by taking into account odorant physical and chemical properties, such as hydrophobicity and volatility. These properties are known to effect the extraction of odorants during sample preparation. Here, work is presented on the statistical modelling of sample preparation extraction efficiencies, showing sample preparation techniques do not extract odorants without bias. This bias may lead to inaccuracy in results, which is attempted to be rectified by the statistical modelling of the GC-O data.

Given the poor correlation of GC-O results to OAV, how does Sensomics validate the results? Within Sensomics, an odour simulation is created and compared to the original material using the human sensory technique of Flavour Profiling®. This ensures simulations are characteristic to the original material. However, error bars and significance testing are not often presented. Here work is presented showing difficulty using Flavour Profiling®, followed by results on a fish liquor using the sensory methodologies of Triangle testing and Napping®. The results show Napping® is able to assess if odour simulations are characteristic of the original material, and also the effect of partially removing groups of odorants from the simulation.

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[P 126] A rapid FT-IR method for monitoring the release of major components of clove essential oil encapsulated into a complex organic matrix.

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Fourier transform infrared (FTIR) attenuated total reflection (ATR) spectroscopy is a simple and rapid technique that provides an overall infrared fingerprint of a matrix and can replace time consuming analysis for monitoring changes in an aroma profile or aroma compounds transfer (Gomez-Carvaca et al., 2013). However, the use of a complex matrix is restricted due to the risk of spectra superposition and the lack of sensibility detection.In this study, clove essential oil, previously identified by GC-MS, was encapsulated into an organic matrix rich in proteins and polysaccharides and the controlled release of major aroma compounds of the essential oil was quantified by a FT-IR method and compared to conventional gas chromatography approach. To achieve the quantification, by FTIR, a calibration curve was carried out by depositing pure clove oil and its major components at different concentrations on a constant mass of matrix without essential oil. Several Partial Least Squares (PLS) regression calibration models were performed to determine the best correlation (R^2 0.90) between the predicted and reference values of clove essential oil major compounds using specific spectral regions. For the best model the limit of detection (LOD) and limit of quantification (LOQ) were determined. With the best PLS method, the release of clove essential oil major compounds was studied and it showed a linear behavior according to time, same as analyzed GC-FID.The FT-IR developed method can be used as an alternative rapid method for the identification and quantification of major aroma compounds in complexes organic samples.

[P 127] The impact of pod storage on the formation of different alkylpyrazines from Ghanaian cocoa liquors roasted at four roasting temperatures

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The typical flavour characteristics of cocoa are related to the cocoa bean genotype and the growing environmental conditions. However the flavour does not exist naturally in the beans, it is generated by a series of procedures that begins with sometimes pod storage, followed by fermentation of the beans and continues during roasting. Pod storage (PS) means storing harvested cocoa pods for a period of time before opening the pods. The effect of pod storage should be beneficial for the subsequent development of cocoa flavour in the resulting cocoa beans [1].
During roasting the formation of several volatile heterocyclic compounds is generated with the most dominant volatiles and also the key odour components, being the alkylpyrazines. Besides tetramethylpyrazine and trimethylpyrazine being the most abundant, several other alkylpyrazines with different substituents are also important. Consequently monitoring the pyrazines can be helpful in optimizing roasting conditions of cocoa beans for attaining the desired aroma of the cocoa liquors.
Several studies have measured cocoa volatiles using gas-chromatography mass spectrometry (GC-MS) frequently using headspace solid phase micro extraction (HS-SPME) to concentrate the volatiles.
The purpose of this study is to investigate the effect of pod storage (0, 3, 7 days of PS) of Ghanaian cocoa beans after roasting at 4 different temperatures (100, 120, 140 and 160°C) on the formation of alkylpyrazines from their liquors. HS-SPME extraction of the alkylpyrazines is carried out with a DVB/CAR/ PDMS fiber. The identified compounds are measured semi-quantitative and the results are statistically treated by multivariate analysis. In this study more than 15 different alkylpyrazines are measured after 7 days of PS. Higher roasting temperatures result in the formation of different alkylpyrazines compared to lower roasting temperatures. For the formation of a specific spectrum of alkylpyrazines, roasting temperatures of 160°C are needed for PS of 0 days, compared to PS of 7 days which reveals the formation of even more alkylpyrazines at lower roasting temperatures.

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[P 128] Method Development for Multiple Partition Coefficients Determination to Understand Headspace Aroma Distribution of Complex Mixture

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Sensory perception is directly related to volatiles from the matrix to the atmosphere. From a physico-chemical point of view, this release may be described by partition coefficients, which correspond to the volatile concentration ratio between the liquid and gaseous phase. Partition coefficients could be determined thanks to Phase Ratio Variation (PRV) method which is based on the fact that, for a volatile, in a closed system, its headspace concentration changes as a function of liquid phase volume [1]. This method is generally applied using HS-GC-FID.For various heavy compounds analysis, some authors proposed a design for low-pressure gas chromatography coupled to mass spectrometry (LP-GC-MS) analysis, consisting in combining a micro-bore column to a mega-bore one, resulting in faster analysis and a better chromatographic resolution and sensitivity [2].
The goal of the present work was to develop a method by coupling the low-pressure and static headspace gas chromatography to a mass spectrometry (LP-HS-GC-MS) in order to calculate simultaneously various partition coefficients [3]. Various parameters were optimised such as the comparison between a micro-bore column and mega-bore column, injection speed, pressure in the injector, or time to reach the thermodynamic equilibrium in the headspace. This method of partition coefficients determination was used in order to study potential modifications of headspace aroma distribution.

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[P 129] Characterization of Wines Produced from Fungus Resistant Grape Varieties

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Like most agriculturally grown products grapes and as a result wine are affected by climate change. The Styrian wine growing area, which belongs to the cool climate regions in Europe, faces a constant increase of the annual average temperature and is forecasted to be about $+1.5°C$ by 2050. This increase will have a significant effect on the vegetation period and also increases the probability for several plant diseases. These changes in the growing conditions can lead to increased dependency on plant protection agents. The amount of agents can be reduced by using fungus resistant grape (FRG) varieties. These are a cross of middle European *vitis vinifera* varieties and American or Asian species which are immune or at least less sensitive to some of the most common fungal diseases like mildew and grey rot.
Even though FRGs have existed for some time, their cultivation is not very common. One of the reasons is the low acceptance from consumers due to their sensory properties ('foxiness'). Breeding efforts during the last decades have led to a substantial change of the sensory quality of the hybrid grape varieties. Some of the breedings show promising properties and are planted in an experimental vineyard for a monitor programme. The wines are processed under controlled conditions using single yeast strains and temperature controlled microvinifcation.
Sensory and analytical data is used to characterize the wines. Solid phase microextraction coupled to different GC systems and detectors (single quadrupole in scan and SIM, triple quadrupole and comprehensive GCxGC) was used to identify the contributing and the key aroma compounds of the wines. In addition the effect of viticulture and viniculture practice on the sensory and analytical data is monitored. The previous steps to characterize the wines should be helpful when identifying the optimum grape selection and processing regime.

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[P 130] Differentiation of less frequent red grape Vitis vinifera varieties by characterization of the aroma precursors

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Glycosydated volatile organic compounds are vital to wine quality, determining their aroma and varietal characteristics. Which are present, and in what quantity, depends on the cultivar, the situation and soil of the vineyard, weather and cultivation methods. In this work, the characterization of non-aromatic grape Vitis vinifera red varieties (Marselan, Arinarnoa, Ancellota, Caladoc, Egiodola and Lacryma Christi) grown in different areas of Uruguay is shown. Sample preparation is a crucial step in the determination of volatile compounds; in an attempt to improve the analytical difficulties on the isolation of the aromatic precursors from these varieties, an optimized procedure using ENV+ cartridge as an alternative to the traditional method with Amberlite XAD-2 resin is proposed. *Vitis vinifera* cv. Arinarnoa was used in order to evaluate the precision and reproducibility of the method. The glycosidic extracts were submitted to enzymatic hydrolysis, and the released aroma compounds were extracted by Solid-Phase Extraction and analyzed by GC-MS. The method proposed seems to be suitable and allows isolating the low concentration compounds with good reproducibility. Among the volatile compounds determined in these varieties we can find C6 alcohols, norisoprenoids (3-hydroxy-β-damascone, 3-oxo-α-ionol, vomifoliol, 4-oxo-7,8-dihydro- α -ionol), volatile phenols (guaiacol, 4-vinyl-guaiacol), vanillins, and others. Results contributed to the valorization of each grape variety through its aromatic potential.

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