Exploring the chemistry of complex samples by tentative identification and semi-quantification: a food contact material case

In fields such as food safety and environmental chemistry, ensuring safety is greatly challenged by large numbers of unknown substances occurring. Even with current state of the art mass spectrometers, dealing with non-identified substances is a very laborious process as it includes structure elucidation of a vast number of unknowns, of which only a fraction may be relevant. Here, we present an exploration and prioritization approach based on high resolution mass spectrometry. The method uses algorithm-based precursor/product-ion correlations on Quadrupole-Time of Flight (Q-TOF) MS/MS data to retrieve the most likely chemical match from a structure database. In addition, TOF-only data is used to estimate analyte concentration via semi-quantification. The method is demonstrated in recycled paper food contact material (FCM). Here, 585 chromatographic peaks were discovered, of which 117 were unique to the sample and could be tentatively elucidated via accurate mass, isotopic pattern, and precursor/product-ion correlations. Nearly 85% of these 117 peaks were matched with database entries, which provided varying certainty of information about the analyte structure. Semi-quantitative concentration ranges of investigated compounds were between 0.7 μg dm-2 and 1600 μg dm-2. With this data, a subgroup of chemicals was risk-categorized and prioritized using the most likely candidate structure(s) obtained. Prioritization based on expected health impact was possible using the tentatively assigned data. Overall, the described method is a valuable chemical exploration tool for non-identified substances, but also may be used as a preliminary prioritization tool for substances expected to have the highest health impact, for example in FCMs.
A framework to estimate concentrations of potentially unknown substances by semi-quantification in liquid chromatography electrospray ionization mass spectrometry

Risk assessment of exposure to chemicals from food and other sources rely on quantitative information of the occurrence of these chemicals. As screening analysis is increasingly used, a strategy to semi-quantify unknown or untargeted analytes is required. A proof of concept strategy to semi-quantifying unknown substances in LC-MS was investigated by studying the responses of a chemically diverse marker set of 17 analytes using an experimental design study. Optimal conditions were established using two optimization parameters related to weak-responding compounds and to the overall response. All the 17 selected analytes were semi-quantified using a different analyte to assess the quantification performance under various conditions. It was found that source conditions had strong effects on the responses, with the range of low-response signals varying from −80% to over +300% compared to centerpoints. Positive electrospray (ESI+) was found to have more complex source interactions than negative electrospray (ESI-). Choice of quantification marker resulted in better quantification if the retention time difference was minimized (12 out of 12 cases error factor <4.0) rather than if the accurate mass difference was minimized (7 out of 12 cases error factor <4.0). Using optimal conditions and retention time selection, semi-quantification in ESI+ (70% quantified, average prediction error factor 2.08) and ESI− (100% quantified, average prediction error factor 1.74) yielded acceptable results for untargeted screening. The method was successfully applied to an extract of food contact material containing over 300 unknown substances. Without identification
and authentic standards, the method was able to estimate the concentration of a virtually unlimited number of compounds thereby providing valuable data to prioritize compounds in risk assessment studies.

**General information**

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Organisations: National Food Institute, Research Group for Analytical Food Chemistry
Authors: Pieke, E. N. (Intern), Granby, K. (Intern), Trier, X. (Intern), Smedsgaard, J. (Intern)
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Scopus rating (2014): CiteScore 4.64
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BFI (2013): BFI-level 1
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Web of Science (2013): Indexed yes
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Web of Science (2011): Indexed yes
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BFI (2009): BFI-level 1
Web of Science (2009): Indexed yes
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Web of Science (2008): Indexed yes
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Web of Science (2003): Indexed yes
Web of Science (2002): Indexed yes
Web of Science (2001): Indexed yes
Web of Science (2000): Indexed yes
Original language: English

Electrospray ionization, Liquid chromatography-mass spectrometry, Method optimization, Screening, Semi-quantification, Untargeted analysis, Chemical contamination, Chromatography, Errors, Ionization, Ionization of liquids, Liquid
Big Data fra jord til bord

Danske landmænd og virksomhederne i fødevaresektoren har gode forudsætninger for at drage nytte af den rivende udvikling inden for insamling og bearbejdning af data:

• Danmark har en stærk fødevaresektor. Det skyldes bl.a., at alle dele af værdikæden arbejder tæt sammen. Fra primærpædproducenterne, over forarbejdindustrien, agroindustrien til videns- og forskningsmiljøerne. Effektiv ressourceudnyttelse og fokus på optimering i hele værdikæden gør sektoren i stand til at konkurrere på verdensmarkedet.

• Danske fødevarevirksomheder har altid været gode til at opdyrke nye forretningsmodeller og finde nye innovative veje til øget værdiskabelse. For eksempel gennem smartere måder at producere på, levere produkterne på eller at indarbejde større værdi i produkterne, så de kan sælges med større forlønnete.

• Dansk landbrug og hele værdikæden i fødevaresektoren producerer store mængder af data. Det skyldes bl.a. et højt automationsniveau og myndighedernes krav til dokumentation af fødevarekvaliteten, når de danske producenter leverer fødevarer til forbrugerne verden over. Der er imidlertid et stort spring fra at råde over store mængder af data til at bruge dem aktivt i forretningsudviklingen. Denne rapport viser, hvordan Big Data kan være ét af omdrejningspunkter

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Organisations: Office for Innovation & Sector Services, Department of Applied Mathematics and Computer Science, Statistics and Data Analysis, National Food Institute, Division of Risk Assessment and Nutrition, Research Group for Analytical Food Chemistry, National Veterinary Institute, Epidemiology, Department of Management Engineering, Management Science, Transport DTU, Operations Management, Department of Bio and Health Informatics, IT Service, High Performance Computing, DI Itek, Landbrug og Fødevarer, City Pressekontor
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Exposure to perfluorononanoic acid combined with a low-dose mixture of 14 human-relevant compounds disturbs energy/lipid homeostasis in rats

Humans are constantly exposed to a significant number of compounds and many are readily detected in human body fluids. Worryingly, several of these compounds are either suspected to be, or have already been shown to be harmful to humans either individually or in combination. However, the potential consequences of low-dose exposure to complex mixtures remain poorly understood. We have profiled the effects on rat blood plasma and liver homeostasis using metabolomics and transcriptomics following 2-week exposure to either a mixture of 14 common chemicals (Mix), perfluorononanoic acid (PFNA) at low (0.0125 mg/kg/day) or mid (0.25 mg/kg/day) doses, or a combination of Mix and PFNA. In blood plasma, 63 and 64 metabolites were significantly changed upon exposure to Mix alone or PFNA + Mix, respectively. Twelve of the metabolites were identified and comprised mainly lipids, with various lipid classes differentially affected across study groups. In the liver, expression of 182 and 203 genes—mainly related to energy homeostasis and lipid metabolism—were differentially expressed upon exposure to PFNA alone or PFNA + Mix, respectively. In general, Mix alone affected lipid metabolism evident in blood plasma, whereas effects on lipid metabolism in the liver were mainly driven by PFNA. This study verifies that a chemical mixture given at high-end human exposure levels can affect lipid homeostasis and that the combined use of metabolomics and transcriptomics can provide complimentary information allowing for a detailed analysis of affected signaling pathways.

General information
**LC-MS analysis of the plasma metabolome—a novel sample preparation strategy**

Blood plasma is a well-known body fluid often analyzed in studies on the effects of toxic compounds as physiological or chemical induced changes in the mammalian body are reflected in the plasma metabolome. Sample preparation prior to LC-MS based analysis of the plasma metabolome is a challenge as plasma contains compounds with very different properties. Besides, proteins, which usually are precipitated with organic solvent, phospholipids, are known to cause ion suppression in electrospray mass spectrometry. We have compared two different sample preparation techniques prior to LC-qTOF analysis of plasma samples: The first is protein precipitation; the second is protein precipitation followed by solid phase extraction with sub-fractionation into three sub-samples; a phospholipid, a lipid and a polar sub-fraction. Molecular feature extraction of the data files from LC-qTOF analysis of the samples revealed 1792 molecular features from the protein precipitation procedure. The protein precipitation followed by solid phase extraction procedure with three sub-samples gave a total of 4234 molecular features. This suggests that sub-sampling into polar, lipid and phospholipid fractions enables extraction of more metabolomic information as compared to protein precipitation alone. Chromatography showed good separation of the metabolites with little retention time drift (< 1s) and a mass accuracy below 3 ppm was observed. The performance of the method was investigated using plasma samples from rats administered the environmental pollutant perfluorononanoic acid.

**General information**

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Organisations: National Food Institute, Division of Food Chemistry, Division of Toxicology and Risk Assessment

Authors: Skov, K. (Intern), Hadrup, N. (Intern), Smedsgaard, J. (Intern), Frandsen, H. L. (Intern)

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Scopus rating (2017): SNIP 0.969 SJR 0.805

Web of Science (2017): Indexed Yes

BFI (2016): BFI-level 1

Scopus rating (2016): SJR 0.799 SNIP 1.061 CiteScore 2.58

BFI (2015): BFI-level 1

Scopus rating (2015): SJR 0.922 SNIP 1.165 CiteScore 2.74

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BFI (2014): BFI-level 1

Scopus rating (2014): SJR 1.065 SNIP 1.317 CiteScore 2.89

BFI (2013): BFI-level 1

Scopus rating (2013): SJR 1.061 SNIP 1.289 CiteScore 2.78

ISI indexed (2013): ISI indexed yes

BFI (2012): BFI-level 1

Scopus rating (2012): SJR 1.166 SNIP 1.266 CiteScore 2.87

ISI indexed (2012): ISI indexed yes

Web of Science (2012): Indexed yes

BFI (2011): BFI-level 1

Scopus rating (2011): SJR 1.296 SNIP 1.291 CiteScore 3.02

ISI indexed (2011): ISI indexed yes

BFI (2010): BFI-level 1

Scopus rating (2010): SJR 1.274 SNIP 1.292

BFI (2009): BFI-level 1

Scopus rating (2009): SJR 1.334 SNIP 1.35
Metabolomics, an analytical strategy for identification of toxic mechanism of action

General information
State: Published
Organisations: National Food Institute, Division of Food Chemistry, Division of Toxicology and Risk Assessment, Research Group for Analytical Food Chemistry
Authors: Skov, K. (Intern), Hadrup, N. (Intern), Smedsgaard, J. (Intern), Frandsen, H. L. (Intern)
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Thesis_with_articles.pdf
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A combined metabolomic and phylogenetic study reveals putatively prebiotic effects of high molecular weight arabino-oligosaccharides when assessed by in vitro fermentation in bacterial communities derived from humans

Prebiotic oligosaccharides are defined by their selective stimulation of growth and/or activity of bacteria in the digestive system in ways claimed to be beneficial for health. However, apart from the short chain fatty acids, little is known about bacterial metabolites created by fermentation of prebiotics, and the significance of the size of the oligosaccharides remains largely unstudied.

By in vitro fermentations in human fecal microbial communities (derived from six different individuals), we studied the effects of high-mass (HA, >1 kDa), low-mass (LA, <1 kDa) and mixed (BA) sugar beet arabino-oligosaccharides (AOS) as carbohydrate sources. Fructo-oligosaccharides (FOS) were included as reference. The changes in bacterial communities and the metabolites produced in response to incubation with the different carbohydrates were analyzed by quantitative PCR (qPCR) and Liquid Chromatography–Mass Spectrometry (LC–MS), respectively.

All tested carbohydrate sources resulted in a significant increase of Bifidobacterium spp. between 1.79 fold (HA) and 1.64 fold (FOS) in the microbial populations after fermentation, and LC–MS analysis suggested that the bifidobacteria contributed to decomposition of the arabino-oligosaccharide structures, most pronounced in the HA fraction, resulting in release of the essential amino acid phenylalanine. Abundance of Lactobacillus spp. correlated with the presence of a compound, most likely a flavonoid, indicating that lactobacilli contribute to release of such health-promoting substances from plant structures.

Additionally, the combination of qPCR and LC–MS revealed a number of other putative interactions between intestinal...
microbes and the oligosaccharides, which contributes to the understanding of the mechanisms behind prebiotic impact on human health.

**General information**

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*Organisations:* National Food Institute, Division of Food Microbiology, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Division of Food Chemistry  
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Web of Science (2018): Indexed yes  
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Scopus rating (2017): SNIP 1.204 SJR 1.144  
Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 1  
Scopus rating (2016): CiteScore 2.75 SJR 0.995 SNIP 0.948  
BFI (2015): BFI-level 1  
Scopus rating (2015): SJR 1.104 SNIP 0.999 CiteScore 2.77  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 1  
Scopus rating (2014): SJR 1.015 SNIP 1.16 CiteScore 2.77  
Web of Science (2014): Indexed yes  
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ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 1  
Scopus rating (2012): SJR 0.984 SNIP 0.937 CiteScore 2.48  
ISI indexed (2012): ISI indexed yes  
BFI (2011): BFI-level 1  
Scopus rating (2011): SJR 0.901 SNIP 0.949 CiteScore 2.48  
ISI indexed (2011): ISI indexed yes  
BFI (2010): BFI-level 1  
Scopus rating (2010): SJR 0.882 SNIP 1.049  
Web of Science (2010): Indexed yes  
BFI (2009): BFI-level 1  
Scopus rating (2009): SJR 0.679 SNIP 0.856  
BFI (2008): BFI-level 1  
Scopus rating (2008): SJR 0.607 SNIP 0.727  
Scopus rating (2007): SJR 0.628 SNIP 0.741  
Web of Science (2007): Indexed yes  
Scopus rating (2006): SJR 0.39 SNIP 0.558  
Scopus rating (2005): SJR 0.327 SNIP 0.444  
Scopus rating (2004): SJR 0.442 SNIP 0.538  
Scopus rating (2003): SJR 0.355 SNIP 0.448  
Scopus rating (2002): SJR 0.276 SNIP 0.288  
Scopus rating (2001): SJR 0.403 SNIP 0.376  
Scopus rating (2000): SJR 0.561 SNIP 0.713
Dynamic Metabolic Footprinting Reveals the Key Components of Metabolic Network in Yeast Saccharomyces cerevisiae

Metabolic footprinting offers a relatively easy approach to exploit the potentials of metabolomics for phenotypic characterization of microbial cells. To capture the highly dynamic nature of metabolites, we propose the use of dynamic metabolic footprinting instead of the traditional method which relies on analysis at a single time point. Using direct infusion-mass spectrometry (DI-MS), we could observe the dynamic metabolic footprinting in yeast S. cerevisiae BY4709 (wild type) cultured on 3 different C-sources (glucose, glycerol, and ethanol) and sampled along 10 time points with 5 biological replicates. In order to analyze the dynamic mass spectrometry data, we developed the novel analysis methods that allow us to perform correlation analysis to identify metabolites that significantly correlate over time during growth on the different carbon sources. Both positive and negative electrospray ionization (ESI) modes were performed to obtain the complete information about the metabolite content. Using sparse principal component analysis (Sparse PCA), we further identified those pairs of metabolites that significantly contribute to the separation. From the list of significant metabolite pairs, we reconstructed an interaction map that provides information of how different metabolic pathways have correlated patterns during growth on the different carbon sources.

General information
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Organisations: National Food Institute, Division of Food Chemistry, Kasetsart University, Institut Pasteur Korea
Authors: Chumnanpuen, P. (Ekstern), Hansen, M. A. E. (Ekstern), Smedsgaard, J. (Intern), Nielsen, J. (Intern)
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- Scopus rating (2015): SJR 1.652 SNIP 1.43 CiteScore 4.52
- Scopus rating (2014): SJR 1.171 SNIP 1.149 CiteScore 2.61
- Scopus rating (2013): SJR 0.639 SNIP 0.72 CiteScore 1.48
- ISI indexed (2013): ISI indexed no
- Scopus rating (2012): SJR 0.667 SNIP 0.552 CiteScore 1.53
- ISI indexed (2012): ISI indexed no
- Scopus rating (2011): SJR 1.578 SNIP 1.239 CiteScore 3.08
- ISI indexed (2011): ISI indexed no
- Scopus rating (2010): SJR 0.936 SNIP 1.005
- Scopus rating (2009): SJR 0.878 SNIP 1.061
- Scopus rating (2008): SJR 0.452 SNIP 0.156
- Scopus rating (2007): SNIP 0.887
- Scopus rating (2006): SNIP 0.525
- Scopus rating (2005): SNIP 0.384
- Scopus rating (2004): SNIP 0.337
- Scopus rating (2003): SNIP 0.4
- Scopus rating (2002): SNIP 0.56
Original language: English

metabolomic, Fungi Plantae (Fungi, Microorganisms, Nonvascular Plants, Plants) - Ascomycetes [15100] Saccharomyces cerevisiae species strain-BY4709, carbon 7440-44-0, ethanol 64-17-5, glucose 58367-01-4, glycerol 56-81-5, 10060, Biochemistry studies - General, 10068, Biochemistry studies - Carbohydrates, 13002, Metabolism - General metabolism
Lactobacillus acidophilus NCFM affects vitamin E acetate metabolism and intestinal bile acid signature in monocolonized mice

Mono-colonization of germ-free (GF) mice enables the study of specific bacterial species in vivo. Lactobacillus acidophilus is a probiotic strain, however many of the mechanisms behind its health-promoting effect remain unsolved. Here, we studied the effects of Lactobacillus acidophilus NCFM (NCFM) on the intestinal metabolome (jejunum, caecum, and colon) in mice by comparing NCFM mono-colonized (MC) mice with GF mice using liquid chromatography coupled to mass-spectrometry (LC-MS). The study adds to existing evidence that NCFM in vivo affects the bile acid signature of mice by deconjugation and dehydroxylation of bile acids. Furthermore, we confirmed that carbohydrate metabolism is affected by NCFM in the mouse intestine. Especially, the digestion of larger carbohydrates (penta- and tetrasaccharides) was increased in MC mice. Interestingly, we also found vitamin E (α-tocopherol acetate) in higher levels in the intestine of GF mice compared to MC mice, suggesting that NCFM either metabolizes the compound or indirectly affects the absorption by changing the metabolome in the intestine. The use of NCFM to increase the uptake of vitamin E supplements in humans and animals is a highly relevant topic for further research.

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BFI (2015): BFI-level 1
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BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.705 SNIP 0.784 CiteScore 2.8
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.519 SNIP 0.724 CiteScore 2.87
ISI indexed (2013): ISI indexed no
Effects of perfluorononanoic acid (PFNA) on the metabolic profiling of rat serum by UHPLC-ESI-Q-TOF MSMS

Endocrine disrupting chemicals are compounds which interfere with normal hormone homeostasis. So far the main concern has been the effect on the reproduction and development. This study has been conducted to find the effect of EDC on the human metabolome, using LC high resolution mass spectrometry and chemical separation of plasma metabolites it is possible to find the difference in the plasma metabolome affected by EDC. The study was conducted given a group of rats an EDC and another group a combination of EDC’s and CYP inhibitors.

General information
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Organisations: National Food Institute, Division of Food Chemistry, Division of Toxicology and Risk Assessment, Technical University of Denmark
Authors: Skov, K. (Intern), Hadrup, N. (Intern), Vestergaard, A. M. (Ekstern), Smedsgaard, J. (Intern), Frandsen, H. L. (Intern)
Number of pages: 1
Publication date: 2013
Event: Poster session presented at 9th International Conference of the Metabolomics Society, Glasgow, United Kingdom.
Main Research Area: Technical/natural sciences
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Bibliographical note
Endocrine disrupting chemicals are compounds which interfere with normal hormone homeostasis. So far the main concern has been the effect on the reproduction and development. This study has been conducted to find the effect of EDC on the human metabolome, using LC high resolution mass spectrometry and chemical separation of plasma metabolites it is possible to find the difference in the plasma metabolome affected by EDC. The study was conducted given a group of rats an EDC and another group a combination of EDC’s and CYP inhibitors.
Source: dtu
Source-ID: u::9873
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Mono-colonization with Lactobacillus acidophilus NCFM affects the intestinal metabolome as compared to germ-free mice

Every single species of the gut microbiota produce low-molecular-weight compounds that are absorbed constantly from the intestinal lumen and carried to systemic circulation where they play a direct role in health and disease. However, very few studies address the host metabolome as a function of colonizing bacteria. In this study the effect of the Lactobacillus acidophilus NCFM strain was investigated by comparing the metabolome of mono-colonized and germ-free mice in several compartments. By liquid chromatography coupled to mass spectrometry, we were able to show that the metabolome differed between the mono-colonized and germ-free mice, not only in ileum, caecum and colon, but also in plasma and liver. These observations suggest that L. acidophilus NCFM highly influence the metabolism in multiple compartments, underlying that the gut microbiota metabolism affects the host systemic metabolism.

General information
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Organisations: National Food Institute, Division of Food Microbiology, Division of Food Chemistry, University of Auckland, University of Copenhagen
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Main Research Area: Technical/natural sciences
Electronic versions:
Mono-colonization with Lactobacillus acidophilus NCFM affects the intestinal metabolome in mice

Mono-colonization of germ-free (GF) mice enables the study of specific bacterial species in vivo. Lactobacillus acidophilus is a probiotic strain, however many of the mechanisms behind its health-promoting effect remain unsolved. Here, we studied the effects of Lactobacillus acidophilus NCFMTM (NCFM) on the intestinal metabolome (jejunum, caecum, and colon) in mice by comparing NCFM mono-colonized (MC) mice with GF mice using liquid chromatography coupled to mass-spectrometry (LC-MS). The study adds to existing evidence that NCFM in vivo affects the bile acid signature of mice by deconjugation and dehydroxylation of bile acids. Furthermore, we confirmed that carbohydrate metabolism is affected by NCFM in the mouse intestine. Especially, the digestion of larger carbohydrates (penta- and tetrasaccharides) was increased in MC mice. Interestingly, we also found vitamin E (α-tocopherol acetate) in higher levels in the intestine of GF mice compared to MC mice, suggesting that NCFM either metabolizes the compound or indirectly affects the absorption by changing the metabolome in the intestine. The use of NCFM to increase the uptake of vitamin E supplements in humans and animals is a highly relevant topic for further research.

Quantification of vitamin D3 and its hydroxylated metabolites in waxy leaf nightshade (Solanum glaucophyllum Desf.), tomato (Solanum lycopersicum L.) and bell pepper (Capsicum annuum L.)

Changes in vitamin D3 and its metabolites were investigated following UVB- and heat-treatment in the leaves of Solanum glaucophyllum Desf., Solanum lycopersicum L. and Capsicum annuum L. The analytical method used was a sensitive and selective liquid chromatography electrospray ionisation tandem mass spectrometry (LC–ESI-MS/MS) method including Diels–Alder derivatisation. Vitamin D3 and 25-hydroxy vitamin D3 were found in the leaves of all plants after UVB-treatment. S. glaucophyllum had the highest content, 200ng vitamin D3/g dry weight and 31ng 25-hydroxy vitamin D3/g dry weight, and was the only plant that also contained 1,25 dihydroxy vitamin D3 in both free (32ng/g dry weight) and glycosylated form (17ng/g dry weight).
Solanum glaucophyllum Desf., Solanum lycopersicum L., Capsicum annuum L., Solanaceae, Vitamin D3, LC–ESI-MS/MS, Heat, UVB

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Bacterial Impact on the Gut Metabolome

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Authors: Sulek, K. (Intern), Licht, T. R. (Intern), Wilcks, A. (Intern), Skov, T. H. (Intern), Smedsgaard, J. (Intern)
Number of pages: 182
Publication date: 2012

Design and Fabrication of Polymer-based Lab-on-a-Chip Devices Towards Applications in Food and Environmental Analysis

Pesticides play a key factor in the high productivity achieved in modern agricultural food production. While increasing productivity and lowering production costs, they are potentially toxic and can have a serious impact on humans and the environment. In general, monitoring of pesticides and other environmental contaminants is performed in analytical laboratories, utilizing a multiplicity of time-consuming and cost-intensive chemical analysis methods like chromatography and mass spectrometry. To ensure food security and to monitor maximum residue levels in a highly globalized market, miniaturized analysis systems could provide inexpensive, portable devices for fast and reliable on-site monitoring of – not only – pesticides. Introduced already more than 20 years ago, lab-on-a-chip (LOC) devices found their way into biological and clinical research. Their fast analysis times, low sample volume and low reagent consumption are attractive for many applications in the life sciences, e.g., for DNA sequencing platforms and screening applications in drug development. It was only recently that the use of LOC systems gained considerable interest in the broad field of environmental analysis. In this work, several polymeric LOC systems for the analysis of dithiocarbamate (DTC) pesticides were designed and their performance was tested. Cyclic olefin polymer (COP) was studied as a potential material for non-aqueous analysis of DTC pesticides. While COP has some outstanding material properties compared to commonly used substrate materials, such as poly(methyl)methacrylate (PMMA) or polycarbonate (PC), it was shown that bonding of COP chips is challenging. Gold microband electrodes were integrated into microfluidic channels for electrochemical detection of the DTCs ziram and nabam. It was found that sulfur-containing DTC pesticides adsorb onto the gold surface of the electrode and thereby passivate it to a high extent. While sulfur-gold interactions of DTC pesticides were a major drawback for electrochemical detections, their high affinity for gold could be exploited in a second microfluidic sensor. Here, the sensor consisted of a polydimethylsiloxane (PDMS) chip for on-chip mixing of DTCs with gold nanoparticle (AuNP), which were functionalized with rhodamine 6G (R6G). While AuNPs act as a fluorescence quencher for the adsorbed R6G, they interact with the sulfur-containing pesticides upon mixing and thus release R6G into the solution. The R6G fluorescence intensity was measured and could be related to ziram concentrations with a limit of detection as low as 16 μg·L−1. Due to its indirect sensing mechanism, the AuNP-based DTC sensor was not specific for ziram and a similar fluorescence response was measured for ferbam, demonstrating that the mechanism can be employed as an indirect detection scheme for several DTC pesticides. Therefore, the nonspecific detection mechanism needs to be combined with a separation step prior to AuNP-mediated detection, to allow quantitative and qualitative analysis of different DTC pesticides. To this end, a capillary electrophoresis (CE) unit was implemented on a third chip, which was fabricated of thiol:ene, a photopolymerizable material. The CE microchip consisted of a separation channel for DTC separation, and side channels for subsequent AuNP probe lamination of the separation bands. Even though a separation of pesticides was not performed, the electrophoretically driven lamination of AuNP, and the feasibility of indirect fluorescence detection of ziram in microfluidic channels with a small detection volume was proven. Furthermore, three different fluorophores could be separated on these chips, demonstrating that chips fabricated from thiol:ene offer a great potential within polymer based CE.
Metabolic footprint of Lactobacillus acidophilus NCFM at different pH

Lactobacillus acidophilus NCFM is a well known microorganism from the genomic and probiotic point of view. In order to analyze the potential interactions of NCFM with the surrounding environment, in vitro tests with the metabolic footprinting approach were performed. It was found that NCFM increased the concentration of lactic acid, succinic acid, adenine and arginine in the medium. The metabolism of NCFM did not change significantly between pH 5 and 7, suggesting that other environmental factors than pH might have bigger impact on its colonization throughout the gastrointestinal tract.
Metabolic footprint of Lactobacillus acidophilus NCFM at different pH

General information
State: Published
Organisations: National Food Institute, Division of Microbiology and Risk Assessment, Division of Food Chemistry
Authors: Sulek, K. (Intern), Frandsen, H. L. (Intern), Skov, T. H. (Intern), Wilcks, A. (Intern), Smedsgaard, J. (Intern), Licht, T. R. (Intern)
Number of pages: 1
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Metabolomics of UC bacterial ecosystem compared to the healthy donors

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Organisations: National Food Institute, Division of Microbiology and Risk Assessment, Division of Food Chemistry, Ghent University, Copenhagen University Hospital, University of Copenhagen
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Vitamin D3 in plants: effect of UVB exposure

General information
State: Published
Organisations: National Food Institute, Division of Food Chemistry, University of Copenhagen
Authors: Jäpelt, R. B. (Intern), Silvestro, D. (Ekstern), Smedsgaard, J. (Intern), Jensen, P. (Ekstern), Jakobsen, J. (Intern)
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Main Research Area: Technical/natural sciences

Poster
LC–MS/MS with atmospheric pressure chemical ionisation to study the effect of UV treatment on the formation of vitamin D3 and sterols in plants

Some plant species are known to cause calcium intoxicification in grazing animals. This has been attributed to the presence of vitamin D3-like activity. However, research into the presence of vitamin D3 in plants has been limited. One reason for this may be limitations in the analytical methods available for unambiguous detection and quantification of vitamin D3. This paper presents a new method for determining vitamin D3 and its sterol precursors. The method is based on saponification and extraction followed by solid phase clean-up of the compounds from plant leaves and detection by APCI-MS. Recoveries ranged from 101% to 114% and precision from 3% to 12%. Detection limits were 2–8ng/g fresh weight for the substances tested. In a pilot study we found that Solanum glaucohyllum Desf. and Solanum lycopersicum L. produced vitamin D3 after UV-treatment. The preliminary results presented suggest that vitamin D3 formation in plants is dependent on light exposure.
Seasonal Variation of Provitamin D2 and Vitamin D2 in Perennial Ryegrass (Lolium perenne L.)

Ergosterol (provitamin D(2)) is converted to vitamin D(2) in grass by exposure to UV light. Six varieties of perennial ryegrass (Lolium perenne L.) were harvested four times during the season, and the contents of vitamin D(2) and ergosterol were analyzed by a sensitive and selective liquid chromatography tandem mass spectrometry method. Weather factors were recorded, and a principal component analysis was performed to study which factors were important for the formation of vitamin D(2). The results suggest that a combination of weather factors is involved and that the contents of ergosterol and vitamin D(2) change more than a factor of 10 during the season. These results demonstrate that grass potentially can be a significant source of vitamin D for grazing animals and animals fed on silage and hay.

General information
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Organisations: Division of Food Chemistry, National Food Institute, DLF-TRIFOLIUM A/S
Authors: Jäpelt, R. B. (Intern), Didion, T. (Ekstern), Smedsgaard, J. (Intern), Jakobsen, J. (Intern)
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Bacterial Impact on the Gut Metabolome

During the last decade, it has become evident that the complex ecosystem of microbes inhabiting the human gut plays an important role for human health. An increasing number of publications have shown that the composition and activity of our intestinal microbiota affects a number of different so-called lifestyle diseases including allergy, obesity, and colorectal cancer, as well as our susceptibility to intestinal infections and inflammation. Additionally, it has become evident that the intestinal microbiota can be modulated by intake of pre- and probiotics. A large number of studies have addressed the effects of dietary interventions on the presence of specific bacterial metabolites, which are anticipated to play a role for gut health. However, such data evidently provide only small parts of the complex puzzle constituting the interactions between diet, microbiota, and mammalian host. This project’s objective is to elucidate the mechanism behind the beneficial effects of pre- and probiotics. This will lead to development of new pre- and probiotics targeting specific lifestyle related disorders. The innovative design of pre- and probiotics will lead to increased value for Danish companies. The major hypotheses to be addressed in the project are as follows: Specific probiotic bacteria growing in an intestinal environment produce metabolites, which are qualitatively and quantitatively different from those produced by the same bacteria in vitro. The production of metabolites by specific probiotic bacteria can be affected by prebiotic substances. The presence of specific prebiotics and/or probiotic bacteria in the intestine induces production of specific metabolites from the host epithelium. These effects will be altered by the presence of other specific bacteria in the gnotobiotic gut. The effects will be different in different gut compartments (e.g. ileum versus colon and mucosa versus lumen). Also metabolites in blood will be affected by probiotic colonization and/or prebiotic administration. To map metabolites, gnotobiotic animal models and in vitro fermentation tests in an anaerobic chamber are used, which allow studies of a simple well-defined intestinal microbiota – in this case Lactobacillus acidophilus NCFM. Usage of Mass Spectrometry makes it possible to measure metabolites in intestinal and other mammalian samples as well as in vitro samples. Newly developed advanced (‘omics-’) methodologies are used for analysis of biological interactions.

General information
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Dynamics in the microbiology of maize silage during whole-season storage

Aims: To monitor seasonal variations in the microbiology of maize silage and to determine whether the risk of fungal spoilage varies during whole-year storage. Methods and Results: A continuous survey of 20 maize silage stacks was conducted over a period from three to 11 months after ensiling. Filamentous fungi, yeasts and lactic acid bacteria (LAB) were enumerated at five time-points, and cultivable species of filamentous fungi were identified. Significant differences in the numbers of filamentous fungi, yeast and LAB were detected. The highest numbers of fungi were five to seven and the lowest 11 months after ensiling, while the LAB decreased in numbers during the study. Filamentous fungi were isolated from all stacks at all time-points. The most abundant toxigenic mould species were Penicillium roqueforti, Penicillium paneum and Aspergillus fumigatus. Conclusions: There are significant variations in the microbiology of maize silage over a whole storage season. The risk of fungal spoilage was highest 5-7 months after ensiling and lowest after 11 months. Significance and Impact of the Study: This information is valuable in the assessment of health risks connected with spoiled maize silage and may be useful in the management of maize silage stacks, when whole-season storage is applied.

General information
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Organisations: Center for Microbial Biotechnology, Department of Systems Biology, Division of Food Chemistry, National Food Institute
Authors: Storm, I. M. L. D. (Intern), Kristensen, N. (Ekstern), Raun, B. (Ekstern), Smedsgaard, J. (Intern), Thrane, U. (Intern)
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BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.56
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.69
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.51
Multi-mycotoxin analysis of maize silage by LC-MS/MS

This paper describes a method for determination of 27 mycotoxins and other secondary metabolites in maize silage. The method focuses on analytes which are known to be produced by common maize and maize-silage contaminants. A simple pH-buffered sample extraction was developed on the basis of a very fast and simple method for analysis of multiple pesticide residues in food known as QuEChERS. The buffering effectively ensured a stable pH in samples of both well-ensiled maize (pH 7). No further clean-up was performed before analysis using liquid chromatography-tandem mass spectrometry. The method was successfully validated for determination of eight analytes qualitatively and 19 quantitatively. Matrix-matched calibration standards were used giving recoveries ranging from 37% to 201% with the majority between 60% and 115%. Repeatability (5-27% RSDr) and intra-laboratory reproducibility (7-35% RSDIR) was determined. The limit of detection (LOD) for the quantitatively validated analytes ranged from 1 to 739 μg kg⁻¹. Validation results for citrinin, fumonisin B-1 and fumonisin B-2 were unsatisfying. The method was applied to 20 selected silage samples and alternariol monomethyl ether, andrastin A, alternariol, citreoisocoumarin, deoxynivalenol, enniatin B, fumigaclavine A, gliotoxin, marcfortine A and B, mycophenolic acid, nivalenol, roquefortine A and C and zearalenone were detected.

General information

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Organisations: Division of Food Chemistry, National Food Institute, Center for Microbial Biotechnology, Department of Systems Biology
Authors: Rasmussen, R. R. (Intern), Storm, I. M. L. D. (Intern), Rasmussen, P. H. (Intern), Smedsgaard, J. (Intern), Nielsen, K. F. (Intern)
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The effect of different in vitro conditions on the metabolic footprint of Lactobacillus acidophilus NCFM
Post-harvest Fungal Spoilage of Maize Silage: Species, growth conditions and mycotoxin detection

General information
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Organisations: Center for Microbial Biotechnology, Department of Systems Biology, Division of Food Chemistry, National Food Institute
Authors: Storm, I. M. L. D. (Intern), Thrane, U. (Intern), Smedsgaard, J. (Intern)
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Metabolome analysis - mass spectrometry and microbial primary metabolites

While metabolite profiling has been carried out for decades, the scope for metabolite analysis have recently been broadened to aim at all metabolites in a living organism – also referred to as the metabolome. This is a great challenge, which requires versatile analytical technologies that are highly sensitive and specific, and to undertake this challenge mass spectrometry (MS) is among the best candidates. Along with analysis of the metabolome the research area of metabolomics has evolved. Metabolomics combines metabolite profiles, data mining and biochemistry and aims at understanding the interplay between metabolites. In this thesis, different topics have been addressed and discussed with the aim of advancing metabolomics to explore the concept in a physiological context. The metabolome comprises a wide variety of chemical compounds that act differently upon sample preparation, and therefore sample preparation is critical for metabolome analysis. The three major steps in sample preparation for metabolite analysis are sampling, extraction and concentration. These three steps were evaluated for the yeast Saccharomyces cerevisiae with primary focus on analysis of a large number of metabolites by one method. The results highlighted that there were discrepancies between different methods. To increase the throughput of cultivation, S. cerevisiae was grown in microtitier plates (MTPs), and the growth was found to be comparable with cultivations in shake flasks. The carbon source was either glucose, galactose or ethanol, and metabolic footprinting by mass spectrometry was used to study the influence of carbon source on the extracellular metabolites. The results showed that footprints clustered according to the carbon source. Advances in technologies for analytical chemistry have mediated increased amounts of data generated in high resolution. One major limitation though is the digestion of data coverting the information into a format that can be interpreted in a biological context and take metabolomics beyond the principle of guilt-by-association. To analyze the data there is a general need for databases that contain metabolite specific information, which will speed up the identification of profiled metabolites. To address the capabilities of electrospray ionization (ESI)-MS in detecting the metabolome of S. cerevisiae, the in silico metabolome of this organism was used as a template to present a theoretical metabolome. This showed that in combination with the specificity of MS up to 84% of the metabolites can be identified in a high-accuracy ESI-spectrum. A total of 66 metabolites were systematically analyzed by positive and negative ESI-MS/MS with the aim of initiating a spectral library for ESI of microbial metabolites. This systematic analysis gave insight into the ionization and fragmentation characteristics of the different metabolites. With this insight, a small study of metabolic footprinting with ESI-MS demonstrated that biological information can be extracted from footprinting spectra. Statistical analysis of the footprinting data revealed discriminating ions, which could be assigned using the in silico metabolome. By this approach metabolic footprinting can advance from a classification method that is used to derive biological information based on guilt-by-association, to a tool for extraction of
metabolic differences, which can guide new targeted biological experiments.

The yeast metabolome addressed by electrospray ionization mass spectrometry: Initiation of a mass spectral library and its applications for metabolic footprinting by direct infusion mass spectrometry

Mass spectrometry (MS) has been a major driver for metabolomics, and gas chromatography (GC)-MS has been one of the primary techniques used for microbial metabolomics. The use of liquid chromatography (LC)-MS has however been limited, but electrospray ionization (ESI) is very well suited for ionization of microbial metabolites without any previous derivatization needed. To address the capabilities of ESI-MS in detecting the metabolome of Saccharomyces cerevisiae, the in silico metabolome of this organism was used as a template to present a theoretical metabolome. This showed that in combination with the specificity of MS up to 84% of the metabolites can be identified in a high mass accuracy ESI-spectrum. A total of 66 metabolites were systematically analyzed by positive and negative ESI-MS/MS with the aim of initiating a spectral library for ESI of microbial metabolites. This systematic analysis gave insight into the ionization and fragmentation characteristics of the different metabolites. With this insight, a small study of metabolic footprinting with ESI-MS demonstrated that biological information can be extracted from footprinting spectra. Statistical analysis of the footprinting data revealed discriminating ions, which could be assigned using the in silico metabolome. By this approach metabolic footprinting can advance from a classification method that is used to derive biological information based on guilt-by-association, to a tool for extraction of metabolic differences, which can guide new targeted biological experiments.
Automated work-flow for processing high-resolution direct infusion electrospray ionization mass spectral fingerprints

The use of mass spectrometry (MS) is pivotal in analyses of the metabolome and presents a major challenge for subsequent data processing. While the last few years have given new high performance instruments, there has not been a comparable development in data processing. In this paper we discuss an automated data processing pipeline to compare large numbers of fingerprint spectra from direct infusion experiments analyzed by high resolution MS. We describe some of the intriguing problems that have to be addressed, starting with the conversion and pre-processing of the raw data to the final data analysis. Illustrated on the direct infusion analysis (ESI-TOF-MS) of complex mixtures the method exploits the full quality of the high-resolution present in the mass spectra. Although the method is illustrated as a new library search method for high resolution MS, we demonstrate that the output of the preprocessing is applicable to cluster-, discriminant analysis, and related multivariate methods applied directly to mass spectra from direct infusion analysis of crude extracts. This is done to find the relationship between several terverticillate Penicillium species and identify the ions responsible for the segregation.

General information
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Authors: Hansen, M. A. E. (Intern), Smedsgaard, J. (Intern)
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**Scopus rating (2015):** SJR 1.318 SNIP 1.113 CiteScore 3.49  
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**Scopus rating (2014):** SJR 1.309 SNIP 1.142 CiteScore 3.74  
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**Scopus rating (2013):** SJR 1.133 SNIP 1.017 CiteScore 4.03  
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**Scopus rating (2009):** SJR 1.279 SNIP 0.819  
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**Scopus rating (2008):** SJR 1.223 SNIP 0.782  
**Web of Science (2008):** Indexed yes  
**Scopus rating (2007):** SJR 0.813 SNIP 0.628  
**Web of Science (2007):** Indexed yes  
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**Fumonisin B2 production by Aspergillus niger**

**General information**

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**Organisations:** Center for Microbial Biotechnology, Department of Systems Biology, CBS-KNAW Fungal Biodiversity Centre  
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Scopus rating (2015): SJR 1.224 SNIP 1.245 CiteScore 3.23
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BFI (2011): BFI-level 2
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ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.42 SNIP 1.391
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.33 SNIP 1.306
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.327 SNIP 1.338
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.252 SNIP 1.44
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.367 SNIP 1.418
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.298 SNIP 1.517
Web of Science (2005): Indexed yes
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Scopus rating (2003): SJR 1.152 SNIP 1.469
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Metabolome Analysis: An Introduction

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Authors: Villas-Bôas, S. G. (Ekstern), Roessner, U. (Ekstern), Hansen, M. A. E. (Intern), Smedsgaard, J. (Intern), Nielsen, J. (Ekstern)
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Production of mycotoxins by Aspergillus lentulus and other medically important and closely related species in section Fumigati

The production of mycotoxins and other secondary metabolites have been studied by LC-DAD-MS from six species in Aspergillus section Fumigati. This includes the three new species Aspergillus lentulus, A. novofumigatus and A. fumigatiaffinis as well as A. fumigatus, Neosartoria fisheri and N. pseudofisheri. A major finding was detection of gliotoxin from N. pseudofisheri, a species not previously reported to produce this mycotoxin. Gliotoxin was also detected from A. fumigatus together with fumagillin, fumigaclavine C, fumitremorgin C, fumiquinazolines, trypacidin, methyl- sulochrin, TR-2, verruculogen, helvolic acid and pyripyropenes. Major compounds from A. lentulus were cyclopiazonic acid, terrein, neosartorin, auranthine and pyripyropenes A, E and O. Thus in the present study A. fumigatus and A. lentulus did not produce any of the same metabolites except for pyripyropenes. The fact that A. lentulus apparently does not produce gliotoxin supports the idea that other compounds than gliotoxin might play an important role in the effective invasiveness of A. lentulus. An overall comparison of secondary metabolite production by strains of the six species was achieved by analysis of fungal extracts by direct injection mass spectrometry and cluster analysis. Separate groupings were seen for all the six species even though only one isolate was included in this study for the two species A. novofumigatus and A. fumigatiaffinis.

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Main Research Area: Technical/natural sciences

Production of mycotoxins by Aspergillus lentulus and other medically important and closely related species in section Fumigati

The production of mycotoxins and other secondary metabolites have been studied by LC-DAD-MS from six species in Aspergillus section Fumigati. This includes the three new species Aspergillus lentulus, A. novofumigatus and A. fumigatiaffinis as well as A. fumigatus, Neosartoria fisheri and N. pseudofisheri. A major finding was detection of gliotoxin from N. pseudofisheri, a species not previously reported to produce this mycotoxin. Gliotoxin was also detected from A. fumigatus together with fumagillin, fumigaclavine C, fumitremorgin C, fumiquinazolines, trypacidin, methyl- sulochrin, TR-2, verruculogen, helvolic acid and pyripyropenes. Major compounds from A. lentulus were cyclopiazonic acid, terrein, neosartorin, auranthine and pyripyropenes A, E and O. Thus in the present study A. fumigatus and A. lentulus did not produce any of the same metabolites except for pyripyropenes. The fact that A. lentulus apparently does not produce gliotoxin supports the idea that other compounds than gliotoxin might play an important role in the effective invasiveness of A. lentulus. An overall comparison of secondary metabolite production by strains of the six species was achieved by analysis of fungal extracts by direct injection mass spectrometry and cluster analysis. Separate groupings were seen for all the six species even though only one isolate was included in this study for the two species A. novofumigatus and A. fumigatiaffinis.
Standard reporting requirements for biological samples in metabolomics experiments: Microbial and in vitro biology experiments

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Authors: van der Werf, M. J. (Ekstern), Takors, R. (Ekstern), Smedsgaard, J. (Intern), Nielsen, J. (Intern), Ferenci, T. (Ekstern), Portais, J. C. (Ekstern), Wittmann, C. (Ekstern), Hooks, M. (Ekstern), Tomassini, A. (Ekstern), Oldiges, M. (Ekstern), Fostel, J. (Ekstern), Sauer, U. (Ekstern)
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Publication date: 2007
Main Research Area: Technical/natural sciences
The exo-metabolome in filamentous fungi

Filamentous fungi are a diverse group of eukaryotic microorganisms that have a significant impact on human life as spoilers of food and feed by degradation and toxin production. They are also most useful as a source of bulk and fine chemicals and pharmaceuticals. This chapter focuses on the exo-metabolome in filamentous fungi, which comprises more than 30,000 known secondary metabolites. Profiles of this diverse range of secondary metabolites have, for more than 25 years, been central in development of fungal systematics, taxonomy, and ecology, today integrated in a multidisciplinary and polyphasic approach to applied mycology. Lead discovery is an example of the successful integration of metabolite profiling and natural product chemistry in mycology.
Host publication information
Title of host publication: Metabolomics
Volume: 18
Place of publication: Berlin / Heidelberg
Publisher: Springer
Edition: 1
ISBN (Print): 35-40-74718-4
Series: Topics in Current Genetics
ISSN: 1610-2096
Main Research Area: Technical/natural sciences
Fungi, metabolomics
DOIs:
10.1007/4735_2007_0230
Source: orbit
Source-ID: 244071
Publication: Research - peer-review › Book chapter – Annual report year: 2007

Elucidating the mode-of-action of compounds from metabolite profiling studies

General information
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology
Authors: Højer-Pedersen, J. (Intern), Smedsgaard, J. (Intern), Nielsen, J. (Intern)
Pages: 105-129
Publication date: 2006

Host publication information
Title of host publication: Systems Biological Approaches in Infectious Diseases : Progress in Drug Research
Volume: 64
Place of publication: Birkhäuser, berlin
Editor: Bostoff, H.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 195495
Publication: Research - peer-review › Book chapter – Annual report year: 2006

Host-derived media used as a predictor for low abundant, in planta metabolites production by necrotrophic fungi.

General information
State: Published
Organisations: Department of Systems Biology, Center for Microbial Biotechnology, Bioscience and Technology
Authors: Overy, D. P. (Intern), Smedsgaard, J. (Intern), Frisvad, J. C. (Intern), Phipps, R. K. (Intern), Thrane, U. (Intern)
Pages: 1292-1300
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Applied Microbiology
Volume: 101
Issue number: 6
ISSN (Print): 1364-5072
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
Identification of an Abscisic Acid Gene Cluster in the Grey Mold Botrytis cinerea

General information
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology
Authors: Siewers, V. (Intern), Kekkelink, L. (Ekstern), Smedsgaard, J. (Intern), Tudzynski, P. (Ekstern)
Pages: 4619-4626
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied and Environmental Microbiology
Volume: 72
Issue number: 7
ISSN (Print): 0099-2240
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.08
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.691 SNIP 1.308 CiteScore 4.14
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.857 SNIP 1.384 CiteScore 4.02
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.899 SNIP 1.414 CiteScore 4.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.975 SNIP 1.429 CiteScore 4.29
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.914 SNIP 1.455 CiteScore 4.12
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.887 SNIP 1.436
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.972 SNIP 1.528
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.156 SNIP 1.572
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.043 SNIP 1.647
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.054 SNIP 1.602
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.074 SNIP 1.653
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.108 SNIP 1.648
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.097 SNIP 1.821
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.046 SNIP 1.754
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.989 SNIP 1.736
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.957 SNIP 1.758
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 2.3 SNIP 1.732

Original language: English
Source: orbit
Source-ID: 194454
Real-time PCR quantification of the AM-toxin gene and HPLC quantification of toxigenic metabolites from Alternaria species from apples

General information
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology
Authors: Andersen, B. (Intern), Smedsgaard, J. (Intern), Jørring, I. (Ekstern), Skouboe, P. (Ekstern), Pedersen, L. (Ekstern)
Pages: 105-111
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: INTERNATIONAL JOURNAL OF FOOD MICROBIOLOGY
Volume: 111
ISSN (Print): 0168-1605
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SJR 1.366 SNIP 1.436
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.97 SJR 1.481 SNIP 1.553
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.614 SNIP 1.683 CiteScore 4.02
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.493 SNIP 1.695 CiteScore 3.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.612 SNIP 1.841 CiteScore 3.8
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.603 SNIP 1.705 CiteScore 3.7
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.607 SNIP 1.713 CiteScore 3.63
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.61 SNIP 1.666
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.475 SNIP 1.539
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.442 SNIP 1.509
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.349 SNIP 1.692
Web of Science (2007): Indexed yes
Soyasaponins resist extrusion cooking and are not degraded during gut passage in Atlantic salmon (Salmo salar L.)

The stability of soyasaponins in fish feed formulations was investigated. The level of soyasaponin Ab, Bb, Bc, Ba-2,3-dihydro-2,5-dihydroxy-6-methyl-4H-pyran-4-one (Ba-DDMP), Bb-DDMP, and Bc-DDMP was quantified in 15 samples of defatted soybean meal, two full fat soybean meals, and two soybean protein concentrates by reverse phase high-performance liquid chromatography. The total level of saponins in the 15 samples of commercial defatted soybean meal ranged from 4.8-6.8 μmol/g (5.1-7.0 g/kg). The two full fat meals contained 4.4 and 4.7 μmol/g whereas no saponins could be detected in the alcohol-extracted soybean protein concentrates. Fifteen batches of fish feed containing 20% defatted soybean meal were produced by twin-screw extrusion from the 15 different samples of defatted soybean meal. Extrusion did not reduce the total level of group B saponins, but the ratio between DDMP-conjugated group B saponins and non-DDMP-conjugated group B saponins was slightly reduced. A soybean-containing diet was fed to seawater adapted Atlantic salmon for 9 weeks. Yttrium oxide was included in the feed as an inert marker in order to estimate the disappearance of saponins during gut passage. High levels of intact non-DDMP-conjugated group B soyasaponins were found in feces whereas only low levels of DDMP-conjugated saponins could be detected. The overall disappearance of saponins was close to zero, and the concentration of intact saponins in dry feces reached levels several fold higher than dietary levels. The present work demonstrates that non-DDMP-conjugated group B soyasaponins resist extrusion cooking and remain intact during gut passage in Atlantic salmon. The latter is contrary to earlier findings in endothermic animals.
A new algorithm for novelty detection and de-replication of spectroscopic analysis of complex mixtures of natural products

General information
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology
Authors: Hansen, M. E. (Intern), Smedsgaard, J. (Intern), Larsen, T. O. (Intern)
Pages: S129-S129
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Biotechnology
Volume: 118
ISSN (Print): 0168-1656
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.86 SJR 0.929
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.88 SJR 1.004 SNIP 0.929
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.068 SNIP 0.988 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.116 SNIP 1.13 CiteScore 2.95
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.183 SNIP 1.175 CiteScore 3.22
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.238 SNIP 1.312 CiteScore 3.4
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.165 SNIP 1.043 CiteScore 2.87
ISI indexed (2011): ISI indexed yes
Automated and unbiased classification of chemical profiles from fungi using high performance liquid chromatography

In this paper we present a method for unbiased/unsupervised classification and identification of closely related fungi, using chemical analysis of secondary metabolite profiles created by HPLC with UV diode array detection. For two chromatographic data matrices a vector of locally aligned full spectral similarities is calculated along the retention time axis. The vector depicts the evaluating of the alikeness between two fungal extracts based upon eluted compounds and corresponding UV-absorbance spectra. For assessment of the chemotaxonomic grouping the vector is condensed to one similarity describing the overall degree of similarity between the profiles. Two sets of data were used in this study: One set was used in the method development and a second dataset used for method validation. First we developed a method for evaluating the secondary metabolite production from closely related Penicillium species. Then the algorithm was validated on fungal isolates belonging to the genus Alternaria. The results showed that the species may be segregated into taxa in full accordance with published taxonomy.

General information
State: Published
Organisations: Department of Informatics and Mathematical Modeling, Center for Microbial Biotechnology, Department of Systems Biology
Authors: Hansen, M. E. (Intern), Andersen, B. (Intern), Smedsgaard, J. (Intern)
Pages: 295-304
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Microbiological Methods
Volume: 61
Issue number: 3
ISSN (Print): 0167-7012
Ratings:
BFI (2018): BFI-level 1
Automated and unbiased image analyses as tools in phenotypic classification of small-spored Alternaria species.

For more than 25 years, controversy has surrounded the characterization and differentiation of small-spored Alternaria spp. And, therefore, the application of names of several species that are involved in the pathology of diseases related to host-specific toxin production. The name A. alternata often has been broadly applied to various morphologically and chemically distinct groups of isolates from different hosts. The purpose of this study was to develop and evaluate automated and unbiased image analysis systems that will analyze different phenotypic characters and facilitate testing and application of the morphological species concept in Alternaria taxonomy. Host-specific toxin-producing Alternaria isolates assigned to five morpho-species were compared with representative isolates of morphologically distinct A. alternata. Combined results of growth rates at different temperatures, colony morphology, and metabolite profiles were found to be useful in characterization and differentiation of small-spored Alternaria spp. when standardized conditions are applied and representative isolates employed for comparison.

General information
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology
Authors: Andersen, B. (Intern), Hansen, M. E. (Intern), Smedsgaard, J. (Intern)
Pages: 1021-1029
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Phytopathology
Volume: 95
Issue number: 9
ISSN (Print): 0031-949X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.566 SJR 1.345
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.308 SNIP 1.573 CiteScore 2.93
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.436 SNIP 1.769 CiteScore 2.94
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.359 SNIP 1.58 CiteScore 2.99
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.217 SNIP 1.601 CiteScore 2.83
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.423 SNIP 1.548 CiteScore 2.81
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.24 SNIP 1.582 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.192 SNIP 1.301
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.306 SNIP 1.386
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.117 SNIP 1.433
Scopus rating (2007): SJR 1.212 SNIP 1.35
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.283 SNIP 1.504
Global metabolite analysis of yeast: evaluation of sample preparation methods

Sample preparation is considered one of the limiting steps in microbial metabolome analysis. Eukaryotes and prokaryotes behave very differently during the several steps of classical sample preparation methods for analysis of metabolites. Even within the eukaryote kingdom there is a vast diversity of cell structures that make it imprudent to blindly adopt protocols that were designed for a specific group of microorganisms. We have therefore reviewed and evaluated the whole sample preparation procedures for analysis of yeast metabolites. Our focus has been on the current needs in metabolome analysis, which is the analysis of a large number of metabolites with very diverse chemical and physical properties. This work reports the leakage of intracellular metabolites observed during quenching yeast cells with cold methanol solution, the efficacy of six different methods for the extraction of intracellular metabolites, and the losses noticed during sample concentration by lyophilization and solvent evaporation. A more reliable procedure is suggested for quenching yeast cells with cold methanol solution, followed by extraction of intracellular metabolites by pure methanol. The method can be combined with reduced pressure solvent evaporation and therefore represents an attractive sample preparation procedure for high-throughput metabolome analysis of yeasts. Copyright (c) 2005 John Wiley & Sons, Ltd.
LC-MS contra direct infusion-MS for profiling of secondary metabolites in fungi

General information
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology
Authors: Smedsgaard, J. (Intern)
Pages: S159-S159
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Biotechnology
Volume: 118
ISSN (Print): 0168-1656
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.86 SJR 0.929
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.88 SJR 1.004 SNIP 0.929
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.068 SNIP 0.988 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.116 SNIP 1.13 CiteScore 2.95
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.183 SNIP 1.175 CiteScore 3.22
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.238 SNIP 1.312 CiteScore 3.4
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.165 SNIP 1.043 CiteScore 2.87
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.135 SNIP 1.175
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.224 SNIP 1.231
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.147 SNIP 1.265
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.133 SNIP 1.27
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.109 SNIP 1.394
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.193 SNIP 1.358
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.028 SNIP 1.442
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.943 SNIP 1.224
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.787 SNIP 1.038
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.754 SNIP 0.972
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.927 SNIP 0.889
Scopus rating (1999): SJR 0.841 SNIP 1.035
Original language: English
Source: orbit
Source-ID: 196237
Metabolite profiling of fungi of yeast: From phenotype to metabolome by MS and informatics

General information
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology
Authors: Smedsgaard, J. (Intern), Nielsen, J. (Intern)
Pages: 273-286
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Experimental Botany
Volume: 56
ISSN (Print): 1460-2431
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 1.757 SJR 2.822
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.02 SJR 2.859 SNIP 1.717
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.784 SNIP 1.811 CiteScore 5.97
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.77 SNIP 2.052 CiteScore 5.93
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.656 SNIP 1.952 CiteScore 6
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.619 SNIP 1.929 CiteScore 5.47
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.631 SNIP 1.865 CiteScore 5.19
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.373 SNIP 1.802
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.382 SNIP 1.7
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.234 SNIP 1.521
Scopus rating (2007): SJR 2.304 SNIP 1.666
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.847 SNIP 1.392
Scopus rating (2005): SJR 1.748 SNIP 1.623
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.676 SNIP 1.439
Scopus rating (2003): SJR 1.682 SNIP 1.567
Web of Science (2003): Indexed yes
Metabolome analysis by mass spectrometry

General information
State: Published
Organisations: Department of Systems Biology, Center for Microbial Biotechnology
Authors: Villas-Bôas, S. G. (Intern), Mas, S. (Intern), Åkesson, M. F. (Intern), Smedsgaard, J. (Intern), Nielsen, J. (Intern)
Pages: 613-646
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Mass Spectrometry Review
Volume: 24
Original language: English
Source: orbit
Source-ID: 184297
Publication: Research - peer-review › Journal article – Annual report year: 2005

Phenotypic taxonomy and metabolite profiling in microbial drug discovery

General information
State: Published
Organisations: Department of Systems Biology, Center for Microbial Biotechnology
Authors: Larsen, T. O. (Intern), Smedsgaard, J. (Intern), Nielsen, K. F. (Intern), Hansen, M. E. (Intern), Frisvad, J. C. (Intern)
Pages: 672-695
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Natural Product Reports
Volume: 22
Original language: English
Source: orbit
Source-ID: 184091
Publication: Research - peer-review › Journal article – Annual report year: 2005

Roquefortine/Oxaline biosynthesis pathway metabolites in Penicillium SER. Corymbifera: IN PLANTA production and implication for competitive fitness

General information
State: Published
Organisations: Department of Systems Biology, Center for Microbial Biotechnology
Authors: Overy, D. P. (Intern), Nielsen, K. F. (Intern), Smedsgaard, J. (Intern)
Pages: 2373-2390
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Chemical Ecology
Volume: 31
ISSN (Print): 0098-0331
Ratings:
X-hitting: A new algorithm for novelty detection and dereplication by UV spectra of complex mixtures of natural products

A major challenge in lead discovery is to detect well-known and trivial compounds rapidly, a process known as dereplication, so that isolation, structure elucidation, and pharmacological investigations can be focused on novel compounds. In this paper, we present a new algorithm, X-hitting, based on cross sample comparison of full UV spectra from HPLC analysis of highly complex natural product extracts/samples. X-Hitting allows automatic identification of known compounds but more important also allows finding of potentially new or similar compounds. We demonstrate this new algorithm by automatic identification of known structures, a task we call cross-hitting, and tentative identification of potentially new bioactive compounds, a task we call new-hitting, in HPLC data from analysis of fungal extracts. Both tasks are illustrated using 18 important reference compounds and complex fungal extracts obtained from isolates in the IBT Culture Collection held at BioCentrum-DTU, Technical University of Denmark. The receiver operating characteristics statistic is used to evaluate the performance of the compound predictor, and it was found that compounds could be identified with high confidence (AUC approximate to 0.98). Based on high confidence in retrieving identical spectra, the method is extended to include similar but still different spectra.
A new matching algorithm for high resolution mass spectra
We present a new matching algorithm designed to compare high-resolution spectra. Whereas existing methods are bound to compare fixed intervals of ion masses, the accurate mass spectrum (AMS) distance method presented here is independent of any alignment. Based on the Jeffreys-Matusitas (JM) distance, a difference between observed peaks across pairs of spectra can be calculated, and used to find a unique correspondence between the peaks. The method takes into account that there may be differences in resolution of the spectra. The algorithm is used for indexing in a database containing 80 accurate mass spectra from an analysis of extracts of 80 isolates representing the nine closely related species in the Penicillium series Viridicata. Using this algorithm we can obtain a retrieval performance of approximate to 97-98% that is comparable with the best of the existing methods (e.g., the dot-product distance). Furthermore, the presented method is independent of any variable alignment procedures or binning.

General information
State: Published
Organisations: Department of Informatics and Mathematical Modeling
Authors: Hansen, M. E. (Intern), Smedsgaard, J. (Intern)
Pages: 1173-1180
Publication date: Aug 2004
Main Research Area: Technical/natural sciences

Publication information
Journal: JOURNAL OF THE AMERICAN SOCIETY FOR MASS SPECTROMETRY
Volume: 15
Issue number: 8
ISSN (Print): 1044-0305
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.846 SJR 1.058
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.096 SNIP 0.788 CiteScore 2.49
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.266 SNIP 1.011 CiteScore 2.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.281 SNIP 0.978 CiteScore 2.93
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.495 SNIP 1.054 CiteScore 3.28
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.809 SNIP 1.096 CiteScore 3.47
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.966 SNIP 1.186 CiteScore 3.8
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.763 SNIP 1.056
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.641 SNIP 1.173
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.767 SNIP 1.092
Scopus rating (2007): SJR 1.71 SNIP 1.146
A proposed framework for the description of plant metabolomics experiments and their results

The study of the metabolite complement of biological samples, known as metabolomics, is creating large amounts of data, and support for handling these data sets is required to facilitate meaningful analyses that will answer biological questions. We present a data model for plant metabolomics known as ArMet (architecture for metabolomics). It encompasses the entire experimental time line from experiment definition and description of biological source material, through sample growth and preparation to the results of chemical analysis. Such formal data descriptions, which specify the full experimental context, enable principled comparison of data sets, allow proper interpretation of experimental results, permit the repetition of experiments and provide a basis for the design of systems for data storage and transmission. The current design and example implementations are freely available (http://www.armet.org/). We seek to advance discussion and
community adoption of a standard for metabolomics, which would promote principled collection, storage and transmission of experiment data.

**General information**
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology
Authors: Jenkins, H. (Ekstern), Hardy, N. (Ekstern), Beckmann, M. (Ekstern), Draper, J. (Ekstern), Smith, A. (Ekstern), Taylor, J. (Ekstern), Fiehn, O. (Ekstern), Goodacre, R. (Ekstern), Bino, R. (Ekstern), Hall, R. (Ekstern), Kopka, J. (Ekstern), Lane, G. (Ekstern), Lange, B. (Ekstern), Liu, J. (Ekstern), Mendes, P. (Ekstern), Nikolau, B. (Ekstern), Oliver, S. (Ekstern), Paton, N. (Ekstern), Rhee, S. (Ekstern), Roessner-Tunali, U. (Ekstern), Saito, K. (Ekstern), Smedsgaard, J. (Intern), Sumner, L. (Ekstern), Wang, T. (Ekstern), Walsh, S. (Ekstern), Wurtele, E. (Ekstern), Kell, D. (Ekstern)
Pages: 1601-1606
Publication date: 2004
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Nature Biotechnology
Volume: 22
Issue number: 12
ISSN (Print): 1087-0156
Ratings:
- BFI (2018): BFI-level 3
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 2
- Scopus rating (2017): SNIP 6.062 SJR 18.252
- Web of Science (2017): Indexed Yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 13.16 SJR 20.666 SNIP 6.42
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): SJR 18.263 SNIP 5.553 CiteScore 11.88
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 16.609 SNIP 5.37 CiteScore 11.4
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): SJR 13.974 SNIP 5.364 CiteScore 10.45
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 10.87 SNIP 4.914 CiteScore 8.44
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): SJR 11.749 SNIP 6.196 CiteScore 8.21
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- BFI (2009): BFI-level 2
- Scopus rating (2009): SJR 7.942 SNIP 5.603
- BFI (2008): BFI-level 2
- Scopus rating (2008): SJR 6.205 SNIP 5.026
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 5.146 SNIP 4.583
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 5.875 SNIP 4.632
Automatic In-Vial MCF Derivatization Coupled to GC-MS for Simultaneous Determination of Amino and non-Amino Organic Acids

General information
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology
Authors: Hansen, K. K. (Intern), Villas-Bôas, S. G. (Intern), Smedsgaard, J. (Intern), Nielsen, J. (Intern)
Publication date: 2004
Event: Poster session presented at 12th Nordic mass spectrometry Conference, Nyborg, 29 August -1 September, .
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 155068
Publication: Research › Poster – Annual report year: 2004

Chemical diversity of fungi - metabolite profiling and metabolomics

General information
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology
Authors: Nielsen, K. F. (Intern), Smedsgaard, J. (Intern), Larsen, T. O. (Intern), Lund, F. (Ekstern), Thrane, U. (Intern), Frisvad, J. C. (Intern)
Pages: 19-35
Publication date: 2004

Host publication information
Title of host publication: Fungal biotechnology in agricultural, food, and environmental applications
Place of publication: New York
Publisher: Marcel Dekker
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 154981
Publication: Research - peer-review › Book chapter – Annual report year: 2004

Classification of terverticillate Penicillia by electrospray mass spectrometric profiling
429 isolates of 58 species belonging to Penicillium subgenus Penicillium are classified from direct infusion electrospray mass spectrometry (diMS) analysis of crude extracts by automated data processing. The study shows that about 70% of the species can be classified correctly into species using only the analysis of metabolites produced on one growth medium. This classification is in concurrence with the taxonomic delimitation of the accepted species obtained by a polyphasic approach. Other relations between species can be read from the dendrograms and the efficient classification shows the potential of this semi-automated identification system.

General information
State: Published
Emericella astellata, a new producer of aflatoxin B-1, B-2 and sterigmatocystin

To report on aflatoxin B-1 and B-2 production from a species of Emericella. Methods and Results: Aflatoxins and sterigmatocystin were determined by high-pressure liquid chromatography (HPLC) with diode array detection and confirmed by HPLC with mass spectrometry detection. Among 30 known species of Emericella only one species produced aflatoxin. Strains originating from the same geographical source material had different patterns of aflatoxin and sterigmatocystin production on different media, indicating that epigenetic factors may be involved in the regulation of aflatoxin production. However, two cultures from the same original genet were very similar. Conclusions: Emericella astellata can produce small amounts of sterigmatocystin and aflatoxin B-1 and B-2. Significance and Impact of the Study: Emericella has been used extensively in genetic studies and therefore the isolates producing aflatoxin can be used to elucidate the genetic, evolutionary and maybe ecological role of aflatoxins using molecular genetic methods.

General information
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology
Authors: Frisvad, J. C. (Intern), Samson, R. (Ekstern), Smedsgaard, J. (Intern)
Pages: 440-445
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Journal: Letters in Applied Microbiology
Volume: 38
ISSN (Print): 0266-8254
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.82
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.66
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.8
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.09
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.92
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.87
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Identification of novel natural products using intelligent screening based on mass and UV spectometric methods

General information
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology
Publication date: 2004
Event: Poster session presented at International symposium on Marine Natural Products, Sorrento, Italy.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 155090
Publication: Research › Poster – Annual report year: 2004

Mass spectrometry for metabolite fingerprinting

General information
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology
Authors: Højer-Pedersen, J. (Intern), Hansen, M. E. (Intern), Smedsgaard, J. (Intern), Nielsen, J. (Intern)
Publication date: 2004
Event: Poster session presented at Metabolic Engineering V, Lake Tahoe, CA, United States.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 155074
Publication: Research › Poster – Annual report year: 2004

Mycotoxins, drugs and other extrolites produced by species in Penicillium subgenus Penicillium
The 58 species in Penicillium subgenus Penicillium produce a large number of bioactive extrolites (secondary metabolites), including several mycotoxins. An overview of these extrolites is presented with original references to the reports on their production and their chemical constitution. 132 extrolite families are reported from the subgenus with an average of 5 extrolite families per species. This is an underestimate as several pigments, volatiles and uncharacterized extrolites are not included in this average. Several reported producers are reidentified and new producers of known extrolites are reported for the first time. Several extrolites are unique for one species, but most of the metabolites are produced by more than one species. The most widespread extrolites were roquefortine C, which is produced by 25 species, the cyclopensins that are produced by 17 species, patulin which is produced by 13 species, penicillic acid which is produced by 10 species, and terresric acid and 2-methyl isoborneol that are produced by 8 species. Most species produce both polyketides, terpenes and amino acid derived extrolites and a large number of the species produce bioactive metabolites. The nephrotoxic mycotoxin ochratoxin A is produced by P. verrucosum and P. nordicum, and another nephrotoxin, citrinin, is produced by P. expansum, P. radicicola and P. verrucosum. Patulin is produced by P. carneum, P. clavigerum, P. concentricum, P. coprobium, P. dipodomyicola, P. expansum, P. glandicola, P. gladioli, P. griseofulvum, P. marinum, P. paneum, P. sclerotigenum and P. vulpinum. Another polyketide mycotoxin, penicillic acid, is produced by P. aurantiogriseum, P. carneum, P. cyclopium, P. freii, P. melanoconidium, P. neoechinulatum, P. polonicum, P. radicicola, P. terrestric acid and P. viridicatum. The tremorgenic verrucosidin is produced by P. aurantiogriseum, P. melanoconidium and P. polonicum, while another tremorgen, pentrem A, is produced by P. carneum, P. clavigerum, P. crutisoma, P. flavigenum, P. glandicola, P. melanoconidium and P. tulipae. Asteloicin is produced by P. cavernicola, P. concentricum, P. confertum, P. formosanum and P. tricolor. The mutagenic mycotoxin botryodiplodin is produced by P. brevicompactum and P. paneum. The chaetoglobosins are produced by P. discolor, P. expansum and P. marinum. The cytotoxic communesins are produced by P. expansum and P. marinum. Cyclopiazonic acid is produced by P. camemberti, P. commune, P.
dipodomyicola, P. griseofulvum and P. palitans. The fumitremorgins, verruculogen.. isochromantoxins and viriditoxin are produced by P. mononematosum. The immunosuppressive extrolite mycophenolic acid is produced by P. bialowiezense, P. brevicompactum, P. carneum and P. roqueforti. PR-toxin is produced by P. chrysogenum and P. roqueforti. Secalonic acid is produced by P. chrysogenum and P. confertum. The territrems are produced by P. cavernicola and P. echinulatum. Viridic acid is produced by P. nordicum and P. viridicatum, while viridicatumtoxin is produced by P. aethiopicum. The hepatotoxins xanthomegnin, viomellein and vioxanthin are produced by P. clavigerum, P. cyclopium, P. frieii, P. melanoconidium, P. tricolor and P. viridicatum. Apart from these mycotoxins several alkaloids, such as festuclavine, rugulovasine, and roquefortine C are also produced by several species in Penicillium subgenus Penicillium. In most cases these extrolites are produced consistently by all isolates examined in a species. The important antibiotic penicillin is produced by all members of series Chrysogena and P. griseofulvum. The cholesterol-lowering agent compactin is produced by P. so A large number of interesting lead-compounds are produced by species in the subgenus.
Penicillium expansum: Consistent production of patulin, chaetoglobosins, and other secondary metabolites in culture and their natural occurrence in fruit products

Penicillium expansum is known for its destructive rot and patulin production in apple juice. According to the literature, P. expansum can, among other compounds, produce citrinin, ochratoxin A, patulin, penitrem A, and rubratoxin B. In this study the qualitative production of metabolites was examined using TLC (260 isolates), HPLC (85 isolates), and MS (22 isolates). The results showed that none of the 260 isolates produced ochratoxin A, penitrem A, or rubratoxin B. However, chaetoglobosin A and communesin B were produced consistently by all 260 isolates. Patulin and roquefortine C were produced by 98% of the isolates. Expansolides A/B and citrinin were detected in 91 and 85% of the isolates, respectively. Chaetoglobosins and communesins were detected in naturally infected juices and potato pulp, whereas neither patulin nor citrinin was found. Because most P. expansum isolates produce patulin, citrinin, chaetoglobosins, communesins, roquefortine C, and expansolides A and B, foods contaminated with this fungus should ideally be examined for chaetoglobosin A as well as patulin.

General information
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology
Authors: Andersen, B. (Intern), Smedsgaard, J. (Intern), Frisvad, J. C. (Intern)
Pages: 2421-2428
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Agricultural and Food Chemistry
Volume: 52
Issue number: 8
ISSN (Print): 0021-8561
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 1.343 SJR 1.269
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.45 SJR 1.305 SNIP 1.343
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.224 SNIP 1.245 CiteScore 3.23
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.267 SNIP 1.413 CiteScore 3.25
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.43 SNIP 1.47 CiteScore 3.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
The p450 monooxygenase BcABA1 is essential for abscisic acid biosynthesis in Botrytis cinerea

The phytopathogenic ascomycete Botrytis cinerea is known to produce abscisic acid (ABA), which is thought to be involved in host-pathogen interaction. Biochemical analyses had previously shown that, in contrast to higher plants, the fungal ABA biosynthesis probably does not proceed via carotenoids but involves direct cyclization of farnesyl diphosphate and subsequent oxidation steps. We present here evidence that this "direct" pathway is indeed the only one used by an ABA-overproducing strain of B. cinerea. Targeted inactivation of the gene bccpr1 encoding a cytochrome P450 oxidoreductase reduced the ABA production significantly, proving the involvement of P450 monooxygenases in the pathway. Expression analysis of 28 different putative P450 monooxygenase genes revealed two that were induced under ABA biosynthesis conditions. Targeted inactivation showed that one of these, bcaba1, is essential for ABA biosynthesis: DeltaBcaba1 mutants contained no residual ABA. Thus, bcaba1 represents the first identified fungal ABA biosynthetic gene.

General information
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology
Authors: Siewers, V. (Ekstern), Smedsgaard, J. (Intern), Tudzynski, P. (Ekstern)
Automated data processing of high-resolution mass spectra

There has been an almost explosive growth in performance and applications of Electrospray Ionization (ESI) Time of Flight (TOF) mass spectrometry, which today is one of the most efficient tools for screening of metabolites in complex bio-samples. Most efficiently ESI-MS can be used by directly infusion of crude extracts into the source taking advantage of the high sensitivity, high mass resolution and accuracy and the limited fragmentation. Unfortunately, there has not been a comparable development in the data processing techniques to fully exploit gain in high resolution and accuracy of the massive amounts of data. We present an automated data processing method to quantitatively compare large numbers of spectra from the analysis of complex mixtures, exploiting the full quality of high-resolution mass spectra. By projecting all detected ions - within defined intervals on both the time and mass axis on to a fixed one-dimensional array, we obtain a vector that can be used directly as input in multivariate statistics or library search methods. We demonstrate that both cluster- and discriminant analysis as well as PCA (and related methods) can be applied directly on mass spectra from direct infusion analyses of crude extract to find the relationship between species from several species terverticillate Penicillium, and also that the ions responsible for the segregation can be identified. Furthermore the process can automate the process of detecting unique species and unique metabolites.

Flavor release measurement by atmospheric pressure chemical ionization ion trap mass spectrometry, construction of interface and mathematical modeling of release profiles

An instrumental on-line retronasal flavor analysis was developed to obtain information about the release of flavor compounds in expired air from humans during eating. The volatile flavor compounds were measured by ion trap mass spectrometry with an atmospheric pressure chemical ionization source (APCI). An interface was designed to sample the breath directly from the nose. The repeat-ability in vitro for seven different flavor compounds came out with relative standard derivation less than 10% in most cases, which is acceptable. In vitro quantification was carried out by a determination of the concentration in the gas phase over a flavor solution by GC/MS, followed by measurements of intensities by the APCI ion trap. Ion suppression by acetone in the breath was negligible at concentration levels relevant in these experiments. The instrumental limits of detection for menthone and menthol coincide with that of the flavor detection threshold. An application study on the release of menthone and menthol from chewing gum by a group of six test persons was performed. Flavored chewing gum was used as a model matrix because of the long chewing periods and the simplicity of the system. It is concluded that the interface and the method can be used to measure breath from the nose. A mathematical model of the data was developed to give a quantitative method for description and characterization of the release of flavor compounds. The release profiles consisted of two sequences, one for a chewing period, and one for a phasing out process. The proposed method for modeling provided a reasonable description of the release process. In addition flavor compounds, this new interface and mathematical application could provide information on chemicals in the human breath which could be interesting, for example, within medical diagnosis.
From Fungal Biodiversity to Novel Natural Products - using intelligent screening based on mass and UV spectrometric methods

General information
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology
Authors: Larsen, T. O. (Intern), Hansen, M. E. (Intern), Smedsgaard, J. (Intern)
Publication date: 2003
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 155075
Publication: Research › Paper – Annual report year: 2003

Fungal metabolite screening: database of 474 mycotoxins and fungal metabolites for dereplication by standardised liquid chromatography-UV-mass spectrometry methodology
A standardised LC-UV-MS micro-scale method for screening of fungal metabolites and mycotoxins in culture extracts is presented. The paper includes data for detection and dereplication of >400 fungal metabolites to facilitate detection and identification when standards are not available. The data also shows the types of components that can be analysed by positive electrospray (ESI+) mass spectrometry (MS) along with common fragments and adducts of these, as well as giving suggestions on whether UV or ESI+ -MS methods should be used. Examples of dereplication of penitrems and macro-cyclic trichothecenes, and detection of several novel compounds are shown. This was done by UV spectroscopy combined with accurate mass determination of adduct and fragment ions obtained by high-resolution orthogonal time-of-flight MS.

General information
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology
Authors: Nielsen, K. F. (Intern), Smedsgaard, J. (Intern)
Pages: 111-136
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Chromatography A
Volume: 1002
Issue number: 1-2
ISSN (Print): 0021-9673
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.212 SJR 1.378
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.97 SJR 1.463 SNIP 1.318
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.693 SNIP 1.398 CiteScore 4.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.823 SNIP 1.507 CiteScore 4.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.006 SNIP 1.613 CiteScore 4.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.298 SNIP 1.697 CiteScore 4.6
ISI indexed (2012): ISI indexed yes
Use of intelligent screening and biocombinatorial libraries in fungal metabolite discovery

General information
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology, Department of Informatics and Mathematical Modeling, Center for Biomedical Microbiology
Authors: Larsen, T. O. (Intern), Hansen, M. A. E. (Intern), Smedsgaard, J. (Intern), Rasmussen, T. B. (Intern), Gibskov, M. (Ekstern), Frisvad, J. C. (Intern)
Publication date: 2003
Event: Poster session presented at 8th Danish Biotechnology Conference.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 46225
Publication: Research - peer-review › Journal article – Annual report year: 2003

Chemical Image Analysis (CIA): Distance based identification

General information
State: Published
Organisations: Department of Informatics and Mathematical Modeling, Center for Microbial Biotechnology, Department of Systems Biology, Image Analysis and Computer Graphics
Authors: Hansen, M. A. E. (Intern), Smedsgaard, J. (Intern), Larsen, T. O. (Intern), Carstensen, J. M. (Intern), Frisvad, J. C. (Intern)
Mikrosvampe leverer ny kemi

General information
State: Published
Organisations: Department of Systems Biology, Department of Informatics and Mathematical Modeling
Authors: Nielsen, K. F. (Intern), Hansen, M. E. (Intern), Larsen, T. O. (Intern), Smedsgaard, J. (Intern), Frisvad, J. C. (Intern)
Pages: 14-17
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: Dansk kemi
Volume: 83
Issue number: 5
ISSN (Print): 0011-6335
Ratings:
ISI indexed (2013): ISI indexed no
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
Web of Science (2007): Indexed yes
Web of Science (2004): Indexed yes
Original language: Danish
Links:
Source: orbit
Source-ID: 58131
Publication: Research › Journal article – Annual report year: 2002

Skimmelsvampe leverer ny kemi

General information
State: Published
Organisations: Department of Systems Biology
Authors: Nielsen, K. F. (Intern), Hansen, M. E. (Intern), Larsen, T. O. (Intern), Smedsgaard, J. (Intern), Frisvad, J. C. (Intern)
Pages: s14-s17
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: Dansk Kemi
Volume: 83
Issue number: 5
ISSN (Print): 0011-6335
Ratings:
ISI indexed (2013): ISI indexed no
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
Web of Science (2007): Indexed yes
Web of Science (2004): Indexed yes
Original language: Danish
Source: orbit
Source-ID: 116740
Publication: Communication › Journal article – Annual report year: 2002
Biochemical characterization of ochratoxin A-producing strains of the genus Penicillium

In order to explore the biochemical scope of ochratoxin A-producing penicillia, we screened 48 Penicillium verrucosum isolates for the production of secondary metabolites. Fungal metabolites were analyzed by high-pressure liquid or gas chromatography coupled to diode array detection or mass spectrometry. The following metabolites were identified: ochratoxins A and B, citrinin, verrucolones, verrucines, anacines, sclerotigenin, lumpidin, fumiquinazolines, alantyripinones, daladin D, dipodazine, penigequinolines A and B, 2-pentanone, and 2-methyl-isoborneol. By use of average linking clustering based on binary (nonvolatile) metabolite data, the 48 isolates could be grouped into two large and clearly separated groups and a small outlying group of four non-ochratoxin-producing isolates. The largest group, containing 24 isolates, mainly originating from plant sources, included the type culture of P. verrucosum. These isolates produced ochratoxin A, verrucolones, citrinin, and verrucines and had a characteristic dark brown reverse color on yeast extract-sucrose agar medium. Almost all of a group of 20 isolates mainly originating from cheese and meat products had a pale cream reverse color on yeast extract-sucrose agar medium and produced ochratoxin A, verrucolones, anacines, and sclerotigenin. This group included the former type culture of P. nordicum. We also found that P. verrucosum isolates and three P. nordicum isolates incorporated phenylalanine into verrucine and lumpidin metabolites, a finding which could explain why those isolates produced relatively lower levels of ochratoxins than did most isolates of P. nordicum.

General information
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology, Center for Biomedical Microbiology
Authors: Larsen, T. O. (Intern), Svendsen, A. (Intern), Smedsgaard, J. (Intern)
Pages: 3630-3635
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied and Environmental Microbiology
Volume: 67
Issue number: 8
ISSN (Print): 0099-2240
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Web of Science (2015): Indexed yes
Scopus rating (2016): CiteScore 4.08
BFI (2014): BFI-level 2
Web of Science (2014): Indexed yes
Scopus rating (2015): SJR 1.891 SNIP 1.308 CiteScore 4.14
BFI (2013): BFI-level 2
Web of Science (2013): Indexed yes
Scopus rating (2013): SJR 1.899 SNIP 1.414 CiteScore 4.25
ISI indexed (2013): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2012): SJR 1.975 SNIP 1.429 CiteScore 4.29
ISI indexed (2012): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2011): SJR 1.914 SNIP 1.455 CiteScore 4.12
ISI indexed (2011): ISI indexed yes
Web of Science (2010): Indexed yes
Scopus rating (2010): SJR 1.887 SNIP 1.436
Consistent production of penigequinolate A and B by Penicillium scabrosum

General information
State: Published
Organisations: Department of Biotechnology, University of Copenhagen
Authors: Larsen, T. O. (Intern), Smedsgaard, J. (Intern), Frisvad, J. C. (Intern), Anthoni, U. (Ekstern), Christophersen, C. (Ekstern)
Pages: 329-332
Publication date: 1999
Main Research Area: Technical/natural sciences

Publication information
Journal: Biochemical Systematics and Ecology
Volume: 27
Issue number: 3
ISSN (Print): 0305-1978
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.679 SJR 0.373
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.405 SNIP 0.719 CiteScore 1.13
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.396 SNIP 0.732 CiteScore 1.14
BFI (2014): BFI-level 1  
Scopus rating (2014): SJR 0.375 SNIP 0.824 CiteScore 1.1  
BFI (2013): BFI-level 1  
Scopus rating (2013): SJR 0.44 SNIP 0.951 CiteScore 1.32  
ISI indexed (2013): ISI indexed yes  
BFI (2012): BFI-level 1  
Scopus rating (2012): SJR 0.427 SNIP 0.815 CiteScore 1.25  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 1  
Scopus rating (2011): SJR 0.436 SNIP 0.809 CiteScore 1.11  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 1  
Scopus rating (2010): SJR 0.499 SNIP 1.053  
BFI (2009): BFI-level 1  
Scopus rating (2009): SJR 0.525 SNIP 0.957  
Web of Science (2009): Indexed yes  
BFI (2008): BFI-level 1  
Scopus rating (2008): SJR 0.488 SNIP 0.892  
Web of Science (2008): Indexed yes  
Scopus rating (2007): SJR 0.453 SNIP 1.012  
Web of Science (2007): Indexed yes  
Scopus rating (2006): SJR 0.506 SNIP 0.889  
Web of Science (2006): Indexed yes  
Scopus rating (2005): SJR 0.537 SNIP 0.92  
Web of Science (2005): Indexed yes  
Scopus rating (2004): SJR 0.508 SNIP 0.852  
Scopus rating (2003): SJR 0.593 SNIP 0.963  
Web of Science (2003): Indexed yes  
Scopus rating (2002): SJR 0.642 SNIP 0.838  
Web of Science (2002): Indexed yes  
Scopus rating (2001): SJR 0.568 SNIP 0.884  
Scopus rating (2000): SJR 0.504 SNIP 0.773  
Web of Science (2000): Indexed yes  
Scopus rating (1999): SJR 0.503 SNIP 0.88  

Original language: English  
DOIs:  
10.1016/S0305-1978(98)00078-7  
Source: orbit  
Source-ID: 173367  
Publication: Research - peer-review » Journal article – Annual report year: 1999

Full second order chromatographic/spectrometric data matrices for automated sample identification and component analysis by non-data-reducing image analysis

A data analysis method is proposed for identification and for confirmation of classification schemes, based on single- or multiple-wavelength chromatographic profiles. The proposed method works directly on the chromatographic data without data reduction procedures such as peak area or retention index calculation. Chromatographic matrices from analysis of previously identified samples are used for generating a reference chromatogram for each class, and unidentified samples are compared with all reference chromatograms by calculating a resemblance measure for each reference. Once the method is configured, subsequent sample identification is automatic. As an example of a further development, it is shown how the method allows identification of characteristic sample components by local similarity calculations thus finding common components within a given class as well as component differences between classes from the reference chromatograms. This feature is a valuable aid in selecting components for further analysis, The identification method is demonstrated on two data sets: 212 isolates from 41 food-borne Penicillium species and 61 isolates from 6 soil-borne Penicillium species. Both data sets yielded over 90% agreement with accepted classifications. The method is highly accurate and may be used on all sorts of chromatographic profiles. Characteristic component analysis yielded results in
good agreement with existing knowledge of characteristic components, but also succeeded in identifying new components as being characteristic.

**General information**
State: Published
Organisations: Department of Biotechnology, Technical University of Denmark
Authors: Nielsen, N. V. (Ekstern), Smedsgaard, J. (Intern), Frisvad, J. C. (Intern)
Pages: 727-735
Publication date: 1999
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Analytical Chemistry
Volume: 71
Issue number: 3
ISSN (Print): 0003-2700
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.08
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 6
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.79
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 6.01
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 5.8
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 5.86
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Web of Science (2005): Indexed yes
Web of Science (2004): Indexed yes
Web of Science (2003): Indexed yes
Web of Science (2002): Indexed yes
Web of Science (2000): Indexed yes

Original language: English
Source: orbit
Source-ID: 173938
Aligning of single and multiple wavelength chromatographic

The use of chemometric data processing is becoming an important part of modern chromatography. Most chemometric analyses are performed on reduced data sets using areas of selected peaks detected in the chromatograms, which means a loss of data and introduces the problem of extracting peak data from the chromatographic profiles. These disadvantages can be overcome by using the entire chromatographic data matrix in chemometric analyses, but it is necessary to align the chromatograms, as small unavoidable differences in experimental conditions causes minor changes and drift. Previous aligning methods either fail to utilise the entire data matrix or rely on peak detection, thus having the same limitations as the commonly used chemometric procedures. The method presented uses the entire chromatographic data matrices and does not require any preprocessing e.g., peak detection. It relies on piecewise linear correlation optimised warping (COW) using two input parameters which can be estimated from the observed peak width. COW is demonstrated on constructed single trace chromatograms and on single and multiple wavelength chromatograms obtained from HPLC diode detection analyses of fungal extracts. A copy of the C program containing the COW implementation used in this work may be obtained at http://www.imm.dtu.dk/~jmc/papers/cow/cow.html
Aligning on single and multiple wavelength chromatographic profiles for chemometric data analysis using correlation optimised warping

General information
State: Published
Organisations: Department of Biotechnology, Department of Informatics and Mathematical Modeling
Authors: Nielsen, N. V. (Intern), Carstensen, J. M. (Intern), Smedsgaard, J. (Intern)
Pages: 17-35
Publication date: 1998
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of chromatography
Volume: A
Issue number: 805
Original language: English
Source: orbit
Source-ID: 170538
Publication: Research - peer-review › Journal article – Annual report year: 1998

Fungal metabolites in chemotaxonomy

General information
State: Published
Organisations: Department of Biotechnology
Authors: Larsen, T. O. (Intern), Smedsgaard, J. (Intern)
Pages: 389-391
Publication date: 1998

Host publication information
Title of host publication: Natural product analysis. Chromatography,spectroscopy,biological testing
A chemosystematic study of the terverticillate Penicillia using electrospray mass spectrometry

General information
State: Published
Organisations: Department of Biotechnology
Authors: Smedsgaard, J. (Intern)
Publication date: 1997

Micro-scale extraction procedure for standardized screening of fungal metabolite production in cultures

General information
State: Published
Organisations: Department of Biotechnology
Authors: Smedsgaard, J. (Intern)
Pages: 264-270
Publication date: 1997
Terverticillate Penicillia studied by direct electrospray mass spectrometric profiling of crude extracts: I. Chemosystematics

A chemosystematic study of 339 isolates from all known terverticillate Penicillium taxa was performed using electrospray mass spectrometric analysis of extractable metabolites. The mass profiles were made by injecting crude plug extracts made from cultures grown on Czapek Yeast Autolysate agar (CYA) and Yeast Extract Sucrose agar (YES) directly into the electrospray source of the mass spectrometer. A data matrix was made from each substrate by transferring the complete centroid mass spectrum from 200 to 700 amu as 501 variables to individual columns. No attempt was made to identify ions in the mass profile, but a noise level was applied. Cluster analysis using the correlation coefficient resulted in dendrograms where approximately 75% of the included taxa could be considered segregated in distinct clusters. Standard normalized data (mass spectra) resulted in clear clusters, but grouped taxa dominated by a single intense ion together, whereas logarithmized data revealed finer detail but with a shorter distance between clusters. The overall results showed that substantial taxonomic information can be extracted from mass profiles even when the identity of ions is unknown. Ions corresponding to known secondary metabolites were, however, found in all mass profiles. (C) 1997 Elsevier Science Ltd.

General information
State: Published
Organisations: Department of Biotechnology
Authors: Smedsgaard, J. (Intern), Frisvad, J. C. (Intern)
Pages: 51-64
Publication date: 1997
Main Research Area: Technical/natural sciences

Publication information
Journal: Biochemical Systematics and Ecology
**Terverticillate penicillia studied by direct electrospray mass spectrometric profiling of crude extracts II. Database and identification**

A mass spectral database was built using standard instrument software from 678 electrospray mass spectra (mass profiles) from crude fungal extracts of terverticillate taxa within the genus Penicillium. The match factors calculated from searching all the mass profiles stored in the database were used as a distance measure for grouping into taxa. Isolates from more than 75% of the taxa were placed correctly, that is with the highest match factors to other isolates of the their own species by library searches. The database was used as an expert system based on correct identification of the isolates stored according to classical taxonomic criteria. Mass profiles collected in previous studies could be identified by a search in the database. (C) 1997 Elsevier Science Ltd.
Using direct electrospray mass spectrometry in taxonomy and secondary metabolite profiling of crude fungal extracts

General Information
State: Published
Organisations: Department of Biotechnology
Authors: Smedsgaard, J. (Intern), Frisvad, J. C. (Intern)
Pages: 5-17
Publication date: 1996
Main Research Area: Technical/natural sciences

Publication Information
Journal: Journal of Microbiological Methods
Volume: 25
ISSN (Print): 0167-7012
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SJR 0.696 SNIP 0.781
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.05 SJR 0.742 SNIP 0.817
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.819 SNIP 0.86 CiteScore 2.04
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.91 SNIP 1.032 CiteScore 2.28
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.924 SNIP 1.015 CiteScore 2.5
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.867 SNIP 0.997 CiteScore 2.32
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.903 SNIP 0.963 CiteScore 2.29
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.954 SNIP 1.05
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.001 SNIP 1.157
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.936 SNIP 1.023
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.003 SNIP 1.111
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.144 SNIP 1.258
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.976 SNIP 1.13
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.933 SNIP 1.051
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.939 SNIP 1.213
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.887 SNIP 1.008
Scopus rating (2001): SJR 0.87 SNIP 0.888
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.711 SNIP 0.862
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.732 SNIP 0.702
Original language: English
Source: orbit
Source-ID: 167193
Publication: Research - peer-review › Journal article – Annual report year: 1996

Projects:

Sample preparation for screening analyses by high resolution mass spectrometry

National Food Institute
Period: 01/06/2016 → 31/05/2019
Number of participants: 3
PhD Student:
Eyring, Philipp (Intern)
Supervisor:
Smedsgaard, Jørn (Intern)
Main Supervisor:
Frandsen, Henrik Lauritz (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Screening of unknown compounds for food monitoring by high resolution mass spectrometry
National Food Institute
Period: 01/06/2016 → 31/05/2019
Number of participants: 3
Phd Student:
Wang, Tingting (Intern)
Supervisor:
Frandsen, Henrik Lauritz (Intern)
Main Supervisor:
Smedsgaard, Jørn (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Proof of food authenticity by chemical methods

National Food Institute
Period: 01/05/2016 → 30/04/2019
Number of participants: 3
Phd Student:
Wilde, Amelie Sina (Intern)
Supervisor:
Fromberg, Arvid (Intern)
Main Supervisor:
Smedsgaard, Jørn (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Miniaturization of food safety analysis

National Food Institute
Period: 15/03/2016 → 14/03/2019
Number of participants: 3
Phd Student:
Zhai, Demi Shuang (Intern)
Supervisor:
Boisen, Anja (Intern)
Main Supervisor:
Smedsgaard, Jørn (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Predictive food microbiology - new models for safety and quality assessment of a broad range of dairy products

National Food Institute
Period: 01/08/2015 → 18/03/2019
Number of participants: 3
Phd Student:
Martinez Rios, Veronica (Intern)
Supervisor:
Smedsgaard, Jørn (Intern)
Main Supervisor:
Dalgard, Paw (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

SERS based Sensing and Centrifugal Microfluidics
Department of Micro- and Nanotechnology
Period: 15/01/2015 → 03/05/2018
Number of participants: 8
Phd Student:
Durucan, Onur (Intern)
Supervisor:
Matteucci, Marco (Intern)
Rindzevicius, Tomas (Intern)
Schmidt, Michael Stenbæk (Intern)
Main Supervisor:
Boisen, Anja (Intern)
Examiner:
Smedsgaard, Jørn (Intern)
Golcuk, Kurtulus (Ekstern)
Hakonen, Aron (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet

Relations
Publications:
Surface-Enhanced Raman Spectroscopy Integrated Centrifugal Microfluidics Platform
Project: PhD

Identification and risk assessment of unknown contaminants migrating from Food Contact Materials
National Food Institute
Period: 01/12/2014 → 16/05/2018
Number of participants: 6
Phd Student:
Pieke, Eelco Nicolaas (Intern)
Supervisor:
Smedsgaard, Jørn (Intern)
Main Supervisor:
Granby, Kit (Intern)
Examiner:
Vinggaard, Anne Marie (Intern)
Grob, Koni (Ekstern)
Nielsen, Nikoline Juul (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

The presence of spores, micro-particles and metabolites in the indoor environment
Department of Systems Biology
Period: 01/03/2013 → 26/05/2016
Number of participants: 7
Phd Student:
Dosen, Ina (Intern)
Supervisor:
Clausen, Geo (Intern)
Nielsen, Kristian Fog (Intern)
Main Supervisor:
Andersen, Birgitte (Intern)
Examiner:
Smedsgaard, Jørn (Intern)
Miller, J. David (Ekstern)
Stadler, Marc (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)

Relations
Publications:
LC-MS based analysis of secondary metabolites from Chaetomium and Stachybotrys growth in indoor environments
Project: PhD

Intestinal Microbial Metabolomics
National Food Institute
Period: 15/12/2012 → 21/04/2016
Number of participants: 7
Phd Student:
Roager, Henrik Munch (Intern)
Supervisor:
Skov, Thomas Hjort (Intern)
Smedsgaard, Jørn (Intern)
Main Supervisor:
Licht, Tine Rask (Intern)
Examiner:
Sommer, Morten Otto Alexander (Intern)
Dragsted, Lars Ove (Ekstern)
Kleerebezem, Michiel (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Metabolomics study of endocrine disrupting chemicals
National Food Institute
Period: 15/12/2011 → 29/02/2016
Number of participants: 7
Phd Student:
Skov, Kasper (Intern)
Supervisor:
Hadrup, Niels (Intern)
Smedsgaard, Jørn (Intern)
Main Supervisor:
Frandsen, Henrik Lauritz (Intern)
Examiner:
Harrison, Scott James (Intern)
Christensen, Lars Porskjaer (Ekstern)
Dunn, Warwick (Ekstern)

Financing sources
Source: Internal funding (public)
Multivariate and multi-target analysis of UHPLC-TOFMS data for linking of fungal metabolites to their biosynthetic genes and for revealing of crosstalk between pathways

Department of Systems Biology
Period: 01/12/2011 → 25/03/2015
Number of participants: 7
Phd Student:
Klitgaard, Andreas (Intern)
Supervisor:
Andersen, Mikael Rørdam (Intern)
Frisvad, Jens Christian (Intern)
Main Supervisor:
Nielsen, Kristian Fog (Intern)
Examiner:
Smedsgaard, Jørn (Intern)
Sørensen, Jens Laurids (Intern)
Wolfender, Jean-Luc (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Tackling challenges in food safety with lab-on-chip technologies

Department of Micro- and Nanotechnology
Period: 01/10/2009 → 04/04/2013
Number of participants: 6
Phd Student:
Senkbeil, Silja (Intern)
Supervisor:
Smedsgaard, Jørn (Intern)
Main Supervisor:
Kutter, Jörg Peter (Intern)
Examiner:
Rozlosnik, Noemi (Intern)
Merkoci, Arben (Ekstern)
Petersen, Nickolaj Jacob (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Bacterial Impact on Gut Metabolomics
The complex ecosystem of microbes inhabiting the human gut plays an important role for human health. An increasing number of publications show that the composition and activity of our intestinal microbiota affects a number of so-called lifestyle diseases including allergy, obesity, colorectal cancer, and susceptibility to intestinal infections. Additionally, it has become evident that the intestinal microbiota can be modulated by intake of probiotic bacteria or prebiotic carbohydrates. Recently developed approaches allow simultaneous mapping of multiple bacterial metabolites present in gut contents. Our intention is to use these state-of-the-art approaches to elucidate the impact of selected bacteria and carbohydrates, which will be supplied by dietary interventions, on the intestinal metabolome. For this purpose, we will use gnotobiotic animal models, which allow establishment of a simple, well-defined intestinal microbiota.

National Food Institute
Period: 01/08/2009 → 31/07/2011
Number of participants: 4
Project participant:
The complex ecosystem of microbes inhabiting the human gut plays an important role for human health. An increasing number of publications show that the composition and activity of our intestinal microbiota affects a number of so-called lifestyle diseases including allergy, obesity, colorectal cancer, and susceptibility to intestinal infections. Additionally, it has become evident that the intestinal microbiota can be modulated by intake of probiotic bacteria or prebiotic carbohydrates. Recently developed approaches allow simultaneous mapping of multiple bacterial metabolites present in gut contents. Our intention is to use these stage-of-the-art approaches to elucidate the impact of selected bacteria and carbohydrates, which will be supplied by dietary interventions, on the intestinal metabolome. For this purpose, we will use gnotobiotic animal models, which allow establishment of a simple, well-defined intestinal microbiota.

Division of Microbiology and Risk Assessment
National Food Institute
Period: 01/08/2009 → 31/07/2011
Number of participants: 4
Project participant:
Sulek, Karolina (Intern)
Licht, Tine Rask (Intern)
Smedsgaard, Jørn (Intern)
Project Manager, organisational:
Wilcks, Andrea (Intern)

Bacterial Impact on Gut Metabolomics
National Food Institute
Period: 01/08/2009 → 06/02/2013
Number of participants: 6
PhD Student:
Sulek, Karolina (Intern)
Supervisor:
Skov, Thomas Hjort (Intern)
Smedsgaard, Jørn (Intern)
Main Supervisor:
Licht, Tine Rask (Intern)
Examiner:
Bahl, Martin Iain (Intern)
Dragsted, Lars Ove (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Vitamin D in plants
National Food Institute
Period: 01/09/2008 → 29/02/2012
Number of participants: 6
PhD Student:
Jäpelt, Rie Bak (Intern)
Supervisor:
Smedsgaard, Jørn (Intern)
Main Supervisor:
Biosynthesis of cancer-preventive organoselenium compounds by metabolically engineered yeast (YESSEL)

Selenium is an essential element that may have cancer-preventive properties. By using biotechnological research methods, the YESSEL project will develop yeast strains as cell factories for synthesis of organic selenium compounds with promising properties towards prevention of disease. The hypothesis is that yeast can be engineered for improved production of target selenium species such as methylselenocysteine or selenium-sulphur conjugates. Furthermore, the project will test if these target compounds are safer than selenomethionine that is predominant in natural yeast. The project will map, engineer and optimise the metabolic routes in yeast leading to the target selenium compounds. The selenium compounds produced by the various strain modifications of yeasts will be characterised by advanced mass spectrometric methods, such as HPLC-ICP-MS and Q-TOF-MS.

Department of Systems Biology
Division of Food Chemistry
National Food Institute
Laboratoire Bio-inorganique et Environnement
University of Copenhagen

Pharma Nord Aps.
Period: 01/01/2007 → 31/12/2009
Number of participants: 11
Project participant:
Olsson, Lisbeth (Intern)
Smedsgaard, Jørn (Intern)
Lobinski, Ryszard (Ekstern)
Krath, Britta (Ekstern)
Dragsted, Lars Ove (Ekstern)
Vanelli, Valeria (Ekstern)
Paulin, Helge (Ekstern)
Moesgaard, Sven (Ekstern)
Nellemann, Christine (Intern)
Sloth, Jens Jørgen (Intern)
Project Manager, organisational:
Larsen, Erik Huusfeldt (Intern)

Carry-Over of Mycotoxins from Cattle Feed into Dairy Products

Department of Systems Biology
Number of participants: 5
Phd Student:
Storm, Ida Marie Lindhardt Drejer (Intern)
Supervisor:
Smedsgaard, Jørn (Intern)
Main Supervisor:
Thrane, Ulf (Intern)
Examiner:
O'Kiely, Pádraig (Ekstern)
Schnürer, Johan (Ekstern)

**Financing sources**
- Source: Internal funding (public)
- Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
- Project: PhD

**Metabolomanalyse**
Department of Systems Biology
- Period: 01/03/2003 → 07/11/2008
- Number of participants: 6
- Phd Student: Højer-Pedersen, Jesper Juul (Intern)
- Supervisor: Smedsgaard, Jørn (Intern)
- Main Supervisor: Nielsen, Jens (Intern)
- Examiner: Larsen, Thomas Ostenfeld (Intern)
- Arneborg, Nils (Ekstern)
- Heinemann, Matthias (Ekstern)

**Financing sources**
- Source: Internal funding (public)
- Name of research programme: DTU-lønnet stipendie
- Project: PhD

**Multivariate Statistics in Predictive Biotechnology**
The aims of the studies are based on the main hypothesis that the combination of multivariate statistics and image analysis of features can be used as a tool in (visual and chemical) database identification processes within isolates from the fungal genera Penicillium and Aspergillus. Databases of functional characteristics are expected to be complementary to the known DNA-sequence based databases. The identification is based on visual as well as secondary metabolite profiles. Secondary metabolites are end products of the bio-chemical processes that take place within cells of all living organisms, and they are therefore indirectly descriptive of the cells metabolic processes. If different cells use different processes, there will also be a difference in the variety of metabolites produced. Furthermore the chemical variation in the metabolites can be directly related to ecology and habitat.

Department of Informatics and Mathematical Modeling

Department of Biotechnology
- Period: 01/01/2000 → 31/12/2003
- Number of participants: 4
- Project participant: Carstensen, Jens Michael (Intern)
- Frisvad, Jens Christian (Intern)
- Smedsgaard, Jørn (Intern)

**Use of secondary metabolites and volatiles from filamentous fungi in quality assessment of foods**
Chemical and spectrometric methods, viz. HPLC with diode array detection, flow injection electrospray mass spectrometry and capillary electrophoresis have been used in projects on the chemotaxonomy of species in the genera Aspergillus, Penicillium, Fusarium, Alternaria and Trichoderma. Chemometric methods have been used for the evaluation of the resulting chemotaxonomic data. Based on the results of the current investigations of different series in these genera, we have started to evaluate which secondary metabolites can be used as specific indicators of fungal growth. This is based on knowledge of the normal fungi of the different foods and the chemical and spectrometric characteristics of the different secondary metabolites combined with data on possible interferences from the food matrix. While several chemical analytical methods have been developed for particular mycotoxins in foods, determination of the whole profiles of mycotoxins and other secondary metabolites in foods have rarely been attempted. We wish to detect which mycotoxins are to be expected in different foods and find specific sensitive indicators of their presence rather than developing accurate multi-mycotoxin methods with optimal recovery of all mycotoxins.
Anvendelse af LC-MS til specifik Bestemmelse af skimmelsvampe metabolitter i cerealier

Department of Systems Biology
Period: 01/04/1992 → 14/01/1996
Number of participants: 2
PhD Student:
Smedsgaard, Jørn (Intern)
Main Supervisor:
Frisvad, Jens Christian (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Program-stipendium
Project: PhD

Activities:

32nd Mycotoxin Workshop: Mycotoxins and other secondary metabolites in maize silage
Period: 14 Jun 2010
Jørn Smedsgaard (Speaker)
National Food Institute
Division of Food Chemistry

Description
Place: Technical University of Denmark
Documents:
2010 Presentation 32nd Mycotoxin Workshop DTU_Rasmussen_Mycotoxins and other secondary metabolites in maize silage.pdf

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Press clippings:

Fremtidige kompetencebehov for laboranter
Jørn Smedsgaard
05/05/2017
National Food Institute, Research Group for Analytical Food Chemistry

Media coverage (1)

Fremtidens kompetencebehov for laboranter
05/05/2017
Laboranten, Denmark, Print
Gunnar Lomborg
Jørn Smedsgaard
National Food Institute, Research Group for Analytical Food Chemistry
Press / Media
Meget høje indhold af PCB fundet i hvaler.
Jørn Smedsgaard
12/01/2016

Subject
Meget høje indhold af PCB fundet i hvaler.
National Food Institute, Research Group for Analytical Food Chemistry

Media contribution (1)

Meget høje indhold af PCB fundet i hvaler.
12/01/2016
Videnskab.dk, Web
Charlotte Price Persson
Jørn Smedsgaard
National Food Institute, Research Group for Analytical Food Chemistry
Press / Media

DTUs sektorudviklingsrapport for Big Data der kommer den 28/10 2015
Jørn Smedsgaard
28/10/2015

Subject
DTUs sektorudviklingsrapport for Big Data der kommer den 29/10 2015
National Food Institute, Research Group for Analytical Food Chemistry

Media contribution (1)

DTUs sektorudviklingsrapport for Big Data der kommer den 29/10 2015
28/10/2015
DR2 Dagen, Television
Malte
Jørn Smedsgaard
National Food Institute, Research Group for Analytical Food Chemistry
Press / Media

Test på æg
Jørn Smedsgaard
07/06/2013
National Food Institute, Division of Food Chemistry

Media contribution (1)

Test på æg
07/06/2013
DR Detektor, Print
Tine Maria Borresø
Jørn Smedsgaard
National Food Institute, Division of Food Chemistry
Press / Media