Metabolic profiling allows comprehensive phenotyping of genetically or environmentally modified plant systems

U Roessner, A Luedemann, D Brust, O Fiehn… - The Plant …, 2001 - Am Soc Plant Biol

Metabolic profiling using gas chromatography–mass spectrometry technologies is a technique whose potential in the field of functional genomics is largely untapped. To demonstrate the general usefulness of this technique, we applied to diverse plant genotypes …

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Measuring the metabolome: current analytical technologies

WB Dunn, NJC Bailey, HE Johnson - Analyst, 2005 - pubs.rsc.org

The post-genomics era has brought with it ever increasing demands to observe and characterise variation within biological systems. This variation has been studied at the genomic (gene function), proteomic (protein regulation) and the metabolomic (small …

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Systems level studies of mammalian metabolomes: the roles of mass spectrometry and nuclear magnetic resonance spectroscopy

WB Dunn, DI Broadhurst, HJ Atherton… - Chemical Society …, 2011 - pubs.rsc.org

The study of biological systems in a holistic manner (systems biology) is increasingly being viewed as a necessity to provide qualitative and quantitative descriptions of the emergent properties of the complete system. Systems biology performs studies focussed on the …

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[HTML] The human urine metabolome

S Bouatra, F Aziat, R Mandal, AC Guo, MR Wilson… - PloS one, 2013 - journals.plos.org

Urine has long been a “favored” biofluid among metabolomics researchers. It is sterile, easy-to-obtain in large volumes, largely free from interfering proteins or lipids and chemically complex. However, this chemical complexity has also made urine a particularly difficult …

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Metabolomics: from pattern recognition to biological interpretation

W Weckwerth, K Morgenthal - Drug discovery today, 2005 - Elsevier

Metabolomics is a technology that aims to identify and quantify the metabolome–the dynamic set of all small molecules present in an organism or a biological sample. In this sense, the technique is distinct from metabolic profiling, which looks for target compounds …

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Construction and application of a mass spectral and retention time index database generated from plant GC/EI-TOF-MS metabolite profiles

C Wagner, M Sefkow, J Kopka - Phytochemistry, 2003 - Elsevier

The non-supervised construction of a mass spectral and retention time index data base (MS/RI library) from a set of plant metabolic profiles covering major organs of potato (Solanum tuberosum), tobacco (Nicotiana tabaccum), and Arabidopsis thaliana, was …

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[HTML] Quantitative metabolomics based on gas chromatography mass spectrometry: status and perspectives

MM Koek, RH Jellema, J van der Greef, AC Tas… - Metabolomics, 2011 - Springer

Metabolomics involves the unbiased quantitative and qualitative analysis of the complete set of metabolites present in cells, body fluids and tissues (the metabolome). By analyzing differences between metabolomes using biostatistics (multivariate data analysis; pattern …

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Metabonomics classifies pathways affected by bioactive compounds. Artificial neural network classification of NMR spectra of plant extracts

KH Ott, N Aranîbar, B Singh, GW Stockton - Phytochemistry, 2003 - Elsevier

The biochemical mode-of-action (MOA) for herbicides and other bioactive compounds can be rapidly and simultaneously classified by automated pattern recognition of the metabonome that is embodied in the 1 H NMR spectrum of a crude plant extract. The ca. 300 …

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[CITATION] Metabolic profiling: a Rosetta Stone for genomics?

RN Trethewey, AJ Krotzky, L Willmitzert - Current Opinion in Plant Biology, 1999 - Elsevier

Man has always aspired to understand the nature of life and the chances of achieving this, at least at the molecular level, have never looked better. As a technolog) i-driven revolution sweeps through the life sciences and we are submerged in an avalanche of new information …

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High-resolution metabolic phenotyping of genetically and environmentally diverse potato tuber systems. Identification of phenocopies

U Roessner, L Willmitzer, AR Fernie - Plant physiology, 2001 - Am Soc Plant Biol

We conducted a comprehensive metabolic phenotyping of potato (Solanum tuberosum L. cv Desiree) tuber tissue that had been modified either by transgenesis or exposure to different environmental conditions using a recently developed gas chromatography-mass …

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Principal component analysis of urine metabolites detected by NMR and DESI–MS in patients with inborn errors of metabolism

Z Pan, H Gu, N Talaty, H Chen, N Shanaiah… - Analytical and …, 2007 - Springer

Urine metabolic profiles of patients with inborn errors of metabolism were examined with nuclear magnetic resonance (NMR) and desorption electrospray ionization mass spectrometry (DESI–MS) methods. Spectra obtained from the study of urine samples from …

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Metabolic Profiling of Root Exudates of Arabidopsis thaliana

TS Walker, HP Bais, KM Halligan… - Journal of Agricultural …, 2003 - ACS Publications

This paper was withdrawn on October 7, 2009 (J. Agric. Food Chem. 2009, 57, 9346). In addition to accumulating biologically active chemicals, plant roots continuously produce and secrete compounds into their immediate rhizosphere. However, the mechanisms that drive …

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[BOOK] Metabolome analysis: an introduction

SG Villas-Boas, J Nielsen, J Smedsgaard… - 2007 - books.google.com

Providing information on the main approaches for the analysis of metabolites, this textbook: Covers basic methodologies in sample preparation and separation techniques, as well as the most recent techniques of mass spectrometry. Differentiates between primary and …

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Comprehensive analysis of metabolites in Corynebacterium glutamicum by gas chromatography/mass spectrometry

S Strelkov, M von Elstermann, D Schomburg - Biological Chemistry, 2004 - degruyter.com

An analytical method based on gas chromatography/mass spectrometry was developed for metabolome investigation of Corynebacterium glutamicum. For the first time a fast method for metabolic screening that can be automated is described for this organism. More than …

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Diagnosis of inborn errors of metabolism using filter paper urine, urease treatment, isotope dilution and gas chromatography–mass spectrometry

T Kuhara - Journal of Chromatography B: Biomedical Sciences …, 2001 - Elsevier

This review will be concerned primarily with a practical yet comprehensive diagnostic procedure for the diagnosis or even mass screening of a variety of metabolic disorders. This rapid, highly sensitive procedure offers possibilities for clinical chemistry laboratories to …

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Gas chromatographic–mass spectrometric urinary metabolome analysis to study mutations of inborn errors of metabolism

T Kuhara - Mass spectrometry reviews, 2005 - Wiley Online Library

Urine contains numerous metabolites, and can provide evidence for the screening or molecular diagnosis of many inborn errors of metabolism (IEMs). The metabolomic analysis of urine by the combined use of urease pretreatment, stable-isotope dilution, and capillary …

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Diagnosis and monitoring of inborn errors of metabolism using urease-pretreatment of urine, isotope dilution, and gas chromatography–mass spectrometry

T Kuhara - Journal of Chromatography B, 2002 - Elsevier

To diagnose inborn errors of metabolism, it would be desirable to simultaneously analyze and quantify organic acids, purines, pyrimidines, amino acids, sugars, polyols, and other compounds using a single-step fractionation; unfortunately, no such method currently exists …

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Gene discovery via metabolic profiling

RN Trethewey - Current Opinion in Biotechnology, 2001 - Elsevier

Biochemical analysis is adding a new dimension to the process of gene discovery. Two major developments have recently taken place in the emerging science of biochemical genomics. The first is an approach that uses a combination of tagged fusion proteins and …

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Metabolic profiling and biochemical phenotyping of plant systems

U Roessner, L Willmitzer, A Fernie - Plant Cell Reports, 2002 - Springer

Over the last two decades incredible progress has been made in the development of technologies to both create and characterise genetic diversity. In plant systems, the development of knockout populations, transposon insertions and chemical mutagenesis …

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Simplified screening for organic acidemia using GC/MS and dried urine filter paper: a study on neonatal mass screening

X Fu, M Iga, M Kimura, S Yamaguchi - Early human development, 2000 - Elsevier

A simplified method for organic acidemia screening using GC/MS, the urease/direct method, is now available. To establish a practical screening system for organic acidemias, we studied the usefulness of dried urine filter paper (filter paper urine) and the application of a …

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Automated metabolic profiling and interpretation of GC/MS data for organic acidemia screening: a personal computer-based system

M Kimura, T Yamamoto, S Yamaguchi - The Tohoku journal of …, 1999 - jstage.jst.go.jp

We have developed a personal computer-based system designed for automated metabolic profiling of urinary organic acids by gas chromatography-mass spectrometry (GC/MS) and data interpretation for organic acidemia screening. For the automated profiling …

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Pilot study of gas chromatographic–mass spectrometric screening of newborn urine for inborn errors of metabolism after treatment with urease

T Kuhara, T Shinka, Y Inoue, M Ohse… - … of Chromatography B …, 1999 - Elsevier

Gas chromatographic–mass spectrometric (GC–MS) techniques for urinary organic acid profiling have been applied to high-risk screening for a wide range of diseases, mainly for inborn errors of metabolism (IEM), rather than to low-risk screening or mass screening …

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Noninvasive human metabolome analysis for differential diagnosis of inborn errors of metabolism

T Kuhara - Journal of Chromatography B, 2007 - Elsevier

Early diagnosis and treatment are critical for patients with inborn errors of metabolism (IEMs). For most IEMs, the clinical presentations are variable and nonspecific, and routine laboratory tests do not indicate the etiology of the disease. A diagnostic procedure using …

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Automated mode-of-action detection by metabolic profiling

N Aranîbar, BK Singh, GW Stockton, KH Ott - Biochemical and Biophysical …, 2001 - Elsevier

Rapid classification and identification of the mode-of-action of bioactive compounds applied to plants can be achieved by a robust and easy-to-use metabolic-profiling method. This method uses artificial neural network analysis of one-dimensional proton NMR spectra of …

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Computational strategies for metabolite identification in metabolomics

DS Wishart - Bioanalysis, 2009 - Future Science

Most metabolomic data are characterized by complex spectra or chromatograms containing hundreds of peaks or features. While there are many methods for aligning or comparing these spectral features, there are few approaches for actually identifying which peaks match …

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Determination of the spectrum of low molecular mass organic acids in urine by capillary electrophoresis with contactless conductivity and ultraviolet photometric …

P Tůma, E Samcová, K Štulík - Analytica chimica acta, 2011 - Elsevier

A mixture of 29 organic acids (OAs) occurring in urine was analyzed by capillary electrophoresis (CE) with capacitively coupled contactless conductivity detection (C 4 D) and UV photometric detection. The optimized analytical system involved a 100 cm long …

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Sarcosine as a marker in prostate cancer progression: a rapid and simple method for its quantification in human urine by solid-phase microextraction–gas …

B Cavaliere, B Macchione, M Monteleone… - Analytical and …, 2011 - Springer

Sarcosine is an amino acid derivative of N-methylglycine and is involved in the amino acid metabolism and methylation processes that are enriched during prostate cancer progression. It could also serve as a new target to be measured during therapeutic …

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