Corporate Poster Session

P-001

Software For Pathway Focused Multi-Omics Analysis

Steven Fischer, Agilent Technologies

We have developed data analysis tools and workflows to facilitate the analysis of metabolomics, genomics and proteomics data in a new Integrated Biology software. Starting with the assumption that the researcher is interested in translational biology, a more directed approach to data mining and interpretation can be taken. We will demonstrate a metabolomics workflow that is based on pathway knowledge. The results of the metabolomics analysis can be visualized in a pathway analysis software package

P-002

The impact of high-resolution MS and NMR techniques on the discovery of novel natural products from myxobacteria

Aiko Barsch, Bruker Daltonik GmbH

Microbial natural products represent a rich and still largely untapped resource for novel chemical scaffolds. Their discovery enables characterization of the underlying biosynthetic pathways and at the same time chances are good to find compounds with potent biological activity. UHPLC-coupled UHR-TOF mass spectrometry and LC-NMR represent most valuable analytical tools for the discovery of novel natural products, efficient dereplication, comprehensive mining of metaboloms and rapid structure elucidation of novel metabolites.

P-003

Metabolomic Fingerprinting of Three Strains of Rats Using Ultra-High Resolution TOFMS

Jeffrey S Patrick, LECO Corporation

Metabolomic profiling in animals is a challenging and rapidly growing area of research with the objective of providing potential dynamic markers of disease states. This presentation will demonstrate the use of UHPLC and GC high resolution time-of-flight mass spectrometry as well as GCxGC-TOFMS in the comparative analysis of metabolomic profiles of serum from three strains of Zucker rats. High-speed acquisition capabilities facilitate substantially faster analysis times than those typically achieved in serum metabolomics, with minimal loss of coverage.

P-004

Re-integration Across Samples in Sample Sets for Better Accuracy in Metabolite Analysis

Sarada Tanikella, Metabolon, Inc.

With high throughput and sensitivity, GC/MS and UHPLC/MS/MS2 are widely used in metabolomic studies, and such high throughput analyses produce a large amount of raw scan data that need to be automatically processed from sample to sample. Ion peak re-integration across all samples in the sample set is a novel technique capable of detecting and correcting such inconsistency and therefore achieving better accuracy in metabolite analysis.

P-005

Applying Q Exactive Benchtop Orbitrap LC-MS/MS and SIEVE 2.0 Software for Cutting-Edge Metabolomics and Lipidomics Research

Yingying Huang, Thermo Fisher Scientific

This poster describes the application of a unique LC-MS/MS system comprised of a UHPLC, a Q Exactive hybrid quadrupole-Orbitrap mass spectrometer, and application-specific software (SIEVE, Mass Frontier, and TraceFinder) to a highly diverse group of differential analysis studies. The performance of the entire system is demonstrated through the metabolomic analyses of lean and obese Zucker rat serum and California wine, and lipidomic analysis of mitochondrial lipids in yeast.

P-006

Multidimensional lipidomics for untargeted and targeted analyses

Giuseppe Astarita, Waters Corporation

One of the main challenges for a global lipid analysis – lipidomics – is the separation of the wide array of lipid species present in biological samples. The ability to perform multi-dimensional separations in one injection prior to MS analysis could improve our ability to map and measure complex lipid mixtures. Here, we present a complete workflow for the extraction, separation, identification and quantification of lipid species in complex matrices using HILIC in combination with ion mobility MS.

Medicinal Metabolomics

P-007

Potent Inhibitor of 17β-Hydroxysteroid Dehydrogenase Type 1 Causes Changes in Metabolite Profile in Breast Cancer Cell Lines as Revealed by Targeted Metabolomics

Pauline Banachowicz, Helmholtz Zentrum Muenchen

We tested a new steroid metabolism inhibitor and a less potent carbenexolone, with T47D and MCF-7) cancer cell lines. Targeted metabolomics analysed amino acids, acylcarnitines, phospholipids, hexoses and sphingomyelins by high throughput LC-MS/MS. Significant changes in metabolite profile of challenged cells were found.

P-008

A comprehensive understanding of thioTEPA metabolism in the mouse using UPLC-ESI-QTOFMS-based metabolomics

Li Fei, National Institutes of Health

To understand the mechanism of thioTEPA-induced encephalopathy, the metabolism of thioTEPA was comprehensively investigated using UPLC-ESI-QTOFMS based-metabolomics. The result indicated that SCMC and TDGA were produced from thioTEPA from two novel metabolites 1,2,3-trichloroTEPA (VII) and dechloroethyltrichloroTEPA (VIII). The increased amylase and decreased glucose in the mice serum treated by thioTEPA and TDGA suggested that the increased TDGA might be responsible for high-dose thioTEPA-induced encephalopathy in the clinic.

P-009

Metabolomic map and bioactivation of noscapine, a promising anti-tumor drug

Zhongze Fang, National Cancer Institute, National Institutes of Health

The present study aims to investigate the metabolism and bioactivation of noscapine, a promising anti-tumor drug. Many phase I metabolites and glucuronides were detected. Cytochrome P450 (CYP2C9, CYP3A4/5, CYP1A1/2,CYP2C19), flavin-containing monooxygenase 1 and UDP-glucuronosyltransferases (UGT1A1, UGT1A3 and UGT1A9) were involved in noscapine metabolism. The bioactivation of noscapine occurred in vitro but not in vivo.

P-010

Metabolomic Study of Neuropeptide Y and Corticotropin-Releasing Treatment in an Immortalized Rat Hypothalamic Cell Line

Sumitra Pati, Claflin University

We sought to determine the metabolites produced by treatment with neuropeptides (NPY and/or CRF) to study the effect of activation and inhibition of metabolic pathways in a rat hypothalamic cell line. To study changes in intra and extra cellular metabolites in response to these treatments, 1D 1H-NMR spectra of both hydrophilic cell extracts and growth medium were recorded. PCA indicated that changes in intracellular concentrations of several metabolites were effected by NPY and/or CRF treatment.

P-011

Rifampicin-Induced Urinary Steroid Profiles in Healthy Male Subjects using UPLC-TOFMS- and GC-MS-based metabolomics

Kim Bora, Seoul National Univ.

Activation of the pregnane X receptor (PXR) is associated with increased the expression of metabolic enzymes and transporters involved in the metabolism of xenobiotics and endobiotics and is commonly targeted to the drug-drug interactions. The aim of this study is to identify endogenous biomarkers of PXR activation in human, rifampicin, a strong PXR activator.

P-012

A Metabolomic Study of Traditional Chinese Medicine with Cold and Hot nature

Jing Guo, Keio University

Chinese medicinal herbs are classified into four groups based on their hot, warm, cool, or cold natures. The objective of this study is to explore the difference in metabolic properties between medicinal herbs with hot and cold natures using capillary electrophoresis time-of-flight mass spectrometry (CE-TOFMS). 2,5-dihydroxybenzoate, 2-hydroxypentanoate, N-acetyl glucosamine and uracil showed significantly higher concentrations in herbs with hot nature. And glutamine was found higher in herbs with cold nature.

Medicinal Metabolomics

P-013

Global Metabolomics Profiling of Human Urine Reveals Change in Endogenous Metabolites after Metformin and Pioglitazone Administration

HyangHee Yang, Seoul National University College of Medicine

Metformin and Pioglitazone are oral antihyperglycemic agents. The aim of this study is to identify the changes of urinary endogenous metabolites by metformin or pioglitazone treatment using untargeted metabolomic multivariate analysis. High abundance correlation of retinyl β-glucuronide and L-pipecolic may contribute to endogenous metabolism according to insulin regulation in treatment group. Therefore, these metabolites could be considered as biomarkers for treatment effects of metformin or pioglitazone.

P-014

Pharmacometabolomics of Ginseng Extracts on Vascular Injury Induced by Chronic Homocysteine Treatment

Ed Lui, University of Western Ontario

Homocysteine (Hcy) is an independent risk factor for vascular diseases. Several studies have demonstrated the protective nature of ginseng against vascular injury; however, the underlying mechanism(s) are poorly understood. We use a pharmacometabolomics approach to study endogenous metabolite responses. HRMS workflow was used for simultaneous non-targeted global metabolite profiling and hypothesis-driven targeted data processing. The objective is to interpret metabolite profile from the multivariate analysis, identify and quantify known markers of vascular injury by Hcy.

P-015

Metabolomics Analysis of Mature Leukemia Blasts and Leukemia Initiating Cells Using High Resolution Accurate Mass Spectrometry

Ahmed Aman, Ontario Institute for Cancer Research

The objective of this metabolomics study is to identify any potential endogenous metabolite differences between acute myeloid leukemia (AML) initiating cells, progenitor cells and terminally differentiated blasts using a high resolution accurate mass spectrometry and non-targeted data acquisition with multiple data processing approach. The ultimate goal is to identify potential biomarkers and novel drug targets for AML.

P-016

An LC-MS assay for measurement of L-asparaginase kinetic parameters

Preeti Purwaha, MD Anderson Cancer Center

In order to characterize asparaginase/glutaminase kinetics of our newly synthesized L-ASP analogs, we have developed an LC-MS MRM assay to optimize quantitation of the key metabolites from this pathway, Asn, Asp, Gln, and Glu. Standards were used to optimize LC-MS conditions on an Agilent 1290 infinity UHPLC coupled to Agilent 6460 triple quadrupole mass spectrometer. This assay enables sensitive and reproducible quantitation of the four amino acids with a large linear dynamic range.

P-017

Untargeted Plasma Metabolite Profiling Suggests a Relative NO-sparing Action of Nebivolol vs. Metoprolol in Patients Receiving β-blocker Drug Therapy for Hypertension

Qiuying Chen, Weill Cornell Medical College

Untargeted metabolite profiling offers the potential to discover both on-target and off-target actions of therapeutic drugs. The present clinical study evaluated the metabolic consequences of treatment with either of two beta-adrenergic receptor blockers in clinical use for hypertension therapy, nebivolol vs. metoprolol. Findings revealed multiple significant differences in drug effects, including a lesser potential of nebivolol to promote endothelial dysfunction by increasing plasma levels of the endogenous NO synthase inhibitor, asymmetric dimethylarginine.

Medicinal Metabolomics

P-018

GC-TOF-MS Metabolomic Study on a New Model of Streptozocin-sodium Chloride-induced Diastolic Heart Failure

Dong Fangting, National Center of Biomedical Analysis

Streptozocin(STZ) and sodium chloride induced diastolic heart failure(DHF) model was studied by a GC-TOF-MS based metabolomics study to characterize the changes in metabolic pathway. The acquired data were exported to SIMCA-P Plus software for further multivariate recognition analysis. Significant differences were founded in the plasma of the DHF among the different models. The potential biomarkers for DHF were demonstrated, and might be the new clues for the pathogenesis and early diagnosis.

P-019

Metabolite Profiling: an Encouraging Novel Diagnostic Tool in Heart Failure

Henning Witt, Metanomics GmbH

Chronic heart failure has become the most prevalent cardiovascular disorder in the ageing population of western countries. However, specific and reliable biomarkers are missing to diagnose CHF early, to predict clinical outcome and to guide therapeutic intervention. We therefore aimed to identify metabolomic markers to distinguish heart failure patients from healthy controls and to evaluate exercise testing for improving diagnostic performance.

P-020

Metabolomics as a Tool for Understanding and Improving Protein Expression in the CHO System

Michael Reily, Bristol-Myers Squibb Co.

NMR-based metabolomics analysis was performed on supernatants and cell pellets of recombinant CHO cells expressing therapeutic proteins. The cells grown at different scales and processes present different metabolomic patterns and time trajectories. Endpoints such as cell count, viability or titer were also measured throughout the culture period. Quantitative analysis allowed us to understand changes in various metabolic pathways, which shed light into culture parameters that can be manipulated to optimize cell growth and protein production.

P-021

Biochemical comparison of two neuronal cell lines using metabolomics.

Ian Mullaney, Murdoch University

Using single-quadrupole GC-MS, we have obtained a baseline metabolic profile in two neuronal cell lines. Cells yielded approximately 200 unique metabolites, while medium extracts yielded approximately 250 metabolites. Principal component analysis showed that the two cell lines, and their media, differed in key areas such as carbohydrates, amino acids and organic acids. The use of these cell lines as biosensors to detect biochemical changes caused by a variety of exogenous compounds will be discussed.

P-022

A GC/MS-based metabolomic approach for identifying the pathway of triflusal response in the urine of healthy individuals

Jeonghyeon Park, Kyungpook National University Hospital

Triflusal is a platelet aggregation inhibitor that inhibits cyclooxygenase-1, and cAMP and cGMP phosphodiesterases in platelets. The aim of this study was to apply the metabolomics approach using GC/MS in the urine samples of healthy volunteers for identifying the pathway of triflusal response. The metabolites, such as pseudouridine, citric acid, phosphoric acid, D-fructose, D-galactose, were significantly decreased or increased. These metabolic phenotypes can be used to understand biochemical pathways that were affected by triflusal.

Medicinal Metabolomics

P-023

Mass Spectrometry-based Metabolomics as a Tool for Cardiac Research: The Effect of Perhexiline on the Myocardial Metabolome in Patients undergoing Cardiac Surgery

Ralf Weber, University of Birmingham

This study analyzed the effect of perhexiline on the myocardial metabolome as part of a clinical trial to improve myocardial protection during coronary artery bypass graft surgery. Full thickness biopsies of the left ventricular wall were obtained from 43 patients (perhexiline n=22, control n=21) prior to ischaemia and analyzed using Fourier transform ion cyclotron resonance mass spectrometry. We found that perhexiline has no significant effect on the mass spectrometry-visible myocardial metabolome in vivo in humans.

P-024

The Role of PPARgamma in the Control of Sebogenesis In Vitro: Prospective for Novel Treatments of Acne

Emanuela Camera, San Gallicano Dermatology Institute

Acne lacks of pharmacological treatments targeting specific lipidogenic pathways, rather than generalized sebum production. Peroxisome proliferators-activated receptor gamma (PPAR[illegible]) can be targeted for the modulation of the sebaceous lipids production. We have investigated the effects of newly designed PPARgamma agonists (GMG-43AC) in regulating sebum biosynthesis in vitro by means of lipidomics approaches. The collected data highlighted the ability of GMG-43AC to interfere with the major pathways of neutral lipids formation and FA biotransformation.

P-025

Pharmacometabolomics Informs Pharmacogenomics

Rima Kaddurah-Daouk, Duke Univeristy Medical Center

The Pharmacometabolomics Research Network was established with funding from NIH with the goal to test the hypothesis that the application of metabolomics analyses and the inclusion of metabolomics data would significantly enhance pharmacogenomic research by providing broad-based, biochemically precise phenotypes capable of supplementing and extending the clinical phenotypes currently used as pharmacogenomic “endpoints”. We will exemplify our approach from metabolomics studies of drugs used for the treatment of neuropsychiatric and cardiovascular diseases.

Environment & Ecology

P-026

Evaluation of NMR Spectroscopy as a Novel Tool for Assessing Stress in Broiler Chickens (Gallus Domesticus)

Karen Machin, University of Saskatchewan

Light is an important management technique in broiler production. Heterophil/Lymphocyte ratio, corticosterone and NMR-based metabolomics was compared in chronically stressed broilers fed a corticosterone diet, birds exposed to 4 photoperiods (14 (L)ight:10 (D)ark, 17L:7D, 20L:4D, 23L:1D) or 4 light intensities (1, 10, 20, 40 Lux). Metabolomics was able to differentiate chronically stressed from control birds. Use of NMR in lighting experiments aided in differentiating among groups that had evidence of compromised welfare, whereas, traditional measures of stress (H/L ratio and CORT) were not good indicators.

P-027

Using Metabolomics to Solve Problems in Environmental Microbiology

Aalim Weljie, University of Calgary

Over the past few years our group has been developing and using metabolomics to study environmental stress in bacteria. Separate studies have provided a metabolic basis for understanding tellurite hyperresistance in a mutant, increased metal resistance in phenotypic variants isolated from a biofilm and differences in the exertion of metal toxicity between planktonic and biofilm cultures. Current work is focusing on understanding the combined toxic effects of both organic and metal pollutants for bioremediation purposes.

P-028

Improvment of Barren Soil Characters By Using Of Blue- Greens.

Monerah Al-Othman, King Saud University

In this study, synthetic and biological soil conditioners were used to screen their abilities to improvise the barren soil characters. These soil conditioners based on treatment of barren soil samples with urea and/or compost as synthetic soil conditioner or by inoculating the soil samples with Spirulina meneghiniana Zanrd. ex Gomon and/or Anabaena oryzae Fritsch as a biological soil conditioner.

P-029

1-D and 2-D NMR-based Metabolomics of Endosulfan and Endosulfan Sulfate to Earthworms in Soil Environments

Jimmy Yuk, University of Toronto

1-D and 2-D NMR-based metabolomics were used to investigate the toxic mode of action (MOA) of an organochlorine pesticide, endosulfan, and its degradation product, endosulfan sulfate, to earthworms, Eisenia Fetida, after sub-lethal soil exposure. PCA scores results reveal a similar trajectory separation of both contaminants to the control and identical metabolites of response were detected. A neurotoxic and apoptotic MOA was delineated and this highlights the potential of NMR-based metabolomics to understand contaminated soil environments.

P-030

1H NMR-based metabolomic analysis of sub-lethal perfluoroalkyl acid exposure to the earthworm Eisenia fetida

Brian Lankadurai, University of Toronto

1H NMR-based metabolomics was used to determine the toxic mode of action of perfluorooctanoic acid (PFOA) and perfluorooctane sulfonate (PFOS) after sub-lethal exposure to Eisenia fetida earthworms. NMR-based metabolomic analysis revealed heightened earthworm responses with higher PFOA and PFOS concentrations. Potential increase in fatty acid oxidation and an interruption of ATP synthesis were observed. This study shows that NMR-based metabolomics shows promise as a powerful ecotoxicological tool for elucidating the mode of action of environmental contaminants.

Environment & Ecology

P-031

Environmental metabolomics approach to alteration of urinary steroid metabolism which prolonged exposure to low concentration of bisphenol-A

Jeongae Lee, Korea Institute of Science and Technology

The present study was designed to analyze urinary steroid and bisphenol-A(BPA). The concentration of estrogen in high concentration level of BPA was increased, while the level of androgen was decreased in women. Especially, hydroxylated estrogens in women were increased, which the activity of 4-hydroxylase was more active than 2-hydroxlase. Prolonged exposure to low concentration of BPA as one of environmental endocrine disrupting chemicals may alter estrogen metabolism by acting as a steroid receptor agonists.

P-032

1H NMR-Based Metabolomics for Determining Changes in Daphnia magna in Response to Three Metal Contaminants in Water

Edward Nagato, University of Toronto

1H NMR was used to determine the metabolome changes in the Daphnia magna, in response to sublethal concentrations of three metal contaminants: copper, lithium and arsenic. It was found that copper accounted for the greatest metabolome change, and arsenic induced the least change. Metabolite concentrations altered in response to the metal stress included alanine, methionine, leucine, lactate valine and betaine. Currently effort is under way to frame these changes in the greater biochemical context.

P-033

Lipidomic Approach to Investigate Systemic Effects of Zinc Oxide Nanoparticles in Serum of Rats via Inhalation

Huiming Lin, Institute of Environmental Health, National Taiwan University, Taipei, Taiwan.

To understand systemic metabolic effects of nano-sized zinc oxide (nZnO), one of the most widely used nano-materials, rats were treated with nZnO particles via inhalation. After rats were exposed to 2 sizes (250 and 35 nm) and 3 concentration of nZnO, blood samples were collected for lipid analysis using UPLC-QTOFMS. Partial least squares discriminant analysis demonstrated lipidome variation among rats treated with different sizes and doses. We intend to identify biomarkers to examine nZnO toxicity.

P-034

Metabolomics in Aquaculture

Tracey Schock, National Institute of Standards and Technology

NMR-based metabolomics is a useful tool for the aquaculture industry. Finfish health was assessed during an alternative feed study which reduced fishmeal inclusion and substituted plant and animal based protein. Metabolomics techniques provided evidence that low fishmeal diets were nutritionally lacking for normal growth and also revealed evidence of a beneficial gut microflora community from a formulated control diet.

P-035

Use of 1H-Nuclear Magnetic Resonance to Investigate the Metabolic Profile of the Freshwater Bivalve Elliptio complanata.

Jennifer Hurley-Sanders, NC State University

We investigate the use of 1H-NMR spectroscopy to describe the metabolome of Elliptio complanata as a preliminary step to better understand freshwater bivalve physiology and metabolic response. Variability between mussels and across tissue types are evaluated using principal components analysis. Tissue type metabolomes are distinctly different and digestive gland varies notably between individuals. The metabolome of E. complanata varies from reported marine species. 1H-NMR is a promising tool for the study of freshwater bivalve metabolism.

Environment & Ecology

P-036

Glycerophosphocholine Profiling of Thermal Fluctuation-Adaptation for a Reef Coral Seriatopora hystrix from the Tide-Induced Upwelling Region in Taiwan

Chuan-Ho Tang, National Museum of Marine Biology & Aquarium

Does oscillating temperature develop coral membrane to face two-sided thermal stresses? The results here, membrane composed of more ether-glycerophosphochlolines and less polyunsaturated ester-glycerophosphochlolines in the coral inhabited in the upwelling region compared to the contrastive region, can be a cue. The membrane of coral tip portion is further composed with more ether-lysoglycerophosphochlolines from the upwelling region. The coral development well in this upwelling region can be correlated with such lipid's biochemical and biophysical roles.

P-037

Sublethal metabolic impacts of a red tide alga on competing phytoplankton

Jessie Roy, Georgia Institute of Technology

We investigated the sublethal impacts of exposure to compounds produced by the harmful alga Karenia brevis on neighboring phytoplankton. Diatoms were grown in co-culture with K. brevis; profiles of polar metabolites from these diatoms were collected using 1H NMR spectroscopy. Principal component analysis showed that exposure to K. brevis led to significant changes in concentrations of aromatic and aliphatic metabolites. Future work will expand upon these preliminary results with mass spectrometry-based metabolomics and proteomics.

P-038

Calanoids as Relevant Model Species for Risk Assessment in the North Atlantic and Barents Sea

Trond Røvik Størseth, SINTEF Fisheries and Aquaculture AS

The micro-crustacean Calanus finmarchicus and other calanoids are key organisms in the north Atlantic Ocean and the Barents Sea. The estimated annual production in the Norwegian Sea of C. finmarchicus alone is 300 million tons. The role of calanoids as model species for the North Atlantic and Barents Sea is discussed. Both sources of calanoids can be used for environmental metabolomics studies and we have observed good and identifiable responses in the metabolome.

Short Abstract Listing

Human Disease and Health Biomarkers I - Metabolomics in Women's and Children's Health

P-039

Characterization of Metabolic Changes During and After Pregnancy by 1H-NMR of Urine from a Large Population-based Cohort Study of Gestational Diabetes in a Multiethnic Population

Daniel Sachse, Department of Medical Biochemistry, University of Oslo

The STORK Groruddalen Research Program is a population-based cohort study of 823 pregnant women with diverse ethnic background. Using 1H-NMR we find that the progression of pregnancy leads to considerable changes of the urinary metabolite profile. Ethnic background has a small but significant influence. Gestational diabetes may lead to an increased excretion of BCAA, sugars and two unidentified compounds, but NMR Metabolomics was unable to predict or trace the condition.

P-040

To waste or not to waste (placental tissue) – that is the question

Warwick Dunn, School of Biomedicine, The University of Manchester

More than 200 million pregnancies are reported each year. The placenta plays an important role during pregnancy including transfer of nutrients and waste products, protection from infection and hormone production. Placental dysfunction can lead to pregnancy complications including pre-eclampsia. The presentation will discuss the application of the placenta (tissue and tissue cultures) to the study of normal pregnancies (normal first trimester biochemical changes) and pregnancy complications (hypoxia, oxidative stress and antiphospholipid antibodies).

P-041

Metabolic Profiling of Human Serum in Relation to the Presence of Human Papillomavirus

Lashia Wilson, Claflin University

NMR-based metabolomics was used to identify and compare the metabolic profiles of serum from South Carolina, college-age, females with and without human papillomavirus (HPV). The serum samples used in this experiment were categorized into five groups corresponding to HPV infection states. Principal component analysis (PCA) indicated the presence of unique metabolic profiles in each of the five groups, and several metabolites were associated specifically with HPV(-) and HPV(+) at initial and final stages.

P-042

NMR based screening of neonatal urines

Manfred Spraul, Bruker BioSpin GmbH

With the high throughput capabilities of modern NMR spectrometers, NMR can deliver targeted and nontargeted results from one measurement of neonate urine in short time, thus combining quantification of a large set of compounds indicative of inborn errors with the statistical analysis of deviations from normality. In this case all kinds of deviations are accessible, be the reason known or unknown. This NMR analysis allows to deliver a general health assessment of the neonate.

P-043

Determination of serum estrogen depurinating DNA-adducts as potential biomarker for breast cancer risk: results from a case-control study

Li Yang, University of Pittsburgh

The goal is to detect and identify serum estrogen depurinating DNA adducts as potential early biomarker of breast cancer. Serum samples from 74 controls, 79 breast cancer cases and 80 high risk subjects (Gail scale > 1.66%) were partially purified by solid phase extraction and analyzed by ultra-performance liquid chromatography-electrospray ionization mass spectrometry. Result show that estrogen dupurinating DNA adducts are significantly higher in cases, high risk group than controls ($p<0.001$).

Short Abstract Listing

Human Disease and Health Biomarkers I - Metabolomics in Women's and Children's Health

P-044

MetaboLipidomics Profiling of Plasma Samples from Human Insulin Resistance in an Obese Population using Ultra Performance LC and Ion Mobility TOF/MS

Isaac Giorgis, Waters Corporations

Here we introduce a simple and rapid UPLC™ ion mobility/time-of-flight MS and novel informatics tools for automated identification of lipids and polar metabolites from a well characterized obese pediatric population (n=30, insulin resistance and insulin sensitive). The use of UPLC coupled to ion mobility provides multiple degrees of orthogonal separation, required for the separation of chromatographically co-eluting isobaric lipids and polar metabolites for confident identification. Preliminary PCA suggests statistically relevant separation between the two cohorts.

P-045

Metabolic Signatures Associated with the Progression of Breast Cancer by Ultra High Pressure Liquid Chromatography Time-of-Flight Mass Spectrometry

Yufeng Jane Tseng, National Taiwan University

Ultra high pressure liquid chromatography combined with time-of-flight mass spectrometry with computational metabolomics techniques was applied to identify metabolites associated with the progression of breast cancer in Taiwanese populations. Serum samples from 38 postmenopausal females with different grades, PR and ER status were analyzed. Identification of differential metabolites between each group was performed. Fourteen metabolites were significantly different between patients in different groups. These metabolites were involved in choline phospholipid metabolism, sphingolipid metabolism and etc.

P-046

Targeted Metabolomics reveal changes in Serum Acylcarnitine profiles in Children and Adolescents with Acute Acetaminophen Toxicity

Sudeepa Bhattacharyya, University of Arkansas for Medical Sciences

Acetaminophen (APAP) is the most common cause of acute liver failure in the US and Great Britain. In this study targeted profiling of serum acylcarnitine levels was performed by liquid chromatography-mass spectrometry in 54 children that were hospitalized following acute APAP intoxication. Our data demonstrate that serum acylcarnitine levels associate with other known markers of APAP-induced liver injury (ALT, APAP-protein adducts) and suggest that fatty-acid β-oxidation may be a component of the toxicity.

P-047

Steroid Metabolic Pathways in Human Breast

Nilesh Gaikwad, University of California

In humans many physiological processes are controlled by steroids but they are also implicated in the development and progression of many diseases. We have performed UPLC-MS/MS based targeted metabolomic analysis on human breast tissue to investigate estrogen anabolic/catabolic pathways. Our results suggest that all major classes of steroids viz. progestins, androgens, cortisones and estrogens, are present in breast tissue. In addition, estrogen derivatives, such as glucuronates, hydroxyestrogens, methoxyestrogens, conjugates and adducts are also detected.

Plant I - Developments in Plant Metabolomics

P-048

Phytochemical profiling of Indian plant Phyllanthus niruri and microbial susceptibility profile against food borne/spoiling pathogens

K Swapna Kumari, Center of Biotechnology

Phytochemical profiling of Phyllanthus niruri was found to contain alkaloids, carbohydrates, glycosides, reducing sugars, fixed oils and fats, phenolic compounds and tannins, saponins and resins as its active constituents. Highest IZD was obtained by Alternaria sp. against acetone extract, followed by ethanol, petroleum ether and benzene. Alternaria sp. was found to be most susceptible to different extract (highest susceptibility index 9.05) and Aspergillus niger was found to be resistant to all extracts.

P-049

Metabolomics Analysis of non-GMO Commercial Maize Lines: A Multisite Study

Vincent Asiago, Pioneer Hi-Bred, DuPont Agricultural Biotechnology

Our study was designed to document the biological variation of many metabolites due to environment, genotype or both. Metabolomic data were collected from grain and forage samples from 50 genetically diverse non-GMO Pioneer maize hybrids grown at six locations in US and Canada. This study demonstrate that the combination of GC/TOF-MS and advanced multivariate analysis is a powerful approach that regulators could use to evaluate substantial equivalence and safety assessments for GM crops.

P-050

Purification and chemical characterization of secondary metabolites from xylem sap of Brassica napus infected with Verticillium longisporum

Husam Ibrahem Aroud, University of Goettingen

Verticillium longisporum (VL) is a soil-borne, phytopathogenic fungus that colonizes xylem vessels of oilseed rape (Brassicas napus).Chemical signals exchanged between plant and pathogen play an important role in the infection. We used differential metabolic profiling to study changes in the occurrence and concentration of secondary metabolites in xylem vessels of infected plants. Several infection-specific metabolites were identified. One of these metabolites with a molecular weight of 612 was purified by Prep-HPLC for structure elucidation.

P-051

NMR Discrimination of Ginseng Landraces

Marc Wolff, Bruker BioSpin GmbH

Raw material from plants vary widely due to agricultural, harvesting, or processing methods. Nuclear Magnetic Resonance (NMR) provides a powerful non-destructive technique for analyzing both pure compounds and mixtures. Efforts are underway to establish a non-targeted quality control screen for plant extracts used as dietary supplements. Such a screen will improve the safety and efficacy to the consumer. Here screening of ginseng extracts is used as an example of discriminating geographically separate and naturally divergent landraces.

P-052

Metabolite Profiling of Curcuma Species Grown in Different Regions by 1H NMR Analysis

Youngae Jung, Korea Basic Science Institue

Metabolite profiling was applied to characterize the differences between Curcuma species (C. aromatica and C. longa) grown in different regions (Jeju-do and Jin-do) by 1H NMR spectroscopy coupled with multivariate analysis. The concentrations of sugars (glucose, fructose, and sucrose) and essential oils (eucalyptol, curdione, and germacrone) were significantly different between the two species. However, the samples from two regions were different mainly in their concentrations of organic acids (fumarate, succinate, acetate, and formate) and sugars.

Short Abstract Listing

Plant I - Developments in Plant Metabolomics

P-053

Dereplication of Brazilian Chrysobalanaceae plant species using Interval MCR-ALS based on recovery of pure compounds from HPLC-DAD-ESI-QToF-MS/MS metabolomics data

Fausto Carnevale Neto, Chemistry Institute - UNESP Araraquara

The dereplication of six Brazilian Chrysobalanaceae plant species with cytotoxic potential was perfomed by combination of Interval Multivariate Curve Resolution (MCR) with on-line high-performance liquid chromatography (HPLC) coupled with a diode array detector (DAD) and a high-resolution electrospray quadrupole time-of-flight tandem mass spectrometer (ESI-QToF-MS/MS) leading to the in situ identification of 30 known metabolites, mainly flavonoids glycosides.

P-054

NMR-based metabolite profiling in potato and rice plants

Yasuyo Sekiyama, NARO Food Research Institute

Nuclear magnetic resonance (NMR) spectroscopy is a powerful, widely used technique in metabolomics. In order to apply NMR techniques to crop metabolomics, we performed metabolite profiling in (1) the leaves of six potato cultivars with different susceptibilities to late blight using 1H-NMR spectra, and (2) rice plants (cultivar Nipponbare) labeled with 13CO2 using 1H-13C heteronuclear single quantum coherence (HSQC) spectra. The 13C incorporation was compared over different sampling days.

P-055

GC-MS based metabolite profiling in microalgae

Rahul Kapoore, The University of Sheffield

Metabolomics aims to quantify all metabolites within an organism, thereby providing valuable insight into the metabolism of cells. Here, we present a novel strategy for harvesting, quenching and extraction procedures for the global GC/MS analysis of microalga. Our work mainly focuses on microalgal species like Chlamydomonas reinhardtii, Dunaleilla salina & Nannochloropsis oculata. We have identified several new metabolites in microalgal species which were not reported in past with the previously published benchmark protocols.

P-056

Strong Metabolite Diversity in Glandular Trichomes of the Wild Tomato Solanum habrochaites

Jeongwoon Kim, Michigan State University

Acylsugars are polyesters with acyl chains on sucrose or glucose produced in secretory glandular trichomes of Solanaceous plants including cultivated tomato. The diversity of acylsugars was assessed for the wild tomato species Solanum habrochaites using liquid chromatography-mass spectrometry. These approaches revealed distinct phenotypic classes varying sugar backbone, numbers and lengths of acyl chains and total acylsugar amount. Chemically similar accessions clustered geographically suggesting that they might have evolved in response to different regional selective pressures.

P-057

How to separate the wheat from the chaff? Exploring Brazilian biodiversity using NMR dereplication techniques.

Ian Castro-Gamboa, IQ-UNESP

New and innovative analytical methods that may shed information towards the composition of complex natural mixtures is critical for bioprospection programs. Our research group has incorporated the use of molecular virtual design using Nuclear Magnetic Resonance (NMR) aiming to increase the understanding of molecular relationships of highly active crude extracts. We have a library of extracts from Cerrado and Atlantic Rainforest specimens as well as endophytic fungi and microorganisms derived from specific rizhosphere habitats.

P-058

Development for VOC profiling of Arabidopsis using HS-SPME-GC-TOF-MS analysis

Yumiko Iizuka, RIKEN PSC

Plants produce various volatile organic compounds (VOCs) to respond toward various factors, e.g., herbivores, nutrition. To identify the kinds of VOCs that can be emitted when the plants are grown under different nutrition condition, we established a method for VOC profiling of Arabidopsis thaliana involving headspace-solid-phase microextraction－gas chromatography－time-of-flight－mass spectrometry (HS-SPME-GC-TOF-MS). The VOC profiles clearly showed a distinct pattern with respect to each condition.

Systems Biology & Pathways

P-059

Metabolomics and Transcriptomics Evaluation of Preclinical Biomarkers of Hepatotoxicity: An Update

Laura Schnackenberg, Biomarkers and Alternative Models Branch,

To discover new biomarkers of hepatotoxicity, metabolomics and transcriptomics evaluated urine, serum, and/or liver tissue from rats dosed with acetaminophen, carbon tetrachloride, felbatol, meloxicam, or penicillin. Histopathology and clinical chemistry data were considered in conjunction with the omics data. Initial results indicated disruptions in several pathways noted previously to be altered after dosing with acetaminophen. Additionally, urinary 2-oxoarginine and serum arginine were identified as potential markers of hepatotoxicity that are inversely correlated with ALT.

P-060

Investigating Anti-radiation Action of Bacillithiol Biosynthesis in Deinococcus radiodurans using Trans-omics Approachs

He-Mi Luan, BGI

We sequenced the 5.4-Mb genome of P. korlenisis using Illumina high-throughput sequencing-based technology and obtained transcriptomic and metabolomic data for D. radiodurans and P. korlenisis with radiation treatment by Illumina HiSeq 2000 and Thermo ORBITRAP platform. On the basis of differential expression analysis of genes and metabolites, key genes and metabolites involved in the pathway of bacillithiol biosynthesis were significantly increased in D. radiodurans. However, P. korlenisis have not found these key genes or metabolites.

P-061

An NMR-Based Metabolomics Approach to Understanding Cold Tolerance in Drosophila melanogaster

Aaron Shepard, Claflin University

Metabolic profiles of male and female samples from a cold-susceptible line of D. melanogaster were analyzed at three time points: before, during, and after induction of chill coma. Results from NMR spectroscopy and PCA showed unique metabolic profiles in each group. Several metabolites were identified to be affected by the cold shock treatment, including a large shift from β-alanine to alanine, which is one of the major end products of anaerobic metabolism in D. melanogaster.

P-062

Pesticide Neurotoxicity: Mechanistic Insight Using a Systems Approach

James Roede, Emory University

Epidemiological studies have reported that repeated exposure to agricultural chemicals is a potential risk factor for developing Parkinson's disease (PD). Using a systems biology approach, specifically the integration of transcriptomics and metabolomics, we aimed to gain further insight into the complex mechanisms of pesticide neurotoxicity in vitro. Integration of transcriptomic and metabolomic data indicated that altered transporter expression and potential redox modification of transporter function resulted in modified amino acid homeostasis and subsequent cell death.

P-063

From metabolomics to the metabolic network: converting metabolite profile into stoichiometric reactions

Raphael Aggio, The University of Auckland

Recently, much attention has been directed towards the use of metabolomics data in the reconstruction of metabolic models. However, there is no well-established methodology for that. We will present a novel function in Matlab that uses metabolite profiles, KEGG database and BLAST to automatically predict and visually display potential enzymes related to the metabolism of a specific organism. Our approach speed up substantially the process of combining metabolomics data with metabolic networks.

P-064

Elucidation of Normal Human Epidermal Keratinocyte (NHEK) Metabolic Pathways using 13C-Stable Isotope Incorporation.

David De Souza, Metabolomics Australia

Normal Human Epidermal Keratinocytes(NHEK) are a model cell line for the study of dermal toxicology. Comparatively little is known about the carbon metabolism of human epidermal cells, with existing research giving conflicting opinions as to whether epidermal metabolism is aerobic or anaerobic. Here, we investigate the metabolism of cultured NHEK cells using 13C-stable isotope tracer approaches and analysis of intracellular metabolites by gas chromatography-mass spectrometry.

Systems Biology & Pathways

P-065

Bayesian Network for Identification of Aberrant Metabolic Pathways

Jinlian Wang, Georgetown University

We investigate a Bayesian network-based approach to analyze changes of metabolic pathways by using various sources of data including protein-protein interaction, gene ontology, and literature. The proposed approach is used to identify aberrant metabolic pathways in human hepatocellular carcinoma (HCC). The method leads to identification of pathways relevant to HCC development and progression. We believe that the integration of high-throughput omics data provides better understanding of the relevant mechanisms, targets, and biomarkers of HCC.

P-066

Metabolomics for the identification of pathways of toxicity: Study of developmental neurotoxicity in rat primary aggregating brain cell cultures

Mounir Bouhifd, The Johns Hopkins University, Bloomberg School of Public Health

we aim to develop an in vitro approach using metabolomics and transcriptomics for development neurotoxicity assessment. Our goal is to identify critical pathways based on a systems toxicology approach relying on transcriptomics and metabolomics outcomes. We will show the workflow strategy and the quality control procedures used to deal with such complex data. The results of mass spectrometry based metabolomics experiments will also be presented.

P-067

Metabolic Perturbations of Ovarian Cancer Cells

Kathleen Vermeersch, Georgia Institute of Technology

Despite some targeted study of cancer metabolism, its systems-level dynamics remain unexplored. To explore the systems-level dynamics of cancer metabolism, the dynamic responses of epithelial ovarian cancer cells to perturbations in vitro are profiled. The perturbations reflect biological stresses that normally occur in cancer. Extracellular and intracellular samples are gathered over multiple days and analyzed using gas chromatography-mass spectrometry. The results of these experiments will determine the metabolites that are altered by the biological perturbations.

P-068

Elucidating Protein-Metabolite Interactions via Small Molecule Microarrays

McKenzie Smith, Georgia Institute of Technology

A broad understanding of regulatory interactions in metabolism is needed in order to allow a true systems biology-based approach to metabolic engineering. Small molecule microarrays and a complementary in vitro metabolite binding assay approach will allow for massively-parallel characterization of allosteric regulatory interactions in Saccharomyces cerevisiae. This information will facilitate the construction of a systems-level mathematical model of yeast metabolism.

P-069

UHPLC-SRM Method for Rapid Analysis of Short AcylCoAs in E.coli Lysates. Application to Synthetic Biology Rational Pathway Optimization

Alex Apffel, Agilent Laboratories

The Acetyl-CoA node represents an important, highly regulated control point in central metabolism and thus represents a key parameter for monitoring the metabolic state of the cell and understanding the effects of metabolic engineering and synthetic biological manipulations. In the current work, a rapid (5 minutes), reproducible, sensitive method was developed for 10 Acyl CoAs using Ultra High Pressue Liquid Chromatograph UHPLC-MS/MS and Selected Reaction Monitoring (SRM) on a Triple Quadrupole (QQQ) Mass Spectrometer.

Systems Biology & Pathways

P-070

Integrative metabolic signatures for radiation induced damage

Irwin Kurland, Albert Einstein College of Medicine

The information from this study suggests the metabolic response to radiation damage is an integrative response of the intestine, liver and kidney. The limitations of the PCA approach are highlighted as is the potential benefit in moving to the non-linear SOM approach. The difference in predictive power between supervised methods indicates the need for adopting multiple approaches, while overlap in metabolites in both supervised methods leads to a higher degree of confidence in identified biomarkers.

P-071

Metabolomics of Hepatic Triglyceride synthesis: Role of Iqgap2.

Bhavapriya Vaitheesvaran, Albert Einstein College of Medicine

IQGAPs are multi-domain scaffolding proteins and integral components of cytoskeletal regulation. Iqgap2 is expressed predominantly in the liver. Mice with genetic deletion of Iqgap2 are obese, glucose intolerant and exihibit metabolic inflexibility. Metabolomics of plasma, liver and skeletal muscle revealed Iqgap2 deletion leads to significant alterations of plasma acylcarnitines and increased accumulation of metabolites critical for triglyceride synthesis in the tissues. Our studies provide a new insight for the role of Iqgap2 in triglyceride synthesis.

P-072

Fuel switching alterations in substrate availability and biosynthesis during the fasted to re-fed transition: Characterization by metabolomics and stable Isotope flux profiling

Kirsten Hartil, Albert EInstein College of Medicine

A stable isotope/metabolomic approach measured rates of hepatic anabolic processes, and changes in plasma substrate availability during the transition from the fasting to the refed state. Refeeding increased hepatic anabolic pathways (glycogen, de novo lipogenesis, protein synthesis). Changes in plasma amino acid and acylcarnitine levels seen to be increased with refeeding may be partially in response, and coordination with, whole body cellular energenics . Therefore, alterations in plasma substrate/metabolites may coordinate the fasting/refeeding biosynthetic “switch”.

P-073

Metabolomic analysis of renal cancer and normal cell lines by capillary electrophoresis time-of-flight mass spectrometry

Mitsuhiro Kitagawa, Institute for Advanced Biosciences, Keio University

We performed metabolome analysis by capillary electrophoresis time-of-flight mass spectrometry. The amounts of ionic metabolites, including glycolysis, TCA cycle, nucleotide synthesis and others were compared among 9 renal cancer and normal cell lines.

P-074

Metabolic diversity of thermophilic enzyme producing bacteria from 15 thermophilic ponds of Odisha, India

Enketeswara Subudhi, Center of Biotechnology

Water and sediment samples from 15 ponds of four thermophilic resources of Odisha were collected. 84 isolates were investigated for presence of range of industrially enzymes viz; amylase, lipase, cellulase, protease, urease, oxidase, catalase etc. and of different carbon utilization capacity viz; glucose, adonitol, arabinose, lactose, sorbitol, mannitol, rhamnose, sucrose and citrate etc. Cluster analysis showed a higher range of metabolic diversity among the bacterial isolates of four major sources of thermophilic environment indicating a rich diverse source of industrially important thermophilic enzymes.

P-075

Untargeted metabolic profiling of yeast extracts by UHR-Q-TOF analysis to study arginine biosynthesis mutants

Friederike Teichert, Bruker Daltonics

Alterations in the arginine biosynthesis pathway in yeast mutants were investigated with an untargeted metabolomics approach employing novel UHR-Q-TOF technology to prove the hypothesis that upstream or downstream metabolites are altered in abundance in gene knock-out mutants. Many primary polar metabolites, such as amino acids, are poorly retained by reversed phase LC column chemistries. Dansylation enables a standard reversed phase (RP)-LC separation with simultaneously enhancement of the signal intensities in electrospray ionization for these compounds.

P-076

Sauvignon blanc metabolomics: Influence of juice manipulations on wine aroma compounds

Farhana Pinu, University of Auckland

The relationship between grape juice composition and wine aroma is poorly understood. As a pioneering metabolomics research for New Zealand wine science, we sought to determine which juice metabolites influence the level of key thiol aroma compounds in Sauvignon blanc wines. Metabolite profiling of 63 grape juices revealed 24 metabolites positively correlated with volatile thiols. Direct juice manipulation confirmed our initial findings and added new insights into aroma development during wine fermentation.

P-077

Development of Yeast Metabolome Sample Preparation Method

Sooah Kim, Korea University

In this study, for the global metabolite profiling of Saccharomyces cerevisiae using gas chromatography-time-of-flight mass spectrometry, we have focused on the development and evaluation of the sampling and extraction methods, which encompassed cold methanol or fast filtration with washing or no washing, cell disruption techniques, and extraction solvents. From these results, metaboloome sample preparation method was optimized for S. cerevisiae.

P-078

Influence of Iron Regulation on Metabolome of Cryptococcus neoformans

MinJu Kim, Konkuk university

Iron plays as a cofactor for key enzymes involved in metabolic pathways. In this study, we analyzed changes of metabolome in a human-fungal pathogen Cryptococcus neoformans associated with iron availability and the regulatory protein Cir1. Our analysis revealed Cir1 influences on the metabolism and iron contents and gene expression in the cir1 mutants contributed metabolite changes. Our study provides a new insight into iron regulation and a role of Cir1 in metabolome of C. neoformans.

P-079

13C Kinetic and Steady State Flux Analysis for Flux Partition Quantification at the Branch Node in Methylobacterium extorquens AM1 Grown on Filters

Song Yang, University of Washington

Methylobacterium extorquens AM1 is a facultative methylotrophic organism, capable of growth on C1 compounds and multi-carbon compounds. A systems biology approach has shown that M. extorquens AM1 is an efficient platform for converting methanol and CO2 to the intermediates of interest for biofuel. 13C kinetic flux simulation and steady state analysis were applied to calculate the flux partition of a key branch node between the ethylmalonyl-CoA pathway and polyhydroxybutyrate cycle for filter cultures of AM1

Short Abstract Listing

Understanding Microbial Metabolism with Metabolomics

P-080

Functional analysis of the methyl jasmonate signaling pathway in the green alga Chlamydomonas reinhardtii

Reid Gustafson, University of California Davis

Evidence shows that biosynthetic genes to produce methyl jasmonate (meja) do exist, but no signaling cascade has ever been found. In a Meja additive experiment we explored the effect of Meja on Chlamydomanas reinhardtii over a 48 hour time course. It was found that Meja did have a profound effect on Chlamydomanas, which suggests an active pathway and an evolutionary relationship to higher plants.

P-081

The use of metabolomics for early detection of Mycobacterium Avium Subspecies Paratuberculosis infection in cattle

Rustem Shaykhutdinov, University of Calgary

“Targeted profiling” NMR metabolomics approach was used for early detection of Mycobacterium Avium subspecies Paratuberculosis infection in cattle. An OPLS-DA model distinguished non-infected calves from infected regardless of time post infection with several metabolites being significantly different between the groups. Longitudinal testing showed that aging causes the most significant alterations in the metabolic profiles of all calves. After 10 months post infection the metabolic profiles can be clearly distinguished between infected and non-infected animals.

Plant II - Plant Physiology and Metabolism

P-082

Polyphenol Oxidase Activates Plant Polyphenols in the Battle against Phytopathogens

Tal Luzzatto Knaan, Hebrew University of Jerusalem, Israel

Plant polyphenoloxidases (PPOs) are oxidizing plant polyphenols, which simultaneously accumulates at the site of penetration, to quinonic intermediates. However, only a few reports have related to the production of quinones and the potency of these aromatic derivatives against bacterial pathogens. In our system activated polyphenols were shown to be oxidized to quinones, evidenced by the complete killing of Pectobacterium carotovorum and also captured by the use of cysteine as a trap and identified by QTOF-LC/MS/MS.

P-083

Metabolomic and Targeted Interrogation of Drought and Nitrogen Stresses in Soybean

Jan Hazebroek, Pioneer Hi-Bred International, Inc.

We applied metabolomics to characterize metabolic responses to drought and nitrogen stresses in soybean. Biomass, growth rate, root nodule characteristics, and leaf chlorophyll content were all affected by nitrogen, and/or drought stress. A mutant line that lacks root nodules and thus cannot fix N2 from air accumulates less ureides. An increase of amino acids with greater N in well watered wild-type plants and increased hexose alcohols with drought across nitrogen treatments were observed.

P-084

Seasonal Variation of Metabolites in Eucalyptus Cambium

Ilara Budzinski, Sao Paulo University

Eucalyptus is a dominant genus in commercial plantation in many parts of the world. However, little information is available about the physiological changes that occur in the wood forming tissues in response to seasonal variation. To observe the dynamic changes in metabolite accumulation, we compared, by GC/MS, the metabolite profile of cambial tissue collected on summer and winter in Brazil. In total 53 metabolites were detected and statistical analysis are being performed in R.

P-085

Molecular Changes in the Metabolome of Medicago truncatula Induced by Short Term Salt and Drought Stress

Vlora Mehmeti, University of Vienna

The effects of abiotic stress on the proteome, the transcriptome as well as the metabolome of plants are subject of several studies at present. However, time and degree of response, the role of symbiotic interaction, nutritional status and the correlation of these differences to particular stress conditions, are still not fully understood. Therefore, we compared nitrogen fertilized and nodulated Medicago truncatula with S.meliloti. Seven weeks old plants have been exposed to drought or salt stress.

P-086

Ozone-Induced Changes in Primary Metabolites in Three Populus Genotypes

Sarita Keski-Saari, University of Eastern Finland

Tropospheric ozone is a phytotoxin that causes oxidative stress in plants. We studied ozone tolerance of three euramerican poplar (Populus deltoides x nigra) genotypes. Leaf samples were collected 2, 4, 11, 15 and 17 days after the start of ozone treatment and analyzed by GC-MS. The genotypes differed in growth rate and ozone responses. Many sugars, such as raffinose and galactose, increased in response to ozone. The most sensitive poplar genotype had the earliest responses.

P-087

Studying Suberization in Potato Tuber Periderms Using NMR- and MS-based Metabolomics

Wenlin Huang, City College of New York

Four varieties of potato (Solanum tuberosum L.) have been studied in suberized periderms by metabolomic analysis using both solution NMR spectroscopy and LC-MS spectrometry. Principal component analysis of the polar extracts exhibits a complete separation among the potato varieties, reflecting the distinctive metabolites and corresponding biological pathways involved in forming their periderms. Cross polarization magic-angle-spinning solid-state 13C NMR spectra of the insoluble potato residues from polar extraction confirm the distinctive suberin solids deposited in the periderms of potato varieties.

Plant II - Plant Physiology and Metabolism

P-088

LC-MS-based chemotaxonomic classification of wild-type Lespedeza sp. and its correlation with genotype

EunSung Jung, Konkuk University

The Lespedeza species were classified by LC-ESI-MS-based chemotaxonomy of leaf and stem samples. Metabolome were classified by species with the selected preprocessing method and detected method. The distance between species was identical to the result from the combined ITS and trnL-trnF analysis. We identified and quantified significantly different phytochemicals between species. This study showed a LC-MS-based metabolomics approach is a powerful tool for classifying the Lespedeza species.

P-089

Changes of phenolic secondary metabolites profiles in lupine leaves after infection with pathogenic fungus or/and elicitation with fungal toxin

Anna Staszków, Institute of Bioorganic Chemistry, Polish Academy of Sciences

Processes of infection with spores of Colletotrichum lupini or/and elicitation with fungal toxin of lupine (Lupinusan gustifolius) leaves is an example of different regulation of metabolic processes occurring during defense reactions. Differences in metabolism are observed inside of plant tissue and in cuticular and wax layers present on leaf surface. Application of GC/MS and LC/MS systems permitted to compare profiles of phenolic secondary metabolites and nonpolar natural products present in/on lupine leaves after biotic stress.

P-090

Compositional Changes in Fruit Pericarp of Water-Stressed Tomato in Greenhouse

Annick Moing, INRA Bordeaux

This work is part of the Eranet EraSysBio+ FRuit Integrative Modelling project. We studied the compositional changes in tomato (Solanum lycopersicum L.) fruit pericarp of plants grown in a greenhouse under usual commercial conditions or under water-stress. Major metabolites were determined using targeted enzymatic analyses of polar extracts throughout fruit development. At two stages of development, metabolites were determined using 1H-NMR quantitative profiling of polar extracts and multivariate analysis was used to highlight discriminant analytes.

P-091

Establishing a diagnostic metabolic profile for soggy breakdown, a physiological disorder of stored 'Honeycrisp' apple fruit

Rachel Leisso, USDA-ARS Tree Fruit Research Laboratory

This study establishes a diagnostic metabolic profile for soggy breakdown, an economically significant physiological storage disorder of 'Honeycrisp' apple fruit linked to chilling. The metabolic profile of symptomatic and healthy fruit were evaluated using untargeted GC and LC-MS protocols. Distinct metabolic fingerprints were constructed indicating specific compounds which may be used for discriminating this disorder from other similar disorders. These results are a step towards the ultimate goal of determining predictive biomarkers for soggy breakdown.

P-092

A Integrated Analytical Approach for Determining the Geographical Origin of Medical Herbs Using ICP-MS and 1H NMR Analysis

Yong-kook Kwon, KBSI

In this study, Astragalus membranaceus Bunge and Paeonia albiflora Pallas were analyzed by 1H NMR and ICP-MS and integrated multivariate analysis was carried out to characterize the differences between origins. Four classification methods were applied. The classification result for two medical herbs was more accurate in integrated analysis than typical analysis. Our study suggests that a suitable integration of different type of analytical data is useful for determining geographical origin of crops with high reliability

Plant II - Plant Physiology and Metabolism

P-093

Primary metabolic responses of silver birch (Betula pendula Roth) leaves to increased air humidity

Jenna Lihavainen, University of Eastern Finland

Water vapor acts as a greenhouse gas affecting water and energy economy of plants. We study long term effects of increased air humidity to silver birch and hybrid aspen at FAHM (Free Air Humidity Manipulation) field site in Estonia. Metabolites were analyzed by GC-MS from leaves of silver birch seedlings after four years of humidification at FAHM site. Increased air humidity induced metabolic changes in sugars and organic acids. Humidification increased dehydroascorbic acid and alpha-tocopherol.

P-094

Towards profiling plant hormones in Lactuca sativa (lettuce) seeds

Dominique Ardura, University of California at Davis

Plant hormones in developing seeds affect a wide range of processes such as cell localization and alignment as well as maintenance, induction and release from dormancy. We here present steps towards profiling five classes of plant hormones using liquid chromatograpy-electrospray ionization tandem mass spectrometry with multiple reaction monitoring, comprising abscisic acid, gibberellins, zeatins, auxins and brassinosteroids. Method details are presented on UPLC chromatography and electrospray/tandem mass spectrometry using a QTRAP 4000 mass spectrometer.

P-095

Monitoring Proteins Degradation using Stable Nitrogen Isotope Labeling in Green Alga

Miho Tanaka, Keio university

Under starvation conditions, proteins degradation is strongly induced in eukaryote. For monitoring proteins degradation, radioactively labeled amino acid is individually used to analyze long-lived proteins, and then labeling rate of free amino acids are detected. Here, we propose the new method for monitoring long-lived proteins degradation using stable nitrogen isotope (15NO3) labeling as the only nitrogen source in a green alga culture. This method can be labeled all 20 standard amino acids of proteins.

P-096

Integrated GC- and LC-MS based Metabolomics reveals different Molecular Phenotypes of diploid and tetraploid Poplar Plants

Lena Fragner, University of Vienna

Poplar is one of the most cultivated non-food plant used for the production of second generation biofuels. Poplar plants of diploid (2N) and tetraploid (4N) genotypes are applied to metabolite profiling using GC-TOF-MS and nanoUPLC-Orbitrap MS/MS techniques. Visualization and statistics of obtained data are performed by our COVAIN toolbox. Diploid and tetraploid genotypes show altered morphological as well as molecular phenotypes.

P-097

Metabolism of the Soybean-Pathogen Interaction – A Plant Metabolomics Study

Brian D. McGarvey, Agriculture and Agri-Food Canada

Diseases of soybean caused by the soil-borne pathogens Phytophthora sojae, Pythium ultimum, Fusarium solani and Rhizoctonia solani are well studied though their effect on overall metabolism in soybean is not well understood. We employed untargeted metabolite profiling of infected and non-infected soybean to explore the effect of infection on soybean and pathogen metabolism. Significant differences in metabolite profiles were observed for plants infected with the four diseases after principal components analysis of their GC-MS chromatograms.

P-098

Effect of Irradiance and Acetate on Lipid Composition of Chlamydomonas reinhardtii

Haruka Shinkawa, Keio University

Irradiance and organic nutrients such as acetate affect algal lipid accumulation and its composition. We examined the triacylglycerol (TAG) composition of C. reinhardtii following nitrogen deficiency by liquid chromatography time-of-flight mass spectrometry, under different irradiance and nutritional conditions (presence or absence of acetate). The irradiances and the presence of acetate affected TAG composition, respectively. These results may contribute to the improvement of cultivation methods and TAG yield for biofuel production.

Plant II - Plant Physiology and Metabolism

P-099

Sugarcane Metabolomics: Sugar signaling

Carlos Labate, Universidade de São Paulo - ESALQ/Departamento de Genética

Sugarcane 1+ leaves from 4 and 12 months old-plants were fed for 3 hours with 50 µM of the following sugars: sucrose, glucose, fructose, mannose, 3-o-metilglucose as hexokinase phosphorilation control, manitol and water. Metabolites were analyzed using a GC-TOF/MS and 70 metabolites were identified. PCA, Heat Maps and Fold change analysis showed how leaf development and sugars supplied affect the reconfiguration of the leaf´s metabolic profile.

Short Abstract Listing

Human Disease and Health Biomarkers II - Understanding Complex Diseases through Metabolomics

P-100

GC/MS-based profiling of amino acids and TCA cycle-related molecules in ulcerative colitis

Masaru Yoshida, Kobe University Graduate School of Medicine

The regulation of immunity and inflammation by amino acids is well defined, and the relationship between inflammatory bowel disease (IBD) and certain amino acids has recently attracted attention. In this study, amino acids and trichloroacetic acid (TCA) cycle-related molecules in the colon tissues and sera of patients with ulcerative colitis (UC) were profiled via gas chromatography/mass spectrometry (GC/MS), and the differences in their profiles between UC patients and healthy volunteers were found.

P-101

Metabolic mechanisms of weight loss in overweight and obese adults

Edoardo Saccenti, University of Amsterdam

A survey of the metabolic mechanisms underlying severe weight loss in overweight and obese adults is presented. Before and after weight loss lipidomics and low-molecular weight serum/plasma profiles from the participants of the DiOGenes project were analyzed. The results suggested different regulatory mechanisms underlying weight loss in morbid obese individuals and successful/unsuccessful weight losers.

P-102

Applications of Mass Spectrometry Based Metabolomics in Cell Culture Models of Cancer

David Watson, University of Strathclyde

Wide ranging effects of a sphingosine kinase (SK) inhibitor on a cell culture model of prostate cancer were observed by using mass spectrometric profiling. Of particular interest were the effects on the pentose phosphate pathway suggesting a key role for SK in regulating the cancer cell metabolome.

P-103

Metabolomics defines the function of microRNA-1291 in pancreatic tumor cell metabolism

Huichang Bi, Laboratory of Metabolism, CCR, NCI/NIH

The study aims to investigate the impact of miR-1291 on Panc-1 cell (human pancreatic tumor cell) metabolism. miR-1291 and empty vector (control) stably transfected Panc-1 cells were subjected to metabolomic analyses. 1-methylnicotinamide, carnitine and its derivatives were identified as key up-regulated metabolites in the miR transfected Panc-1 cells. These metabolites were considered as potential biomarkers for disease.

P-104

Strengthening Genomic and Disease Inquiry with Metabolomics

Michael Milburn, Metabolon, Inc.

Genome-wide association studies (GWAS) have identified many risk loci for complex diseases, but with the multiple genes involved in many diseases and/or conditions the effect size is usually quite small. We published the largest human genome wide association study analyzing 500 metabolites for 3000 human blood samples (Nature, 477, pg. 37-41, 2011) and concentration statistics relative to genotyping data. It reported comprehensive analysis of genotype-dependent metabolic phenotypes using GWAS with a non-targeted global metabolomics method.

P-105

Metabolomics as a Biomarker Approach: Application to Disease Progression and Drug Treatment Studies

Michelle Clasquin, Merck Research Laboratories

We have developed a metabolomics platform to discover small, endogenous molecules which may serve as preclinical and clinically translatable biomarkers. The platform couples UPLC with Orbitrap technology for the separation and detection of analytes. We have applied the method to the analysis of biological fluids, coupling hypothesis-driven experiments with unbiased metabolite profiling. Examples of how the approach can be applied to characterize metabolic changes associated with disease state or pharmacological intervention will be described.

Short Abstract Listing

Human Disease and Health Biomarkers II - Understanding Complex Diseases through Metabolomics

P-106

High Performance Metabolic Profiling in Plasma and Urine as a Prognostic Tool in Corticosteroid Insensitive Severe Asthmatic Children

Youngja Park, Emory University

Although CS have been in use for severe asthma, their precise mechanism of action is still not completely understood. Most severe asthmatics are now effectively controlled with inhaled CS. However, approximately 5% of patients with asthma do not respond well to CS or require a high dose inhaled or oral CS to control asthma symptoms. With high performance metabolic profiling, the result showed several pathways and metabolites were identified for discrimination of CS insensitivity.

P-107

Metabolic Profile in Animal Models of Nonalcoholic Steatohepatitis with Different Conditions of Dietary Restriction

Ryuichi Uozumi, Analysis & Pharmacokinetics Labs, Drug Discovery Research, Astellas Pharma Inc.

Metabolome analysis were applied to liver and plasma samples of rat models of nonalcoholic hepatitis (NASH) in order to understand metabolic change upon pathogenesis of NASH. As a result, we elucidated that metabolic changes related to lipid metabolism and glutathione synthesis in liver and plasma occur in diet-induced NASH rat models.

P-108

Characterizing the Metabolic Changes in Serum to Identify Biomarkers for Hepatocellular Carcinoma in Patients with Liver Cirrhosis

Habtom Ressom, Georgetown University

Early-stage diagnosis of hepatocellular carcinoma (HCC) remains difficult due to lack of adequate biomarkers with desired sensitivity and specificity. In this study, both untargeted metabolomics and targeted quantitation of metabolites are investigated to identify metabolic biomarkers in serum samples from HCC cases and cirrhotic patients recruited in the US and Egypt. The samples are analyzed by using LC-MS/MS for identification of candidate metabolites and isotope dilution by selected reaction monitoring on triple quadrupole mass spectrometers.

P-109

Metabolomics of UC bacterial ecosystem compared to the healthy donors

Karolina Sulek, Technical University of Denmark

Ulcerative colitis (UC) is an idiopathic inflammatory bowel disease. As its etiology remains still unknown, it has been shown that patients with UC have an altered bacterial microbiota. The aim of this study was to examine the difference in the metabolites profile of fecal microbiota derived from UC patients and healthy subjects, colonizing a dynamic in vitro gut model. Metabolism of bile acids, fatty acids and some of the amino acids differentiated those two groups.

P-110

Metabolomic biosignatures of mice exposed to ionizing radiation

Evagelia Laiakis, Georgetown University

Biomarkers of acute exposure to ionizing radiation are highly needed, particularly in the case of accidental exposures and terrorist acts. The classic cytogenetic methods available for biodosimetry are laborious and time consuming. Here, we screened mouse sera for alterations in major metabolic pathways following exposure to gamma radiation using a combination of mass spectrometric methods (flow injection-MS/MS, UPLC-TOF and UPLC-MS/MS.

P-111

Metabolite Profiling to Identify Early Indicators of Future Diabetes

Amanda Souza, Broad Institute of MIT and Harvard

We profiled plasma samples from participants of the Framingham Heart Study using LC-MS based methods to elucidate early metabolic indicators of future type 2 diabetes. We identified a signature of elevated branched chain and aromatic amino acids that was present up to 12 years before clinical diagnosis and validated this finding in an independent cohort. Analyses of plasma lipids also revealed a novel relationship between lipid acyl chain content and diabetes risk.

Short Abstract Listing

Human Disease and Health Biomarkers II - Understanding Complex Diseases through Metabolomics

P-112

Benefits and Challenges of Multi-OMICS Approach to Identify Metabolic Abnormalities of Patients with a Common Disease Type

Curtis Oleschuk, Diagnostics Services of Manitoba

In-born errors in metabolism result in derangements in patient's biochemistry that can be observed in plasma and urine. A complementary tool to existing practices is one that could offer layered analyses from a single sample. A sample could be investigated for a short list of well-established disorders, screened to observe new disorders, and once clues of a disorder were found, the data could be reprocessed for additional information. We describe using HMRS for this approach.

P-113

A new benchtop Orbitrap LC-MS/MS system for global metabolomics in applied medical research

David Peake, Thermo Fisher Scientific

Identification of unique biomarkers to distinguish healthy animals or humans compared to those with disease can have an impact on early detection of diseases and personalized medicine. We present an evaluation of a new quadrupole-Orbitrap mass spectrometer for metabolomics analyses using the Zucker fatty rat model for type II diabetes. The data obtained from these experiments provides unique biomarker signatures for the experimental manipulations of disease states of animals.

P-114

A metabolomics study on H1N1 pneumonia using NMR and GC-MS

Mohammad Mehdi Banoei, University of Calgary

By applying NMR and GC-MS, we revealed metabolomics profiling for a total of twenty-one H1N1 pneumonia infected individuals. These results demonstrate how metabolomics analysis can give important insights into the phenotype of H1N1 pneumonia patients separating those who will survive > 90 days from those who will die ≤ 90 days. Our findings suggest that non-targeted metabolomics analysis has potential as a new approach with good sensitivity to define different metabolic phenotypes for H1N1 pneumonia.

P-115

A Metabolomic study of a rat model of Hepatocellular Carcinogenesis to investigate the induction of Non-alcoholic Fatty Liver Disease

Yajing Chu, University of Cambridge

A rat model of non-alcoholic fatty liver disease (NAFLD) induced by choline deficient (CD) diet was studied to elucidate the multiple pathogenic mechanisms of NAFLD. In addition animals were treated with an analogue of the thyroid hormone, GC-1, to investigate the potential reversal of fatty liver by this intervention. A comprehensive metabolomic strategy combining NMR, GC-MS, UPLC-MS and MS imaging techniques was employed, demonstrating perturbations of several fatty acids and amino acids metabolism.

P-116

Discovery and Glycolysis Pathway Targeted Metabolome Profiling by Nano LC-Chip-MS in Colorectal Cancer Cells: Effects of Hypoxia and HIF1-α

Alessandro Valli, Nuffield Department of Medicine, Henry Welcome Building for Molecular Physiology University of Oxford

Wild type and knockout for HIF-1α colorectal cancer cells were cultured in normoxia and hypoxia. We developed two platforms based on nanoflow C18 reverse phase and HILIC for Chip-QTOF MS system. Hypoxia and HIF-1α elevation caused substantial changes in metabolomics profiles and in glycolysis. Nano-LC-Chip-MS can be used as a reliable tool to assess specific changes in the glycolysis pathway and cell metabolome.

Short Abstract Listing

Human Disease and Health Biomarkers II - Understanding Complex Diseases through Metabolomics

P-117

A Pilot Study Characterizing Pre- and Post-treatment Metabolomic Profiles of Lung Cancer Patients

M. Omair Sarfaraz, University of Calgary

This pilot study describes the temporal metabolic profiles of 25 non-metastatic lung cancer patients from pre-treatment to six cycles of chemotherapy all the way up to 6 months post therapy. The time points selected for analysis were; at diagnosis, mid-point of therapy and approximately 3 and 6 months after treatment. Results suggest that significant differences exist in the metabolomic profiles of patients at pre-treatment, therapy and post-treatment as well as in cancer staging and pathophysiology.

P-118

Biomarker for the detection of early hepatic fibrosis in NASH patients

Ooga Takushi, Human Metabolome Technologies Inc

The diagnostic biomarker for Nonalcoholic fatty liver diseases (NAFLD), which is one of the most common liver disease in progressed countries, were obtained by using CE- and LC-TOFMS based metabolomics. In total, NAFLD149 patients were analyzed in initial screening study (44 patients) and secondary validation study (105 patients). Among 293 metabolites measured in serum sample, three hormone metabolism intermediates showed excellent performance for the diagnosis of early stage of the fibrosis.

P-119

Metabolomics investigation of human Schistosoma haematobium infection

Carolus Reinecke, Centre for Human Metabonomics

Bilharzias is a complex parasitic disease affecting approximately 200 million people and declared by the WHO to be eradicated globally, requiring efficient targeting of infected individuals and monitoring of treatment. Here we present the first metabolomics investigation of bilharzias due to S. haematobium infection. Twenty metabolites have been identified as potential markers, using elaborate data pre-treatment of untargeted GC-MS data. The results clarify the potential of this methodology for accurate disease diagnosis and improved disease surveillance.ter a short version of the abstract.

P-120

A Metabolomics Approach for Osteoarthritis Biomarker Discovery via Biomechanical Stimulation of Chondrocytes

Catherine Kirn-Safran, University of Delaware

Osteoarthritis is a common complex joint disease, characterized by severe pain and disability from the loss of articular cartilage. Our research focus is to understand the mechanisms involved in the early progression of the disease. Biomechanical stimulation and altered joint loading are known to deregulate the functional behavior of articular chondrocytes during aging. Therefore, these studies aim to identify novel non-protein biomarkers by metabolomics analysis using in vitro chondrocyte model systems and the IROA technology.

P-121

Metabolome data for mouse model of Social Stress

Aarti Gautam, USACEHR

A social stress (SS) mouse model was used to simulate aspects of post-traumatic stress disorder (PTSD).Global metabolomic profiling was carried out on plasma samples of C57BL/6 mice exposed to either 5 day or 10 day of SS at both early (24h) and late (1.5 weeks for the 5d SS and 4 weeks for the 10d SS) time points. Metabolites involved in redox changes, neuronal damage and /or cell death and energetic alterations were identified.

P-122

Accurate Mass Metabolite Fingerprinting - A Case Study on the Effect of Aspirin and Fish Oil

Christoph Buchholz, Metabolomic Discoveries GmbH

We have developed a high-throughput accurate mass metabolite fingerprinting method. That approach yields hundreds of injections per day. Accurate mass enables the prediction of the responsible metabolites relevant for separation or clustering of samples. A study group of ten diabetic adults were subjected to aspirin, fish oil, aspirin and fish oil. We have used metabolite fingerprinting to screen blood serum for changes in the whole metabolome resulting from those treatments in individuals with diabetes.

Short Abstract Listing

Human Disease and Health Biomarkers II - Understanding Complex Diseases through Metabolomics

P-123

1H NMR metabonomics approach to diabetes type 2 disease for risk assessment and diagnosis with artificial neural network modeling

Mohammad Arjmand, Pasteur Institute of Iran

Diabete mellitus describes a metabolic disorder of multiple etiology characterized by chronic hyperglycemia with disturbances of carbohydrate, fat and protein metabolism resulting from defects in insulin secretion, insulin action or both (WHO 1999). 1H NMR spectroscopy of human serum with the help of artificial neural network (ANN) modeling is widely used in medical studies now days. In the present, investigation, we used ANN modeling to differentiate between T2DM diabetes patients and normal individuals to predict the disease with a clinical diagnosis support system.

P-124

Quantitative metabolomic profiling of serum, plasma and urine by 1H NMR spectroscopy discriminates between patients with inflammatory bowel disease and healthy individuals

Alsu Nazyrova, University of Calgary

NMR metabolomic profiling was used to detect promising biomarkers in inflammatory bowel disease (IBD) in human. Quantitative NMR metabolomic profiling of serum, plasma and urine sample spectra discriminates between healthy subjects and subjects with active Crohn's disease (CD) and ulcerative colitis (UC), but only limited differences were observed between the CD and UC cohorts. Differences in metabolic profiles between cohorts are revealed and discussed.

P-125

Characterizing Human Diseases and Human Biofluids using Multi-Platform Metabolomics Techniques

Constance Sobsey, University of Alberta

Applications of multi-platform metabolomics techniques in disease biomarker studies are presented. The Metabolomics Innovation Centre (TMIC), Canada's national metabolomics platform, specializes in performing quantitative metabolomics assays using a wide range of technologies. TMIC has recently completed several disease biomarker studies including biomarkers of organ transplant rejection and the first trimester prediction of early- and late-onset preeclampsia. These studies are presented in detail to show the potential of multi-platform metabolomics for our improved understanding of health and disease.

P-126

Hepatitis B and C viruses as paradigms of "metabolovirus"

Patrice André, INSERM U851

Viruses are parasites that rely on cells they infect for energy and metabolites necessary for their replication. The metabolism status of the cell does not always fulfill these needs and viruses often actively modify it. Viruses can thus been viewed as "metaboloviruses", which are metabolism engineers that induce dramatic changes of the cell metabolism with a limited number of viral proteins. Hepatitis B and C viruses illustrate two opposite ways metaboloviruses cope with the cell metabolism.

P-127

Metabolomics and Integrated "omics" Analysis of the Mesenchymal-Epithelial Transition in Ovarian Cancer

Mark Styczynski, Georgia Institute of Technology

Transitions between epithelial and mesenchymal states are believed to play pivotal roles in cancer metastasis and recurrence, but have not yet been studied in great depth. Here, we study the mesenchymal-epithelial transition in a metastatic ovarian cancer cell line. Metabolomics analysis indicates distinct intracellular and extracellular changes throughout the transition. Proteomics and transcriptomics analyses are being integrated to more fully understand the metabolism of this transition and its potential as a target for anticancer therapies.

Short Abstract Listing

Human Disease and Health Biomarkers II - Understanding Complex Diseases through Metabolomics

P-128

Common Metabolites Responding to Antihytensive Medication in Young-Onset Hypertension Patients

Wen-Harn Pan, National Health Research Institutes

Phamacometabolomics study compared metabolomic profiles in hypertensive patients with and without antihypertensive treatments with 50 subjects in those without medication and in each of the 4 anti-hypertensive medication groups. We found over 72 metabolites significantly associated with the antihypertensive treatments (p value <10-6). Among them, concentrations of two metabolites were consistently lower in all treatment groups (p value <10-10), compared to those without treatment. These two metabolites may play crucial role in blood pressure regulation.

Plant III - Applied Genetical Metabolomics

P-129

Genetic and Environmental Effects on Polar Metabolites in Corn Grain

Mingjie Chen, University of Missouri

To better understand the influences of genetics versus environment, on polar metabolite levels in corn grain, 50 commercial hybrid varieties grown at six different locations in North America were analyzed. The corn seed samples were lyophilized and ground and polar metabolites were extracted by using a modified two-phase separation method. The metabolites were analyzed by GC-MS after derivatization. The resulting values were normalized. Statistical analysis was performed to identify associations among polar metabolites content/profile with maize genotypes and environmental conditions.

P-130

Characterization of Rice Cultivars under High Night Temperatures using Metabolite Profiling

Ulrike Glaubitz, Max-Planck-Institute of Molecular Plant Physiology

Global warming has an increasing influence on crop productivity. In the past century a stronger increase in night than day temperatures was observed with strong influences on crop physiology. We analyzed the effects of high night temperatures on 12 rice cultivars and a DHL mapping population. GC-MS, LC-MS and HPLC profiling showed differences in metabolite contents between cultivars and conditions, indicating the possibility to identify important metabolic pathways and marker metabolites for breeding programs.

P-131

ReSpect: A Plant-specific MS/MS-based Data Resource and Database

Yuji Sawada, Riken Plant Science Center

RIKEN tandem mass spectral database (ReSpect) is MS/MS data resource (8649 records) and database for phytochemicals. The ReSpect database is primarily composed of MS/MS data obtained from the 163 literatures. An MS/MS fragment search system was established for the annotation of untargeted MS/MS data. All web application and data resource in ReSpect is publicly available (http://spectra.psc.riken.jp/). In the case study of metabolite quantitative trait locus analysis, unknown metabolites were successfully narrowed down to putative structures.

P-132

Genetic Engineering of Flavonoid Pathway through Gene Overexpression and Silencing Approaches in Tobacco (Nicotiana tabacum L.)

Monika Mahajan, IHBT (CSIR), Palampur, INDIA

Here, two approaches were used to engineer the flavonoid pathway in tobacco towards flavan-3-ols production, one is through downregulation of flavonol synthase (FLS) gene and other is through overexpression of Camellia sinensis flavanone-3-hydroxylase (CsF3H) cDNA in tobacco. Silencing of FLS reduced flavonol (quercetin) content and led to generation of less seeded fruits whereas both overexpression of CsF3H and silencing of FLS increased flavan-3-ols content and affects the antioxidant system of transgenic tobacco plants.

Safety Monitoring and Biomarkers

P-133

The Metabolomic Approach Identifies a Biological Signature of Chronic Low-dose Exposure to Cesium 137

Gaëlle Favé, UMR INSERM 1062 / INRA 1260 / AMU

The present study aimed at evaluating the effects of chronic low-dose exposure to cesium 137 on rat health using both conventional toxicological tests, including organs weigh-in and plasma biochemical assays, and a metabolomic approach, using analysis of urinary and plasma LC/MS profiles. No difference could be observed between the control and contaminated groups with the conventional approach, whereas the metabolomic one identified for the first time a discriminant metabolomic signature based on 26 plasma signals.

P-134

Metabolomic Analysis of Zidovudine (AZT)-Induced Toxicity in Mice

Jessica Bonzo, National Cancer Institute

There is accumulating clinical and animal model evidence linking nucleoside reverse transcriptase inhibitor (NRTI) treatment for HIV infection to mitochondrial toxicity and multiple disorders including liver dysfunction, myopathy, and lipodystrophy. An UPLC-QTOF-MS-based metabolomic study was conducted using male mice treated with 400 mg/kg AZT for 4 weeks to determine the full scope of metabolic disruption caused by AZT treatment. Preliminary findings suggest broad activation of hepatic fatty acid metabolism by AZT.

P-135

Non-invasive assessment of gastrointestinal toxicity of methotrexate using NMR based metabolomics

Yong-jin An, Department of Biochemistry, College of Medicine, Inha University

Methotrexate (MTX) has anti-inflammatory and immune-modulating properties, leading to its various uses across multiple specialties. However, MTX has various dose-dependent side effects. We performed metabolomics studies on the urine obtained from MTX-treated male Sprague-Dawley rats. We performed NMR-based metabolomics analysis combined with OPLS-DA for urine samples. We identified 30 metabolites. Our discovery in metabolic markers might have a clinical value in noninvasive detection of intestinal toxicity caused by this commonly used anti-cancer drug.

P-136

1H NMR-based Metabolomics to Study Effects of Naphthalene on Mouse Tissues

Meng-Hsuan Chung, Graduate Institute of Environmental Health, National Taiwan University

Naphthalene, a primary polycyclic aromatic hydrocarbon, can cause respiratory cell injury in mice. To understand the mechanisms of naphthalene-induce toxicity, NMR-based metabolomics was applied to study effects of naphthalene on the lung, liver, and kidney of mouse. The results of multivariate statistical analysis from J-resolved NMR spectra of tissue extracts showed a dose-response relationship. This study can provide information for biomarker development and suggest future direction of mechanistic studies.

P-137

Analysis of hormone levels in H295R cell culture supernatants using LC-MS/MS analysis in agreement with current OECD and OPPTS test guidelines

Bianca Bethan, metanomics GmbH

LC-MS/MS measurement is an efficient alternative to the ELISA analysis for the measurement of steroid hormones produced by H295R cell system not only because it reduces costs, time and avoids cross-reactivity artefacts, but also it enables us to enhance the read-out of the steroidogenesis assay, since in parallel to E2 and T, we can determine further steroid hormones.

Databases & Data Analysis

P-138

Inferring differences in the distribution of reaction rates across conditions

Diana Hendrickx, University of Amsterdam

Elucidating how metabolic pathways function is an important topic in systems biology, because it can contribute to different disciplines by discovering unknown relations between metabolites. In this study, changes in reaction rate distribution are inferred from correlations in time-resolved metabolomics data measured under different conditions, combined with a priori information on topology and directionality of the pathway. This allows for inferring regulation scenarios without detailed knowledge of kinetics.

P-139

Integrative Ionization Mass Spectrometry and Multilateral Scaling for Comprehensive Metabolomics-Based Biomarker Analysis

Daiki Setoyama, Kyushu University

This study is to evaluate the multiple ionization-MS method, especially combined with ESI and MALDI, for high-coverage comprehensive metabolomics and also provide a technique to discover significant metabolite biomarkers from the integrated data set. We found the multilateral scaling method, a pretreatment with multivariate statistical analysis, as a very useful tool to detect a wide range of changing patterns of metabolites.

P-140

High(er) throughput Metabolite Annotation

Steffen Neumann, IPB Halle

We present a workflow for high(er) throughput Metabolite Annotation. This includes the improved acquisition and processing of Tandem-MS data with MetShot, where high-quality compound spectra of only the biologically relevant peaks are obtained, and the following metabolite identification step. The MetFusion approach integrates both MassBank and the in-silico fragmentation tool MetFrag for identification.

P-141

Metabolite Biomarker to identify treatment non-responder in type 2 diabetes

Sophie Narath, HEALTH /JOANNEUM RESEARCH

The aim of this study is the detection of candidate biomarkers in low molecular weight compounds allowing identifying patients with type 2 diabetes with progressive atherosclerosis despite attempts to intensify risk factor treatment. First results, using a holistic approach involving a subgroup (18) show a tendency towards a clustering between responders and non-responders (PCA). We identified 32 features from LC/FTMS-Metabolite Fingerprints, which represent the basis for further research on the whole study group (100 subjects).

P-142

Quality Assessment of LC-MS Metabolomic Data

Mohammad R Nezami Ranjbar, Lombardi Comprehensive Cancer Center, Georgetown University

Liquid Chromatography–Mass Spectrometry metabolomic data need to be carefully preprocessed to remove the effects of systematic bias and noise caused by the complex nature of human samples, presence of large number of metabolites, analytical variability and noise which can mislead the interpretation of results from subsequent statistical analysis. We discuss problems with reproducibility of LC-MS metabolomic data and provide suggestions to detect and overcome these issues through quality assessment approaches and appropriate experimental design.

P-143

Natural product-likeness as a filter for metabolome prediction methods

Kalai Vanii Jayaseelan, European Bioinformatics Institute

We present an open-source engine to calculate Natural Product (NP)-likeness - a score for a given molecular structure based on a statistical model relying on the differences in occurrence of circular fingerprint of atoms in compound collections. In methods enumerating theoretical metabolomes or for filtering the results list from computer-assisted structure elucidation results based on metabolomics experiments, such a score will provide a means to rank the results based on their NP-likeness.

Databases & Data Analysis

P-144

MetaboSearch: a tool for metabolite identification by integrating information from multiple databases

Bin Zhou, Georgetown University

Searching metabolites against databases according to masses is often the first step in metabolite identification for mass spectrometry-based untargeted metabolomics studies. By integration of the search results from multiple databases, it is expected to yield a more comprehensive coverage of metabolome. A web-based software tool, MetaboSearch, is implemented to enable the simultaneous search against four major databases and the integration of the results. The tool utilizes ion annotation information to further aid the identification task.

P-145

Deconvolution of Complex Mixtures by NMR Consensus Trace Clustering

Kerem Bingol, Florida State University

Identification and quantification of each mixture metabolite of a metabolomic mixture represents a key step for their analysis. Nuclear magnetic resonance (NMR) is a powerful analytical tool providing atomic-detail information without requiring extensive fractionation of samples. Identification of metabolites in these non-fractionated samples can be accomplished by acquiring multidimensional NMR spectra followed by labor-intensive manual deconvolution. Here we present an approach that replaces the manual procedure by a semi-automated approach that is fast and accurate.

P-146

H-MS : Wavelet Smoothing, Adaptive Binning and Peak Detection for LC-MS Data

Harriet Muncey, Imperial College London

LC-MS is a key analytical tool in metabolomics. Instruments of higher resolutions are being developed producing vast, unwieldy datasets, creating a necessity for increasingly sophisticated data processing methods. H-MS is a LCMS data processing tool, designed to overcome loss of information in binning and includes novel peak detection using a likelihood test. H-MS competes well against commonly-used package XCMS. Comparisons are ongoing, but H-MS shows promise to improve peak detection in complex metabolomic LCMS data.

P-147

IsoCor & influx_1: Bioinfomatics Tools for High-Throughput 13C-Fluxomics

Fabien Letisse, LISBP - Universite de Toulouse

Fluxomics is a powerful but low-throughput tool for quantitative characterization of the actual operation of metabolic networks. The growing demand for comprehensive phenotyping in systems and synthetic biology, is driving the need for high-throughput approaches to investigate large sets of organisms, strains, or physiological conditions. In addition to experimental & analytical developments, HT fluxomics requires tools for the processing of large datasets. Here, we present IsoCor & influx_s, two software particularly adapted for HT 13C-fluxomics.

P-148

SRM/D: An Online Data Resource for Complex Biological Standard Reference Materials

William Wallace, National Institute of Standards and Technology

To better assist NIST Standard Reference Material customers we have developed a website for viewing compounds found in SRM 1950 'Metabolites in Human Plasma'. The interactive website has a wide variety of ways to search, sort, filter, and display the results. It will be updated as new discoveries are made by NIST and by other institutions investigating SRM 1950. We aim for it to be a focal point of the metabolomics community.

P-149

Ion annotation-assisted analysis of multiple LC-MS based metabolomic experiments

Rency Varghese, Georgetown University

We investigate methods to identify metabolite levels with significant and consistent changes by evaluating the overlaps of ions selected from multiple LC-MS-based experiments. Specifically, we propose an ion annotation-assisted method that takes into account the presence of a large number of derivative ions such as isotopes, adducts, and fragments to determine ions overlapping across multiple experiments. We evaluate the performance of this method with the traditional method that does not utilize the ion annotation information.

Databases & Data Analysis

P-150

MeRy-B: A Plant Metabolomics Database and Knowledge Base

Catherine Deborde, INRA Bordeaux

MeRy-B is the first platform for plant metabolomic profile management and metabolite identification for proton NMR experiments [Ferry-Dumazet et al. 2011 BMC Plant Biol. 11:104]. MeRy-B manages all the data generated by NMR-based plant metabolomics experiments, from description of the biological source to identification of the metabolites and determination of their concentrations. MeRy-B is evolving towards a knowledge base.

P-151

Selective Paired Ion Contrast Analysis: A Novel Algorithm for Analyzing Radiation Metabolomic Datasets Possessing Exceptionally High Noise

Tytus Mak, Georgtown University Medical Center

The primary pitfall in analyzing complex biofluids, such as patient samples, via metabolomics is the sheer variability in the data, which has confounded established statistical analysis methods. Thus, a new algorithm has been developed, called Selective Paired Ion Contrast Analysis, which utilizes ion pairs as its fundamental unit of multivariate analysis. For this study, biofluids from 100 patients undergoing bone marrow transplant were assessed for their responses to radiation therapy.

P-152

Computer-assisted Structure Elucidation for the Identification of Natural Products

Luis F de Figueiredo, European Bioinformatics Institute

We will present an interdisciplinary project aiming at the isolation and structure elucidation of new natural products (NP). The experimental component will consist of the extraction and isolation of NP produced by filamentous fungi. The computational component focuses on the development of new workflows for computer-assisted structure elucidation (CASE). To this end a new database for NMR and MS spectral data is being developed, SpectraDB. Furthermore, recent developments in CASE will be integrated in SENECA.

P-153

A hybrid approach of feature detection from LC-FTMS metabolomics data

Tianwei Yu, Emory University, Department of Biostatistics and Bioinformatics

Databases of known metabolites and historical data contain information that could help boost the sensitivity of LC-FTMS feature detection, especially for metabolites existing in lower concentrations. We describe a new computational method that utilizes databases and preexisting data to improve feature detection from high-resolution LC-MS data. It uses a two-step procedure, and reduces the chance of false-positives by non-parametric local peak detection. The method is implemented in the R package apLCMS at http://www.sph.emory.edu/apLCMS/.

P-154

The Golm Metabolome Database - An Update

Dirk Walther, Max Planck Institute for Molecular Plant Physiology

The GMD was developed to store GC/MS chromatogram and spectra information to serve as reference data for the improved metabolite identification in biological samples. Currently, we focus on consolidating the accumulated diversity of biological samples and experiments. To capture all relevant experimental metadata, we build on the XEML ontology and experiment description facilities. Other developments include the integration of decision tree based spectra interpretation and improved sum formula identification based on accurate molecular mass measurements.

P-155

Libraries of Recurrent Unidentified Spectra for Metabolite Profiling

W. Gary Mallard, NIST

Libraries of recurrent unidentified spectra in a variety of metabolic matrices are being developed. The presentation illustrates the procedure for pediatric urine, human plasma and essential oils samples. Data files are analyzed using AMDIS to deconvolve spectra and the library is built from these spectra along with the RI values.

Databases & Data Analysis

P-156

MetaboLights Repository: Collecting metabolomics experimental data using ISA Tools

Reza Salek, MRC-HNR

MetaboLights is a resource developed to archive metabolomics experimental evidence, covering raw, processed data and ancillary metadata. One of the main submission channels for MetaboLights is the ISA Tools Suite. The ISA software suite comprises several platform-independent components, which run as 'desktop' applications built around ISA-Tab based format. The 'Investigation/Study/Assay' ISA-Tab format, developed to represent experimental metadata independently from the assay technology used, is utilised here to capture the raw file and associated metadata.

P-157

Sorting, Classifying, and Analysis of Metabolomic Data

Corey DeHaven, Metabolon, Inc.

Metabolomics experiments generate copious data files. Collection, sorting, and analysis of the data consume large amounts of time and computational power. Typically, each data file is subjected to peak detection and integration processes sequentially and individually compared to spectral libraries of known metabolites. This approach is labor-intensive and generally includes minimal quality control of peak detection and integration. Further, potentially relevant and/or valuable metabolomic data that may be useful to identify and classify samples may be overlooked or discarded.

P-158

Statistical hypothesis test of factor loading in principal component analysis and its application to metabolite set enrichment analysis

HIroyuki Yamamoto, Human Metabolome Technologies, Inc.

Principal component analysis has been widely used in metabolomics. In many metabolomics research articles, some metabolites (e.g., the top 10 metabolites) have been subjectively selected by using the factor loading. In the present study, we objectively evaluated the number of metabolites by statistical hypothesis test of factor loading. And, metabolite set enrichment analysis can be performed for the significant metabolites. We created an R package "mseapca" to perform these analysis.

P-159

Biological Magnetic Resonance Data Bank NMR Metabolite Spectral Database

Eldon Ulrich, Biological Magnetic Resonance Data Bank

The metabolite NMR spectral database housed at BMRB contains 1D and 2D 1H and 13C NMR spectra for over 1000 compounds. Included are raw time-domain and frequency domain data with peak lists and assigned chemical shifts. The spectra have been collected under standard conditions and at spectrometer field-strengths from 700-250 MHz. Individual data sets or bulk data downloads for research and educational purposes can be retrieved from the BMRB web and ftp sites.

P-160

Building a High Quality and Comprehensive Tandem Mass Spectral Library

Xiaoyu Yang, National Institute of Standards and Technology

A high quality and comprehensive MS/MS library is developed. A clustering algorithm used an adjusted dot product as a measure of spectral similarity to create a 'consensus spectrum' from multiple MS/MS spectra measured with low- and high-resolution, ion-trap and linear collision cell instruments. Consensus spectra were validated based on mass accuracy and fragments. The library contains >50% metabolites with >6,000 compounds, >15,000 precursor ions, >100,000 spectra of positive and negative ions at different collision energies.

P-161

m/z Cloud – A New Type of Mass Spectral Library for the Identification of Unknowns even if the Unknown Compound is not Present in the Library

Robert Mistrik, HighChem

We will present a new type of mass spectral library providing the functionality required for elucidation of unknown metabolic components even if unknowns are not present in the library. The m/z Cloud public domain database aims to provide complete library technology based on spectral ion trees to enable elucidation of unknowns using the precursor ion fingerprinting method.

Databases & Data Analysis

P-162

MassBank: Public Repository for Sharing Mass Spectral Data of Metabolomics

Takaaki Nishioka, Nara Institute of Science and Techonology

MassBank (http://www.massbank.jp) is a public repository of mass spectral data. Contributors to MassBank prepare their data in the MassBank Record Format, and deposit the data in the MassBank system that is installed on their own data servers. Here we report on 1) the chemical annotation of MassBank data, 2) a new repository, Bio-MassBank, for sharing the mass spectra of unknown metabolites.

P-163

Integrating multiplatform metabolomics analyses

Alysha De Livera, The University of Melbourne

Metabolomics research increasingly conducts multi-platform analyses in order to obtain better coverage for the whole metabolome and to enhance the identification of biologically interesting metabolites by considering instrumental and other variations. We present a statistical model for combining the results of multiplatform analyses for the identification of differentially expressed metabolites. The proposed approach is broadly applicable, and can be extended to integrate multiomics studies.

P-164

MMMDB: metabolome database of multiple tissues from single mice

Masahiro Sugimoto, Graduate School of Medicine and Faculty of Medicine Kyoto University

The Mouse Multiple Tissue Metabolome Database (MMMDB) is a web-based database, providing quantitative metabolomic information for multiple tissues from single mice. We conducted non-targeted metabolome analyses, using capillary electrophoresis time-of-flight mass spectrometry, of 10 tissues and plasma from single mice, and developed database including these quantified profiles.

P-165

TNO-LCHRMS-DECO: Deconvolution Tool for Pre-processing Liquid Chromatography High Resolution Mass Spectrometr (LCHRMS) Data

Shaji Krishnan, TNO

TNO-LCHRMS-DECO is a deconvolution tool capable of pre-processing raw LC-HRMS data and produce metabolite peak tables, and the mass spectra. In contrast to the existing tools, TNO-LCHRMS uses less stringent rules and user-defined parameters to format and clean the raw mass chromatogram. To further, lessen the multiple dataset deconvolution load, the signal segmentation method previously used for GC-MS data has been extended to LC-HRMS data.

P-166

Review of Data Mining Tools for Metabolomics Data

Ananda Mondal, Claflin University

Many tools have been explored in mining metabolomics data but the factor analysis (FA) method remains unexplored. Most of the studies used only one set of data. In order to claim the superiority of a technique, it is required to be robust to different set of data with different features. Present study will use at least three different datasets to evaluate the performance of existing methods along with FA to identify a superior technique.

P-167

xMSanalyzer: automated pipeline for downstream analysis of large-scale, non-targeted metabolomics data

Karan Uppal, 2Department of Medicine, Division of Pulmonary, Allergy and Critical Care, Emory University

Multiple algorithms are available to extract m/z features from liquid chromatography-high-resolution mass spectral data. Feature identification criteria for dietary and environmental chemicals, which may be present in only a small fraction of samples, are likely to differ from criteria used to extract information on higher abundance chemicals found in most samples. We present an R package, xMSanalyzer, to maximize detection of low abundance and variable peaks.

Nutritional Metabolomics

P-168

Metabolomics reveals the metabolic effects of whole grain rye products on humans

Ali Moazzami, Swedish University of Agricultural Sciences

Epidemiological studies have shown that whole grain cereals can protect against the development of chronic disease. However, the underlying mechanism is not fully understood. We are reporting the results from NMR-based metabolomics analysis of two human interventions and one postprandial study in which subjects received whole grain rye (RP) or refined wheat (WP) products. Our studies revealed that the consumption of RP products compared with WP causes favourable shifts in energy-, branch amino acid-, and single carbon metabolism.

P-169

An UPLC-QTOF/MS Metabolomic Profiling Unveils Urinary Changes in Humans after a Whole Grain Rye versus Refined Wheat Bread Intervention

Isabel Bondia-Pons, VTT Technical Research Centre of Finland

This study aimed at elucidating novel urinary biomarkers of rye intake by applying a non-targeted UPLC-QTOF/MS approach to samples from an intervention with whole grain rye vs. refined wheat bread. Twenty-two metabolites were revealed as relevant biomarkers, including phenolic compounds, nitrogen-containing metabolites, organic acids and glucuronides. The most discriminative metabolites were identified as metabolites of dihydrocaffeic acid, phenylglycine and tryptophan. Several biomarkers were microbial metabolism products, indicating a role of gut microbiota in whole-grain biotransformations.

P-170

Sulfur-containing metabolite-targeted analysis using liquid chromatography-mass spectrometry

Ryo Nakabayashi, RIKEN Plant Science Center

Plants accumulate human beneficial metabolites such as amino acids, flavonoids and sulfur-containing metabolites (S-metabolites) with a wide range of biological activities related to antioxidation, platelet aggregation inhibition, and anticancer benefit. Profiling methods for such metabolites with high accuracy and throughput are being required. Here, we describe the targeted analysis using liquid chromatography (LC)-mass spectrometry (MS) for S-metabolites.

P-171

Characterization of Traditional Chinese Medicines using high performance time-of-flight mass spectrometry with UHPLC – Metabolomic Analysis of Nutriceuticals

Jeffrey Patrick, LECO Corporation

Comprehensive metabolic profiling using UHPLC with high resolution TOF-MS and high resolution comprehensive fragment ion analysis, was to the characterization of extracts and supplemented extracts from several herbal medicines. The utility o of HR-TOF-MS and comprehensive MS/MS is clearly demonstrated by metabolite identification and differential analysis. The high mass accuracy, resolving power, and relative isotope abundance enable analyte identification and facilitates retrieval of high information content from these complex samples.

P-172

Identification of biomarkers of efficacy for cancer prevention in mouse models of inflammation--induced colorectal cancer by dietary supplement Resveratrol

Shakir Saud, Nutritional Science Research Group, NCI, NIH

Despite resveratrol's well-documented anti-cancer activity, there have been, to date, no studies that detail specific biomarkers that can be utilized to establish efficacy of treatment during clinical trials. Furthermore, the direct targets of resveratrol still remain elusive. We assessed the global changes in fecal metabolites associated with the chemo-preventive effects of resveratrol to generate biomarkers of efficacy of resveratrol, and to illustrate resveratrol's mechanism of action through global metabolic changes.

Nutritional Metabolomics

P-173

Metabolomic analysis for discovery of serum and fecal Molecular Indicators of Dietary Intervention for Colon Cancer

Matthew Young, NCI,

Colorectal cancer results in ~50,000 deaths a year. The Polyp Prevention Trial showed that a high bean intake is inversely associated with advanced colorectal adenoma recurrence. In AOM/DSS treated mice, bean extract showed a significant reduction in tumor number. We identified metabolic biomarkers in serum and feces of mice fed the been extract supplemented diet. We have translated this data to a human feeding study where we identified some of the same biomarkers.

P-174

Metabolomic Assessment of the Protective Effect of M1 in the High Fat Diet-induced Hepatosteatosis in mice

Jung Chao, Institute of Pharmacology, National Yang-Ming University

M1, a naturally active compound in Dioscorea species, has been shown to have potent anti-oxidative and hypolipidemic activity. The aim of this study is to investigate the beneficial effects of M1 administration on nutritional hepatosteatosis by 1H NMR-based metabolomics using an animal model. Our study suggests that M1 ameliorates fatty liver disease through multiple mechanisms and suggest that M1 can be used to ameliorate Nonalcoholic fatty liver disease (NAFLD).

P-175

Characterization of Chinese Traditional Vinegar by NMR and Chemometric Methods

Li Zhenyu, Shanxi University

In China, Vinegar is a kind of well known and important seasonings foods. Three kinds of vinegars, namely Shanxi vinegar, Zhenjiang vinegar and White vinegar, were compared by NMR and chemometric methods in this study. PCA and HCA analysis showed clear seperation between different vinegars, and the characteristic components causing the seperation among different groups were found out by PLS-DA.

P-176

RP-HPLC-DAD-ESI-TOF for the pharmacokinetic study of Quercetin in adipocytes

Isabel Borrás Linares, Research and Development of Functional Food Centre (CIDAF)

A pharmacokinetic study of quercetin in a model of adipogenesis has been carried out. Quercetin was added to the media at the beginning of the study. After that, samples of cytoplasm were taken at different time (0, 3, 6, 12, 18 hours). The presence of quercetin was analyzed by reversed-phase high-performance liquid chromatography coupled with photodiode array and time of flight mass spectrometry detectors. Quercetin was detected in all analyzed samples, except in the control.

P-177

MALDI-MS Imaging for Visualizing Metabolomic State of Aged Mouse Brain after Oral Administration of Green Tea Polyphenol EGCG

Yoshinori Fujimura, Kyushu University

Here we examined metabolomic state of aged mouse brain (C57BL/6J mice, 40-60-week-old) after oral administration of green tea polyphenol (-)-epigallocatechin-3-O-gallate (EGCG) by MALDI-MS imaging. We were able to visualize a broad range of metabolites including nucleotides, phosphorylated sugars, amino acids, and lipids with their unique distributions. Several metabolites in EGCG-administrated mouse showed a different localization compared with control mouse. These results may provide a novel insight into the metabolomic understanding of EGCG's actions in brain.

P-178

The Influence of Polyphenol-Rich Diets in Mice – A Multicompartmental LC-QTOF-Based Metabolomics Approach

Friedrich Mandel, Agilent Technologies

Metabolomics using LC-Q-TOF and novel pathway architect software disclose novel metabolic relationships between different body compartments. As a proof of fact, we demonstrate that the number of metabolites whose levels correlate between digestive contents and plasma is higher than those correlating between plasma and urine. Interestingly, those correlations are sensitive to dietary changes, supporting the complexity of the interactions between nutrient-digestive microflora and host metabolism.

Nutritional Metabolomics

P-179

An in Vitro Vascular Niche Model for Expansion of Hematopoietic Stem Cells:Global Metabolite Profiling Reveals Unanticipated Transcellular Metabolic Networks

Lili Yang, Weill Cornell Medical College

Endothelial cells provide a critical “vascular niche” for in vivo expansion of hematopoietic stem and progenitor cells (HSPCs). This vascular niche was emulated ex vivo, using engineered human umbilical vein endothelial cells (E4+HUVEC) for expansion of HSPCs from cord blood. Untargeted metabolite profiling of co-cultured HSPCs and E4+HUVEC revealed a complex trans-cellular metabolism that we hypothesize is key for productive HSPC expansion. Findings are guiding studies to discover specific E4+HUVEC-derived metabolites that drive HSPC expansion.

P-180

An untargeted metabolic profiling study of plasma compounds affected by apple intake

Daniela Rago, University of Copenhagen

The research aims to investigate whether metabolic profiling may reflect health effects after feeding rats with raw apple for 13 weeks. The results indicate that apples may alter the gut microbial protein fermentation lowering toxic compounds (e.g. protein bound uremic toxins) and increasing metabolism into more protective products (e.g. 3-indole propionic acid).

P-181

Metabolomic profiling of changes in metabolism of CD1 rats from late gestation to early lactation using GC-MS

Umang Agarwal, University of Maryland

Plasma and liver samples were harvested from CD1 rats either at 14-16 days in gestation (n = 3) or 4-5 days in lactation (n = 3), and metabolite profiles determined by GC-MS. Automated analysis with Agilent Mass profiler professional detected 445 and 517 components in plasma and liver, respectively. Six metabolites in plasma and nine in liver were found to be different ($P < 0.10$), reflecting the onset of lipolysis and ketogenesis in lactation.

P-182

Metabolomics of Liver in Developing Chicken Embryos and Post-Hatch Chicks Identifies Metabolic Differences

Qiong Hu, University of Maryland-College Park

In this study, a metabolomic profiling approach using GC-MS and MetaboAnalyst web server was employed to investigate differences in metabolism in the liver of chicken embryos from two egg sizes and from broiler breeders of different maternal ages. Results reveal that liver metabolism involving Linoleic acid, glycerol, cholesterol, gluconeogenic and ketogenic amino acids (threonine, glycine, and serine) were distinct in embryos during later stages of development due to influences of breeder age and egg size.

P-183

Metabolic effects of fructose in human adipocyte – A stable isotope tracer based metabolic pathway analysis

Vijayalakshmi Varma, Biomarkers and Alternative Models Branch,

The metabolic effects of fructose on adipocyte, which can take up fructose, is not fully understood. This study examined the effects of fructose on adipocytes, using genomic and metabolomic approaches with [U-13C6]-D-fructose and [1, 2-13C2]-D-glucose respectively as single tracers. This study suggests that in adipocytes i) fructose has an anabolic role and is a potent lipogenic agent ii) in its presence; fructose pushes more glucose for energy production and alters the metabolism of glucose.

P-184

Metabolomics to Elucidate Food Processing Effects

Ric De Vos, Plant Research International, WUR

We will show that untargeted metabolomics, using both LCMS and GCMS, is a powerful technique to unravel the mechanisms underlying food processing-induced metabolite alterations, and to define and control key steps in food processing that determine product quality. Examples will be provided from industrial processing of fresh tomato fruits towards paste, from comparing food processing methods for their effect on vegetables for soup, and from freshly cut vegetables and fruit upon shelf-life in the supermarket.

Short Abstract Listing

Human Disease and Health Biomarkers III - Pathophysiology and Metabolic Pathways

P-185

Metabolic Profiling of Serum Samples by 1H NMR Spectroscopy as a Potential Diagnostic Approach for Septic Shock

Beata Mickiewicz, University of Calgary, Bio-NMR Centre

Human serum samples were analyzed by 1H NMR spectroscopy using a quantitative metabolomics approach. A multivariate statistical analysis (e.g. OPLS-DA) was applied to compare 59 serum samples. Very clear separation was obtained between patients suffering from septic shock and ICU controls without infection. Additionally a predictive model was build which had an excellent accuracy. Our results indicate that metabolomics might become a promising tool for diagnosis and treatment follow-up of septic shock.

P-186

Comparison of the Serum Metabolic Profiles from Hospitalized Patients with Acute Kidney Injury and a Control Population

Jinchun Sun, Biomarkers and Alternative Models Branch,

Rapid LC/MS-based metabolic profiling of serum demonstrated in a pilot study that metabolomics could provide novel indicators of acute kidney injury (AKI). Metabolic profiles of serum samples from seventeen hospitalized patients with diagnosed AKI were compared with the profiles of serum from age-matched subjects with normal kidney function. The results of this study demonstrate the utility of metabolomics in the discovery of novel serum biomarkers that can facilitate the diagnosis and determine prognosis of AKI.

P-187

1H NMR Metabonomics to Monitor Recovery Profile and Diagnose Malaria: Implications for Plasmodium vivax Infection

Arjun Sengupta, Tata Institute of Fundamental Research

1H NMR metabonomics of the post-hospitalization temporal (day1-5 and day30) urine profile of malaria infected patients was employed to gain insight into the recovery, perturbed biochemical pathways, and to explore the possibility of non-invasive diagnosis. The recovery starts from day 3. Perturbed metabolites suggest an altered guanidoacetate- glycine pathway and gut microbial metabolism. Significant correlation obtained between the parasitemia and urine profile of the patients opens up possibility of non-invasive diagnosis.

P-188

Bile Acid Profiling in Multifunctional Protein 2 (MFP-2) Knockout Mouse Using Liquid Chromatography Tandem Electrospray Mass Spectrometry

Anna Artati, Helmholtz Zentrum Muenchen

Multifunctional protein-2 (MFP-2) plays an important role in peroxisomal beta-oxidation and bile acids metabolism. We quantified the profile of 12 major bile acids in MFP-2 KO mice by LC-MS/MS. The concentrations of most bile acids in MFP-2 KO mice are significantly lower for both gender of mouse with the exception of the concentration of cholic acid in the liver of female mice.

P-189

Investigation of the Metabolic Changes Associated with Fanconi Anemia (FA) in Damaged and Undamaged Patient-Derived Human Keratinocyte Cell Lines

Miki Watanabe, Claflin University

The metabolic changes associated with Fanconi anemia (FA) in patient-derived, immortalized human keratinocytes were investigated in order to detect FA-specific small metabolites by NMR. The metabolic profiles from cell extracts and growth media from FA-deficient and -proficient cells were compared by pattern recognition software and statistical significance analysis. In addition, the cell extracts and media from these cells treated with DNA repair inducing agents were studied in order to obtain additional information on metabolic changes.

Short Abstract Listing

Human Disease and Health Biomarkers III - Pathophysiology and Metabolic Pathways

P-190

Metabolomics in Infectious Disease Research, the Case of Melioidosis

Saskia Decuypere, University of Western Australia

Metabolomics promises to be a powerful tool in infectious disease research for studying the nature of the pathogen driven disruption of the human metabolism during disease, and for identifying biomarkers that can improve the clinical management of infectious diseases. In this study, we evaluate the potential of metabolomics to (i) investigate the variation in disease process amongst bacteremic melioidosis patients with and without underlying diabetes, and (ii) identify clinically useful melioidosis biomarkers.

P-191

Metabolic Investigation of Urine and Plasma Profiles Obtained from Alcohol-Dosed Mice Using Accurate Mass LC-MS-MS

Craig Dorschel, Waters Corporation

Extreme alcohol consumption in man is a significant social and health issue. In this study a rodent “intragastric feeding model” was used together with accurate mass LC/MS/MS analysis to determine changes in the global metabolic profiles in both plasma and urine. The resulting raw data obtained were analyzed by multivariate statistical analysis (PCA). This analysis revealed that there was a significant difference in the between the profile of the control and alcohol treated group.

P-192

Metabolomic study on the myocarditis heart tissues of rat using HR-MAS 1H NMR spectroscopy

Hyun-ju Kim, Korea basic science institute

This study will show the valuable potential of HRMAS technique for investigating the metabolic phenotype of particular diseases and provide useful metabolic information related in myocarditis.

P-193

1H NMR-based Metabolomics to Study Effects of Ionizing Radiation in Human Lymphocytes

Heng-Chun Liu, Institute of Environmental Health

Human lymphoblastoid cell lines: TK6 (wild-type p53) and WTK1 (mutant p53) were used to examine metabolic effects of ionizing radiation. Time-course and dose-response experiments were conducted in cells treated with gamma-ray. Hydrophilic and hydrophobic metabolites were analyzed by 1H and J-resolved NMR followed by principal component analysis. The results showed a time- and dose- dependent effects. The metabolic finding will be compared with the results from transcriptomic studies. The roles of p53 may be suggested.

P-194

NMR- and MS-based Metabolomics to Investigate Effects of Naphthalene on Mouse Serum

Ching-yu Lin, Institute of Environmental Health

NMR and MS followed by multivariate analysis were applied to characterize metabolic effects of naphthalene in leading to cell injury in a susceptible species, mouse. After dose-response experiments, serum samples were collected for metabolomic analysis. CPMG 1H-NMR and validated UPLC-MS2 methods were applied to analyze metabolome and lipidome of serum, respectively. Diacyl-glycerophosphocholines (GPC), and their subclasses including alkyl-acyl- and alk-1-enyl-acyl-GPC, and related lyso-GPC were analyzed by UPLC-MS2 and correlated with naphthalene treatment.

P-195

Evaluation of Plasma and Urinary Steroids as Markers for CYP3A Activity in Healthy Subjects

Joo-Youn Cho, Department of Clinical Pharmacology and Therapeutics, Seoul National University

The endogenous marker for CYP3A activity is useful for prediction of CYP3A metabolic activity before administration of drugs which is metabolized by CYP3A. The 12-hours interval urine and plasma were collected in control, inhibited, and induced period to identify the endogenous markers for CYP3A activity using GC-MS-based quantitative steroid signatures. 16α-OH-DHEA/DHEA, 7β-OH-DHEA/DHEA, 6β-hydroxy cortisol/cortisol, and 6β-hydroxy cortisone/cortisone were well correlated with midazolam clearance.

Short Abstract Listing

Human Disease and Health Biomarkers III - Pathophysiology and Metabolic Pathways

P-196

Metabolic Alterations in Host Caused by Malarial Parasite Infection: 1H NMR Spectroscopic Investigations

Haripal Sonawat, Department of Chemical Sciences, Tata Institute of Fundamental Research

1H NMR investigation of organ and biofluid level metabolomic response towards malarial parasite infection in mice was carried out. The results suggested a clear sexual dimorphism during the disease progression. The female animals could maintain blood homeostasis at early stage while manipulating their excretory metabolite level unlike males. Despite their absence in global profile at early stage, individual brain metabolites showed significant perturbation during disease process.

P-197

Targeted Analysis of Polar Metabolites from Jukat T Cells using Ion Chromatography coupled to Tandem Mass Spectrometry

Sven Baumann, Helmholtz Centre for Environmental Research - UFZ

LC-MS/MS is a valuable tool for separation and identification of metabolites. However, polar compounds like organic acids and nucleotides are difficult to separate. Here we describe the combination of an ion-exchange system with MS/MS detection, which allows studies of polar key metabolites. Different protocols for extraction of intracellular metabolites were evaluated regarding their efficiency, recovery and reproducibility. Currently, investigations on activation and stimulation of Jurkat T cells and their effects on metabolites will be investigated.

P-198

Metabolomic Pathway Analysis reveals pattern of increased amino acid degradation from hyperglycemic pregnancy

Michael Muehlbauer, Duke University Medical Center

Software tools for pathway enrichment analysis in metabolomic studies have been developed to evaluate nontargeted gas chromatographic mass spectrometry (GC/MS) data sets using the UniPathway database. We examined archived samples from the Hyperglycemia and Adverse Pregnancy Outcome (HAPO) study, comparing serum metabolites from fifty pregnant mothers each in the upper and lower distribution of fasting plasma glucose. Hyperglycemic mothers exhibited increased amino acid degradation, a pattern previously seen in other conditions of compromised metabolic health.

P-199

NMR Metabonomics of Lung Tumour Tissues: Biomarker Profiles of Malignancy and Histological Type

Cláudia Rocha, University of Aveiro

Tumour and non-involved adjacent lung tissues, collected from near 50 patients after surgical resection and directly analysed by 1H High Resolution Magic Angle Spinning (HRMAS) NMR, could be clearly differentiated by multivariate analysis and putative biomarkers of malignancy were highlighted. Moreover, consistent metabolic differences were found between adenocarcinoma, carcinoid and epidermoid tumours, adding valuable knowledge on the biochemistry of different histological types of bronchial-pulmonary carcinomas, not available through conventional histopathology.

P-200

Identification of biomarkers for alcoholic liver disease from mice fed with unsaturated fat diets by gas chromatography-high resolution time-of-flight mass spectrometry

Schlegel David, LECO Corporation

High resolution TOF-MS in combination with GC is used to study the role of alcohol and diet in mice. The utility of this technology is demonstrated and its benefits in the context of the investigation of liver metabolites are shown. Several potential modulated metabolites are identified and associated with the changes in diet or chemical stress. High resolution and mass accuracy combined with MetPP processing provide a comprehensive tool for differential metabolomic analysis

P-201

Urine Metabolomic Analysis to Explore the Role of PPARβ/δ in Alcohol Induced Liver Damage

Maryam Goudarzi, Georgetown University

A protective role has been suggested for peroxisome proliferator-activated receptror-β/δ (PPARβ/δ) in alcoholic liver disease (ALD). Thus, this study aimed to examine the role of PPARβ/δ in ALD using metabolomic analysis in wild-type and Pparβ/δ-null mice. The results suggest a distinct separation between the metabolomic profile of mice based on genotype as well as diet. Several amino acid pathways showed significant differences in their urinary excretion levels with respect to genotype and diet.

Short Abstract Listing

Human Disease and Health Biomarkers III - Pathophysiology and Metabolic Pathways

P-202

Development of a Metabolic Biomarker Panel for the Early Diagnosis of Hepatocellular Carcinoma in Hepatitis C Infected Populations

Wendy Baker, UTMB

The objective of this investigation is to discover urinary metabolic biomarkers characteristic for the development of hepatocellular carcinoma (HCC) in hepatitis C virus (HCV) positive individuals. Urine samples from 36 HCC/HCV and 64 HCV patients were examined by 1H NOESY-presat NMR spectroscopy for neoplasia-indicative metabolites. Student's t-test analysis of the targeted data revealed 18 significant HCC-associated metabolites. Multivariate Adaptive Regression Spline analysis yielded an 11 member biomarker panel being 94% accurate for HCC prediction.

P-203

1H NMR-based metabolic profiling of chronic renal failure in rats

Juae Kim, KBSI

Chronic renal failure (CRF) is the gradual loss of the kidney's ability to filter waste and fluids from the blood. In this study, we applied a 1H NMR based metabolomics approach to investigate the altered metabolic pattern in serum from CRF model rats induced by surgical reduction in renal mass.

P-204

Diagnosis of Tuberculosis through a Urinary Metabolic Profile

Young-Sang Jung, KBSI

We investigated urinary metabolic profiles of Tuberculosis (TB), Treatment, Cured, and Control group. One dimensional proton NMR experiment was performed to collect NMR spectra of ~700 urine samples from seven different groups; TB, Treatment-1w, Treatment-1m, Treatment-2m, Treatment-6m, Cured, and Control group. Scores plot showed that the TB group is different with the Treatment groups as well as the Control group. The most significantly discriminating metabolites included hippurate, creatinine and citrate.

P-205

Metabolomic profiling differentiated diabetic nephropathy using capillary electrophoresis-mass spectrometry (CE-MS)

Akiyoshi Hirayama, Keio University

Diabetic nephropathy (DN) is the most common complication of diabetes and the exploration of new biomarkers bearing high sensitivity and specificity for DN diagnosis is of great importance. In this study, we utilized CE-MS for comprehensive analysis of serum metabolites from a total of 78 diabetic patients. The combination of serum metabolomics and multivariate analyses enabled accurate discrimination of DN stages, suggesting a possible novel diagnostic approach for DN.

P-206

Aberrant Fatty Acid Metabolism in Colorectal Cancer

Emily Mackay, Department of Medical Sciences, University of Calgary

Fatty acid profiling of serum samples from individuals with colorectal cancer (N=48) and age-and-gender matched disease-free controls (N=48) was performed using gas chromatography-mass spectrometry. Five biologically relevant fatty acids, palmitic acid, palmitoleic acid, oleic acid, elaidic acid, and cis-11-eicosenoic acid were found to be significantly more abundant in colorectal cancer (p-value<0.05, two-tailed t test). Characterization of aberrant lipid metabolism in cancer may provide the basis for development of preventative and targeted therapeutics.

P-207

Comparative Metabolome Analysis of Vitamin C-sensitive and -insensitive Cancer Cells

Megumi Uetaki, Institute for Advanced Biosciences, Keio University, Japan.

Recent studies suggested high-dose vitamin C exerts pro-oxidant effects and selectively kills the cancer cells. However, the cytotoxic mechanism of vitamin C hasn't been clarified yet. Here, we analyzed the metabolomic changes of vitamin C-sensitive and -insensitive cancer cell lines by CE-TOFMS. As a result, metabolomic changes of both cell lines in response to vitamin C treatment were similar to each other at toxic doses, suggesting that vitamin C toxicity links to the metabolomic changes.

Short Abstract Listing

Human Disease and Health Biomarkers III - Pathophysiology and Metabolic Pathways

P-208

Investigation of Antioxidant Metabolites in Cancer Cells by Capillary Electrophoresis Time-of-flight Mass Spectrometry

Keiko Iino, Institute for Advanced Biosciences, Keio University

Cancer cells are often adapts to stress environment by effectively eliminating reactive oxygen species. Metabolites may have a crucial role in this robust defense mechanism. We applied capillary electrophoresis time-of-flight mass spectrometry to identify the metabolites that potentially serve as antioxidants in cancer cells and found dozens of metabolites whose amounts were significantly high in hydrogen peroxide-resistant cancer cell lines. Interestingly, several of these metabolites indeed exhibited an ability to scavenge ROS in vitro.

P-209

The Human Urine Metabolome

Rupasri Mandal, University of Alberta

A comprehensive characterization of the human urine metabolome is presented. Multiple analytical platforms such as NMR, GC-MS, DFI-MS/MS, HPLC-UV/FLD and ICP-MS together with computer-aided literature mining tools were combined to quantify the metabolites that can be commonly detected in human urine. Our experimental methods yielded a total of 227 unique urinary metabolites that could be quantified. The human urine metabolome database lists these and 600 other literature-derived urinary compounds. It is freely available at http://www.urinemetabolome.ca.

P-210

The role of Metabolomics in pathway elucidation and confirmation using Propionic academia as an example

Barend Christiaan Vorster, Centre for Human Metabonomics, North-West University

The AMDIS compare tool was used to compare the urine organic acid spectra of 5 known propionic acidemia patients with a pooled control. The procedure was done with and without prior fraction separation with thin layer chromatography to confirm its validity. ±200 Compounds were identified. In addition to the known compounds, 21 compounds that have not been previously associated with PA were selected for biochemical pathway elucidation of poorly explained clinical observations.

P-211

Can Metabolite Profiling Identify Patients at Risk for Cancer?

Daniel Raftery, University of Washington

Our recent work has shown that the use of metabolite profiling can identify patients who are at risk for a number of different cancers. Interestingly, we find that this pattern in which at risk patients have intermediate levels of certain metabolite cancer biomarker candidates repeats itself for a variety of cancers. This approach might be useful towards the stratification of patients for diagnostic purposes.

P-212

Haem oxygenase is synthetically lethal with the mitochondrial tumour suppressor fumarate hydratase

Christian Frezza, Hutchison/MRC research center

Germline mutations of the TCA cycle enzyme FH are responsible for Hereditary Leiomyomatosis and Renal-Cell Cancer (HLRCC). Here we used newly characterized Fh1 knock out mouse cells and applied a computer model of the metabolism of these cells to predict and experimentally validate a linear metabolic pathway beginning with glutamine uptake and ending with bilirubin excretion. We predicted and confirmed that targeting this pathway would render Fh1-deficient cells non-viable, while sparing Fh1 wild-type cells.

P-213

Intracellular Metabolomic Study of Estradiol-induced effects in Human Breast Cancer Lines MCF-7

Liang Zhao, Johns Hopkins, School of Public Health, Department of Enviromental Health Sciences

Estradiol (E2) has a critical impact not only on reproductive and sexual functioning, but also on other organs mediated through the estrogen receptors. Our objective is to map pathways of endocrine disruption (ED) by performing an intracellular metabolomics study using human breast cancer cell line MCF-7. These studies should provide more insight into the identification of the metabolomics effects of E2 and may reveal pathways associated with ED.

Short Abstract Listing

Human Disease and Health Biomarkers III - Pathophysiology and Metabolic Pathways

P-214

Metabolic phenotype and its relationship with CYP2D6 genetic polymorphisms and pharmacokinetic variation

Seo Jeong Ju, Department of Biomedical Science, Graduate School, Kyungpook National University

CYP2D6*10 is the most common allele in Asians. Because CYP2D6 is involved in about 70-80% of the metabolism of metoprolol, it has been reported that CYP2D6*10 genetic polymorphism is responsible for the pharmacokinetic (PK) variability. A metabolomic approach can be a useful tool to predict the individual PK variation associated with both genetic and environmental factors. In our studies suggest that this approach may potentially provide a new powerful tool for prediction of PK variation.

P-215

Metabolite Profiling Identifies Early Diabetic Changes Leveraging

Dietrich Rein, Metanomics Health GmbH

Early detection and treatment of type 2 diabetes (T2D) reduces the risk of developing disease-associated complications. A better understanding of the metabolic changes involved might help identifying new ways of preventing or slowing down disease progression. We explored the performance and the value of specific metabolic marker panels for T2D risk assessment as well as the pathophysiological mechanisms contributing to the disease.

P-216

1H NMR-based Metabolic Profiling of Blood Plasma and Milk in Dairy Cows Reveals Physiological Mechanisms Underlying Economically Relevant Traits

Anthony Maher, Department of Primary Industries

We have applied statistical heterospectroscopy and projections to latent structures to 1H NMR data from milk and blood plasma collected from Holstein dairy cows. The results revealed latent intra-individual relationships between metabolites across these biofluids. The results have implications for understanding bovine physiology and potential for predicting economically relevant traits such as milk yield using NMR-based metabolic profiling.

P-217

Metabolic Profiles of Cancer Cells Cultured in the Presence of Endogenous Antiproliferative Metabolites

Amy Su, Department of Chemical and Biomolecular Engineering, Georgia Institute of Technology

Understanding cancer cell metabolism is vital to both cancer diagnostics and treatment. The increased or decreased presence of various endogenous metabolites have been shown to exhibit antiproliferative behavior in cancer cells, but the mechanism that causes growth inhibition is not always known. Analysis of the overall metabolite levels of Jurkat cells grown with additions of these metabolites can reveal connections which give insight to their role in cancer cell metabolism.

New Technology & Measurements Posters

P-218

Development of a High-Throughput Protocol for Metabolite Extraction and Quantification from Tissue to Study Diabetes Related Pathways

Sven Zukunft, Helmholtz Zentrum Muenchen

We present a high-throughput quantification method for the simultaneous quantification of 186 metabolites from tissue. We tested different extraction solvents with 11 different mouse tissues and analysed recovery, quantification, reproducibility, and suppression effects. For proof of concept these extraction conditions were applied to tissue samples from drug treated and non-treated diabetic mice.

P-219

Testing Times for Tuberculosis: A Metabolomics Approach to Characterise and Identify Various Mycobacterium Species

Du Toit Loots, NWU-Centre for Human Metabonomics

Using GC-MS and chemometrics, we built a classification model for various TB causing and non-TB Mycobacterium species, based on Bayes' theorem, using 12 metabolite markers identified via PCA and PLS-DA, after a modified Bligh-Dyer fatty acid extraction. This model subsequently correctly classified the unknown samples of each of the Mycobacterium species, cultured from patient sputum 6 months later, with probabilities ranging from 72-100%, in less than 16h, with a detection limit of 1000 CFU/mL.

P-220

Can We Trust Untargeted Metabolomics: First Results of the Metabo-Ring Study

Jean-Charles Martin, INRA

We designed a ring test to evaluate the convergence of the same biological information extracted from various NMR (n=4) and MS (4 QTOF and 4 orbitraps) in non-targeted metabolomics. The same rat plasma samples were analyzed by all the participants. Convergence within NMR (78 to 91%) were slightly better than within MS (57 to 87%). Convergence between NMR and MS was lower (37 to 87%). Improvement can be easily achieved by a tight standardization.

P-221

The Search for Surface Active Compounds on Native Stingless Australian Bees by Desorption Electrospray Ionisation Mass Spectrometry

Lewis Adler, Bioanalytical Mass Spectrometry Facility

Stingless native Australian bees, Austroplebeia australis and Tetragonula carbonaria are known to have surface active compounds that act as antimicrobials. Previous work extracted these components from whole bees, without distinction between differing body parts. In this study we explore surface compounds on three regions of the bee; head, thorax/wings, and abdomen using Desorption Electrospray Ionization Mass Spectrometry. Data presented here are the initial surface components detected. Also a brief overview of future methodology will be described

P-222

Technological Advances in Metabolomics: the Role of Ultrahigh-Resolution FT-ICR MS

Wiebke Timm, Bruker Daltonik GmbH

Large-scale experiments aimed to identify and quantify metabolites currently suffer from analytical and computational limitations. No single analytical technique can effectively deal with all chemical classes of metabolites. Idnetification by Mass spectrometry (MS) is typically limited by the frequent need to perform MSn analyses. Sub-ppm mass accuracy alone is often insufficient to unambigously assign elemental compositions. We present a method using isotopic fine structure information acquired by ultrahigh-resolution FTMS instrumentation to identify elemental compounds uniquely.

New Technology & Measurements Posters

P-223

Untargeted metabolic profiling using a new generation high-field linear ion trap Orbitrap hybrid mass spectrometer (Orbitrap Elite)

Annie Evans, Metabolon, Inc.

Untargeted metabolic profiling involves identification and quantification of as many metabolites in a biological system as possible. Ultrahigh Performance Liquid Chromatography Mass Spectrometry is the standard for analyzing biological samples, which enables superior chromatographic separation. Advances in high-resolution MS instrumentation incorporate desirable features, including fast spectral acquisition rate, high mass accuracy, and increased detection sensitivity. In this study, the recently introduced Orbitrap Elite equipped with UPLC is evaluated for high-throughput untargeted metabolic profiling.

P-224

Identification of Human Fumarylacetoacetate Hydrolase Domain Containing Protein 1 (FAHD1) as a Novel Mitochondrial Acylpyruvase

Haymo Pircher, Austrian Academy of Sciences

The human fumarylacetoacetate hydrolase (FAH) domain containing protein 1 (FAHD1) is part of the FAH protein superfamily, but its enzymatic function was previously unknown. In quest for a putative enzymatic function of FAHD1, we found that FAHD1 exhibits acylpyruvase activity, demonstrated by the hydrolysis of acetylpyruvate and fumarylpyruvate in vitro. Conserved amino acids D102 and R106 of FAHD1 were found important for its catalytic activity, and Mg2+ was required for maximal enzyme activity.

P-225

A highly sensitive GC-MS/MS method for absolute quantification of amino and non-amino organic acids, including a robotized derivatization step

Hans Fredrik Kvitvang, NTNU (Norwegian University of Science and Technology)

The ultimate requirement for a quantitative description of the metabolite pool - in biological cells and fluids - is absolute concentration determination. We have developed a high-throughput and sensitive gas chromatography-tandem mass spectrometry (GC-MS/MS) targeted metabolite profiling method. This profiling method enables absolute quantification of all detected amino- and non-amino organic acids. The method is based on methyl chloroformate (MCF) derivatization and quantification by spiking samples with metabolite standards separately derivatized with deuterated derivatization reagents.

P-226

Analyzing Aloe vera by NMR in Automation with the Assure-RMS Software Package: Quantitative Measurements of Metabolites and Potential for Classification

Michelle Markus, Bruker BioSpin

1H-NMR spectroscopy is a powerful technique to analyze complex mixtures such as the natural product Aloe vera because individual components can be analyzed without separating the mixture. The previously published NMR method for quantifying components of Aloe vera has been implemented within the Assure-RMS software, which provides full automation from acquisition to final report. The potential to generate a “fingerprint” for Aloe vera based on its metabolic profile as captured by NMR is explored here.

P-227

Targeted Metabolomics Analysis of Animal Plasma Using a Combined Flow Injection and UPLC-MS/MS Assay

Ralf Bogumil, BIOCRATES Life Sciences AG

We analyzed plasma samples from different animal species in comparison to human plasma. A quantitative targeted metabolomics method was applied consisting of a combined flow injection LC-MS/MS method. To improve the turn-around time we have developed a fast UPLC method. A high number of metabolite concentrations were observed to be significantly different in animal plasma compared to human plasma, but most metabolites were found to be still in the specified concentration range of the validated assay for human plasma.

New Technology & Measurements Posters

P-228

Metabolic profiling of a Drosophila melanogaster cytosolic Superoxide dismutase null allele in using Liquid Chromatography/Mass Spectrometry

Thomas Merritt, Laurentian University

We are developing protocols for liquid chromatography/mass spectrometry based metabolomic characterization of genetic variation using the cytosolic superoxide dismutase gene (Sod1) in Drosophila melanogaster as a model. SOD1 is involved in reactive oxygen species scavenging; Sod1 mutants accumulate both ROS and ROS damage. Initial work is targeting “known” metabolites to allow us to develop and optimize protocols. Subsequent work will use these protocols to expand our investigation to a broader, currently unknown, suite of metabolites.

P-229

Sauvignon Blanc Juice Index: Analysis of Phosphorylated Metabolites and Related Compounds in grape juice and wines

Francesca Casu, The University of Auckland

Metabolite profiles of grape juices may provide new tools for prediction of wine properties before fermentation starts. In fact, wine’s features are influenced by the grape juice compounds which affect the yeast metabolism during the fermentation. The objective of this work is to correlate the level of phosphorylated metabolites in the juice with the chemical and sensorial properties of fermented wines. Thus, we will present our method development for high-throughput analysis of phosphorylated metabolites in grape juices and wines.

P-230

Modified fluorescent dyes for glycerophospholipid absolute quantification using LC-FTICR-MS

Sergey Tumanov, The University of Auckland, New Zealand

ESI-MS has become a suitable analytical platform for the analysis of multicomponent lipid fractions from biological samples due to its higher sensitivity and capacity for high throughput analysis. Glycerophospholipid labeling within fluorescent dye followed by LC-FTICR-MS analysis will allow expanding the quantification linear concentration range, analyzing the sample in one positive ion mode, avoiding introduction of inorganic ions and shifting the masses of molecular ions of lipid-dye conjugates to the range of 1100-1600 Da.

P-231

Development of an LC-MS-based Method to Evaluate Bile Acids in Non-Human Primates as Potential Biomarkers of Metabolic Disease.

Aaron Zefrin Fernandis, Merck Sharp & Dohme

We report a LC-MS-based method for quantification of 20 bile acids in plasma. The baseline level of these species in 25 naive Cynomolgus macaque plasma samples serves as a reference for intra-individual variability and distribution of the bile acids in a normal cohort. Animals with progressing diseases will be monitored for these bile acids to determine if any would serve as useful biomarkers for disease progression or treatment efficacy.

P-232

Targeted serum lipidomics by ultra performance liquid chromatography coupled with tandem mass spectrometer

Jun Feng Xiao, Georgetown University

Phospholipids are involved in a variety of human biological processes and have been previously reported as potential disease biomarkers. In order to perform high throughput validation of candidate phospholipids, a fast and accurate quantitation method is needed. In this study, we present LC-ESI-MS/MS based quantitation of selected phospholipids using isotope dilution by selected reaction monitoring. We demonstrate the effectiveness and accuracy of the method in detecting lipidomic changes in serum samples.

New Technology & Measurements Posters

P-233

Exploration and Optimisation of Mass Spectrometric and Chromatographic Parameters for LC-MS Metabolomics Profiling Experiments

Russell Pickford, University of New South Wales

This work details the progress in bringing metabolomics profiling capabilities to our facility, so as to offer them to collaborators. The research compares results obtained from applying different chromatographic and mass spectrometric approaches to two 'test case' metabolomics samples. The overall aim is to establish a 'best practice' approach for new metabolomics experiments employing liquid chromatography and mass spectrometry in our facility.

P-234

Targeted Metabolomics for Bioprocess Optimization

Denise Sonntag, BIOCRATES Life Sciences AG

Targeted metabolomics was used to optimize bioprocesses for the production of biologicals. The metabolomics approach to bioprocess monitoring made it possible to determine the concentration of a multitude of analytes from several metabolite classes in a sample- and time-efficient way by using small sample volumes and a multi-assay strategy on a mass-spectrometry platform. We will present case studies from cell fermentations to point out the feasibility and significance of the metabolomics technology for this application.

P-235

Development of Sampling, Sample preparation and Targeted UPLC-MS/MS method for Eicosanoid and Oxylipins in Cell, Plasma and Apidose Tissue Samples

Sirkku Jäntti, VTT Technical Research Centre of Finland

Eicosanoids are signaling lipids produced by oxidation of essential fatty acids. The goal was to study the lipid composition of adipose tissue, and for this purpose, a novel methodology for the reliable determination of eicosanoids in adipose tissue, as well as in cell and plasma was developed including 49 oxylipins by ultra performance liquid chromatography-tandem mass spectrometry. Several oxylipins could be detected and quantitated from human adipose tissue.

P-236

Metabolomic Profiling of Uremia With an LC-EC Array-MS Parallel Platform

Ian Acworth, Thermo Fisher Scientific

Kidney disease can lead to the uremic syndrome. Novel robust and sensitive analytical methods are capable of accurately and selectively detecting molecules that span a diverse chemical spectrum and an extremely large concentration range, thereby enhancing the likelihood of discovering biomarkers and establishing metabolomic profiles of specific diseases. The objective of this project was to characterize the metabolomic profile of patients with uremia using a novel HPLC-electrochemical (EC) array—mass spectrometry (MS) parallel platform.

P-237

Using Electrochemistry-MS to Investigate Biological Metabolite Identification in Metabolomic Studies

Yingying Huang, Thermo Fisher Scientific

A significant challenge in metabolomics is identification of unknown metabolites in biological matrices. We have investigated the use of electrochemical (EC) flow-cells on-line with LC-MS for their potential to facilitate structural identification of low-level species through biomimetic production of oxidative metabolites. We used EC to generate oxidative products for characterization by EC-Array and MS. These data were guided analytical conditions for targeted analysis in biological tissue obtained from an experimental model of oxidative stress.

New Technology & Measurements Posters

P-238

A Comprehensive Approach to Metabolomics - High Performance Time-of-Flight Mass Spectrometry with Advanced Bioinformatics Tools

Xiang Zhang, University of Louisville

High resolution TOF-MS data is combined with highly effective processing tools and evaluated using liver metabolites from disease models in mice. The benefits of data from high resolution MS interfaced to both GC and LC is demonstrated by the complementary nature of modulated metabolites observed. Our observations in the metabolite profile changes agree with the histological results and indicate that the metabolic effects of PCB 153 were highly dependent on nutrient interactions and antioxidant depletion.

P-239

Repeatability of LECO LC-HRT-MS in Analysis of Metabolite Extract from Mouse Liver

Nick Hall, LECO Corporation

The repeatability, reproducibility, and robustness of a HILIC LC-MS method using high performance TOF-MS is characterized for the analysis of biological samples in metabolomics applications. A pooled metabolite extract was analyzed on each of five days with replicate injections in combination with changes to the system. Experimental data were processed using MetSign and Chromatof HRT softwares. The analytical and mass spectral performance was evaluated over this period to provide an understanding of its inherent capabilities.

P-240

Comprehensive and Complementary Plant Metabolomics using GCxGC-TOF and High Performance Time of Flight Mass Spectrometry Interfaced to UHPLC and GC

Luo Jie, College of Life Science and Technology

Two-dimensional GC interfaced to time-of-flight mass spectrometry and high performance time-of-flight mass spectrometry (HP-TOF-MS) interfaced to UHPLC and GC are used to provide complementary information on the metabolic state of rice and corn strains. Differences in key metabolites are identified with each technique. The combination of these high performance techniques and complement of GC and LC provides comprehensive analyte identification through high mass spectral and GC resolving power.

P-241

Translating Metabolomics into Clinical Practice with the Vantera NMR Clinical Analyzer

Thomas OConnell, LipoScience Inc.

For metabolomics to realize its full clinical potential, the detection of biomarkers has to be translated onto a robust, high-throughput platform that can be deployed in clinical laboratories. The Vantera NMR Clinical Analyzer was developed to enable the advantages of NMR detection in a clinical laboratory. Currently quantification of lipoprotein particles and a number of small molecule metabolites are being validated for the diagnosis and management of cardiovascular disease and diabetes.

P-242

Radiation metabolomics and minimally invasive exposure-prediction modeling with principal components analysis

John B Tyburski, Georgetown University Medical Center

The nation’s medical capacity for handling radiological exposures is inadequate. In this report, we extend our findings in the area of radiation metabolomics and radiation biomarker discovery. We compared urine samples from male mice before and after exposure to near-lethal doses of ionizing radiation and created predictive models with varying number of pre-exposure samples using principal components analysis of time-of-flight mass spectrometric data. These models show substantial promise for discriminating exposed and unexposed mice.

New Technology & Measurements Posters

P-243

Applications of Capillary Ion Chromatography Mass Spectrometry to Metabolomics Research

Mark Sanders, Thermo Fisher Scientific

Ion chromatography (IC) is a complimentary separation technique to HPLC, and recent applications include coupling to mass spectrometry for identification and quantification of metabolites. Capillary IC-MS extends IC capabilities by improving the sensitivity and stability as well as reducing the amount of sample required. This study demonstrates IC application on the targeted analysis of organic acid metabolites, sugar phosphate and energy phosphates, quantitation of isobaric sugar phosphates and the metabolic profiling of 19 nucleotides.

P-244

Combined Genomic-Metabolomic Approach for the Differentiation of Geographical Origins of Natural Products: Deer Antlers as an example

Xing Jin, college of pharmacy, seoul national university

The correct identification of the geographical origin of deer antlers is essential to quality control. In this study, we applied both genomics and motabolomics to the origin identification of 101 samples from Canada, New Zealand, and Korea. The genomics identified deer species in each country but failed to categorize all the samples. NMR-based metabolomics gave clean separations, compounds specific to each country were identified, and the validity was confirmed by prediction analysis.

P-245

Exploring GC/Q-TOF Workflow For Identification of Unknowns in Biological Samples

Mine Palazoglu, UC Davis Genome Center

In metabolomics, identification of unknowns is one of the challenges that would benefit from the improvements in mass spectrometry technologies. In typical metabolomics profiling experiments, only small fraction of annotated peaks are identified. In this study, GC/QTOF and GC-APCI/QTOF are compared for mass accuracy, isotope distribution and MS/MS fragmentation patterns at different collision energy levels. Using accurate mass isotope distribution and MS/MS fragmentation information from both instruments, the compound identification workflow is being tested.

P-246

Accelerating structural annotation: searching candidate (bio)chemical substrate product pairs in the metabolome

Kris Morreel, Plant Systems Biology, VIB-UGent

In metabolomics, thousands of metabolites are profiled but, disappointedly, most of them cannot be structurally characterized as MS database construction occurs at a slow pace. Complementary high-throughput approaches are therefore necessary. Here, we describe a new method employing biochemical information that allowed the characterization of 145 compounds in rosette leaves of Arabidopsis thaliana Col0 using LC-negative ionization-MS. Based on the Scifinder database, half of these compounds have never been described in plants before.

P-247

Metabolomics Strategies Using GC-MS/MS Technology

Anthony Taylor, Thermo Fisher Scientific (Schweiz) AG

The central strategy in metabolomics is described using GC-MS/MS technology. First, a semi-quantitative discovery phase identifies as many metabolites as possible. GC-MS with EI ionization offers distinct advantages in the compound identification employing large commercial general as well as dedicated spectral libraries. Both the discovery phase as well as the targeted phase are performable with one instrument. Very low detection limits and a dynamic range of up to 6 orders of magnitude can be presented.

New Technology & Measurements Posters

P-248

Differential Metabolomic Profiling of Wheat Cultivars by IROA (Isotopic Ratio Outlier Analysis)

Chris Beecher, NextGen Metabolomics Inc

The differential metabolite profiles of the leaves and stems of two very different, cultivars of wheat, 'Halberd' an Australian heat-tolerant spring wheat, and 'Len' an American heat- sensitive hard red spring wheat were determined using the IROA protocol. Metabolite differences of amino acids and sugars observed between the two cultivars will be discussed. These finding demonstrate the potential for a biochemical profiling approach using 13C IROA-based methodologies to characterize metabolites of varietal importance.

P-249

Influence of Hemolysis on Metabolite Profiles of Plasma Samples in LC-MS/MS-based Metabolomics Analysis

Manuela J. Rist, Max Rubner-Institut

Since hemolytic plasma or serum samples may pose problems in metabolomics, we tried to investigate the influence of hemolysis on metabolite profiles. Plasma samples with different degrees of hemolysis were analyzed by LC-MS/MS. For most detected compounds no difference was observed over all samples of the same volunteer, only few masses increased or decreased with increasing hemoglobin concentration. For this generic LC-MS/MS method, slightly hemolyzed plasma samples appear to be tolerable in metabolic profiling studies.

P-250

Implementing Metabolite Profiling in Bioprocessing Applications

Ulrike Rennefahrt, Metanomics GmbH

Manufacturers encounter several challenges towards optimizing bioprocessing processes, e.g. product yield, development and scale-up of biotechnology products and processes, reproducibility of reactor operation, strain improvement and media optimization. Towards this goal, Metanomics Health GmbH, a BASF Group company founded in 2003, offers robust and highly reproducible targeted and non-targeted comprehensive metabolite profiling services (metabolomics).

P-251

Metabolite Profiling Identifies Endogenous Substrates and Products of the Mitochondrial Sulfur Dioxygenase ETHE1

Changyuan Lu, Weill Cornell Medical College

Hydrogen sulfide is a gaseous signaling molecule that can be produced by all cell types. A mitochondrial sulfide oxidizing complex has been identified that serves to limit endogenous sulfide levels. ETHE1 is a critical sulfur dioxygenase found in this sulfide detoxification complex. In this study, we used metabolite profiling to successfully identify the endogenous cellular substrate and product of ETHE1 as glutathione persulfide and glutathione, respectively.

P-252

NMR Based Metabolomics in Clinical Studies of Human Population

David Krings, Bruker BioSpin

NMR over many years was used for structure elucidation of pure compounds, however in the last decade NMR established itself as a major tool for metabolomics analysis based on its unmatched reproducibility and transferability properties. In our contribution, we report on the application of NMR in a cohort of 700 Neonates, where urine samples are taken and analysed between day 1-3 with the aim of a health and disease assessment. Such, we demonstrate the value of NMR for molecular epidemiology with a diagnostic potential.

P-253

MALDI-MS Imaging and LC-MS-based Metabolomics Reveals Spatiotemporal and Detailed Metabolomic Dynamics in MCAO Rat Brain

Daisuke Miura, Kyushu University

In our previous works, spatiotemporal metabolic dynamics of the brain of transient middle cerebral artery occlusion (MCAO) rat during infarct formation after ischemia reperfusion were analyzed by newly developed in situ metabolomic imaging technique. Here we performed LC-MS analysis to trace molecular coverage of the brain of MCAO rat for comprehensive analysis. Integration of MALDI-MS imaging and LC-MS-based matabolomics would visualize drastic changes in spatiotemporal metabolite distribution.

New Technology & Measurements Posters

P-254

Unlocking flavour through metabolomics. A new way of analysing flavour in food and beverages

Nicolas Schauer, Metabolomic Discoveries GmbH

Mangos often need to be harvested early to arrive in ripeness stage in the supermarket. The fruit has therefore little time on the plant to develop flavour. To understand mango flavour and its correlation with ripeness, we have used our Flavour Profiler platform to screen for flavour components contributing to ripe and unripe mangos. A consumer panel scored the taste and ripeness of mangos. The Flavour Profiler platform allowed to model and predict mango flavour.

P-255

Comparison of Extraction Methods for NMR-base Metabolomic Analysis of Mice Liver

Andrey Tikunov, UNC Metabolomic facility

Extraction procedure is the crucial step affecting final sample composition and outcome of the metabolomic analysis. Prior knowledge of an extraction method's capabilities as well as its limitations is a necessary reference invaluable when designing metabolomics experiments or when interpreting results. Within the past 8 years, there have been over 15 NMR-based and 14 MS-based extraction publications however all have failed to reported empirical extraction efficiencies for specific, biologically relevant metabolites.

P-256

Study of small molecules captured in a pellet after protein precipitation of plasma sample

Zheng Ouyang, Bristol-Myers Squibb Company

When preparing plasma for metabolomics analysis, addition of cold acidified methanol results precipitation of dissolved proteins. Re-extraction of this sedimented protein pellet with eight different solvents was performed to study the recovery of individual metabolites that co-precipitate with protein. Our results reveal that the protein pellet contains certain metabolites in amounts comparable with their quantity in supernatant. This observation is important to consider when developing metabolomics methodologies for proteinaceous biolfuids.

P-257

In situ Metabolomics via Vapour-mediated Ion Activation Enhanced SIMS

John Pugh, The University of Sheffield

Time-of-flight secondary ion mass spectrometry (ToF-SIMS) imaging is increasingly generating interest in the field of bioanalysis. The technique can provide metabolomic information, through the detection of molecular species in biological samples. We report our recent investigations to increase the ionisation probabilities of metabolites. Results provide evidence for examining vapour-mediated ion activation approaches, to enhance ToF-SIMS analyses, for use as a tool in metabolic research.

Workshop - Software Showcase

P-258

Concurrent Metabolites for Global Metabolomics from Accurate MS

Hongping Dai, Metabolon, Inc.

Global metabolomics profiling is strived to detect and identify as many metabolites as possible in biological samples. Still, more unknown are detected than known metabolites. Correlation methodology was used to uncover various forms of ions from each of the concurrent metabolites across sample. Accurate mass spectrometry has much better resolution and so many more ions are differentiated and detected. Applying the correlation methodology to accurate mass would result in identification of more unknown metabolites.

P-259

A New Integrated Bioinformatics Tool for Metabolomic Data Handling

Gunnar Libiseller, HEALTH / JOANNEUM RESEARCH

There are now several programs and databases for managing metabolomics data, including tools for peak detection, alignment, normalization, statistics and many more. But there has been no single tool that can handle everything from data conversion to compound identification, let alone individualized storage of results, statistical analysis along with management of projects, studies and experiments within one graphical user interface—until now: We have created an integrated bioinformatics tool – the Joanneum Research metabolomics database (JRMDb).

P-260

Automated Analysis of High Resolution LC-MS Profiles of Biological Samples in Metabolomics Studies

Serhiy Hnatyshyn, Bristol-Myers Squibb Company

High resolution LC-MS provides a practical way to analyze highly complex biological samples. It enables the detection of a wide variety of molecules and facilitates a quantitative evaluation while also being amendable to high throughput. Data analysis automation is required for the conversion of a high information content LC-MS datasets into meaningful lists of metabolites. Automated analysis includes spectral interpretation, alignment and comparison across many samples. Recent advances in automation of metabolomics data analysis are discussed and illustrated with the examples.

P-261

Related Seasonal and Geographical Differences in Wine from California's Central Coast

Michael Athanas, Thermofisher

We investigate factors that may influence organoleptic properties of wine including micro-climate and soil conditions. Vintage must and wine samples were collected from central California vineyards during the 2007 through 2011 growing seasons. Samples were analyzed using LC-MS differential analysis to determine the relative levels of various expected flavonoids as well as unexpected constituents. The results from this study provide a catalogue and differential statistical analysis of the compounds present across the samples.

Short Abstract Listing

Workshop - Analytical QC Measures for Interlaboratory Comparability

P-262

Quality Control with High Resolution Metabolomics on a Dual Chromatography Fourier Transform Mass Spectrometer

ViLinh Tran, Emory University Dept of Pulmonary

High-resolution metabolomics measures thousands of m/z features (accurate mass of m/z features within 5 ppm range, retention time, and associated integral). Because of the large number of features measured, most represents unidentified chemicals; it is impractical to use traditional quality control procedures. Daily determination of CV for total ion intensities and a selected internal standard, along with ∆ppm of 5 internal standards provides a simple means to assure quality control for high resolution metabolomics data.