

## Mass spectrometry- based metabolomics

K Dettmer, PA Aronov... - *Mass spectrometry ...*, 2007 - Wiley Online Library

This review presents an overview of the dynamically developing field of mass spectrometry-based metabolomics. Metabolomics aims at the comprehensive and quantitative analysis of wide arrays of metabolites in biological samples. These numerous analytes have very ...

Cited by 1476

## Gas chromatography/mass spectrometry in metabolic profiling of biological fluids

KK Pasikanti, PC Ho, ECY Chan - *Journal of Chromatography B*, 2008 - Elsevier

One of the objectives of metabolomics is to identify subtle changes in metabolite profiles between biological systems of different physiological or pathological states. Gas chromatography mass spectrometry (GC/MS) is a widely used analytical tool for metabolic ...

Cited by 258

## 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 ...

Cited by 163

## Metabolomics in the study of kidney diseases

RH Weiss, K Kim - *Nature Reviews Nephrology*, 2012 - nature.com

Metabolomics—the nontargeted measurement of all metabolites produced by the body—is beginning to show promise in both biomarker discovery and, in the form of pharmacometabolomics, in aiding the choice of therapy for patients with specific diseases. In ...

Cited by 169

## [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 ...

Cited by 143

## Mass spectrometry- based holistic analytical approaches for metabolite profiling in systems biology studies

G Theodoridis, HG Gika... - *Mass spectrometry reviews*, 2011 - Wiley Online Library

Metabolomics and metabolomics represent one of the three major platforms in systems biology. To perform metabolomics it is necessary to generate comprehensive “global” metabolite profiles from complex samples, for example, biological fluids or tissue extracts ...

Cited by 132

## Recent and potential developments in the analysis of urine: a review

D Ryan, K Robards, PD Prenzler, M Kendall - *Analytica Chimica Acta*, 2011 - Elsevier

Abstract Analysis of urine is a widely used diagnostic tool that traditionally measured one or, at most, a few metabolites. However, the recognition of the need for a holistic approach to metabolism led to the application of metabolomics to urine for disease diagnostics. This ...

Cited by 123

## [HTML] Ejaculatory disorder caused by alpha- 1 adrenoceptor antagonists is not retrograde ejaculation but a loss of seminal emission

SI HISASUE, R Furuya, N Itoh... - ... *journal of urology*, 2006 - Wiley Online Library

Aim: The etiology of the ejaculatory disorder induced by alpha-1 blockers is still controversial, although it has been suggested to be retrograde ejaculation. The aim of this study was to investigate the distribution of alpha-1 adrenoceptor subtype mRNA in human ...

Cited by 115

## Metabolomics study of stepwise hepatocarcinogenesis from the model rats to patients: potential biomarkers effective for small hepatocellular carcinoma diagnosis

Y Tan, P Yin, L Tang, W Xing, Q Huang, D Cao... - *Molecular & Cellular ...*, 2012 - ASBMB

The aim of this study is to find the potential biomarkers from the rat hepatocellular carcinoma (HCC) disease model by using a non-target

metabolomics method, and test their usefulness in early human HCC diagnosis. The serum metabolic profiling of the diethylnitrosamine ...

Cited by 104

### [Inhibition of Seminal Emission Is the Main Cause of Anejaculation Induced by a New Highly Selective \$\alpha\$ 1A- Blocker in Normal Volunteers](#)

[K Kobayashi, N Masumori, S Hisasue...](#) - *The journal of sexual ...*, 2008 - Wiley Online Library

Aim. We evaluated the effect of a new, highly selective  $\alpha$ 1A-blocker, silodosin, on ejaculatory function of normal volunteers. Methods. The study included 15 healthy male urologists who voluntarily participated in the study. They took 4 mg of silodosin or a placebo twice daily for 3 ...

Cited by 88

### [Monitoring the health to disease continuum with global metabolic profiling and systems biology](#)

[LK Schnackenberg, RD Beger](#) - 2006 - *Future Medicine*

Global metabolic profiling, which includes both metabolomics and metabonomics studies, is the latest 'omics' research platform that is being applied to understand the health and disease continuum. Metabolic profiling analyses have been demonstrated for the ...

Cited by 88

### [A practical approach to detect unique metabolic patterns for personalized medicine](#)

[JM Johnson, T Yu, FH Strobel, DP Jones](#) - *Analyst*, 2010 - pubs.rsc.org

Information-rich technologies have advanced personalized medicine, yet obstacles limit measurement of large numbers of chemicals in human samples. Current laboratory tests measure hundreds of chemicals based upon existing knowledge of exposures, metabolism ...

Cited by 88

### [Serum metabonomics study of chronic renal failure by ultra performance liquid chromatography coupled with Q-TOF mass spectrometry](#)

[L Jia, J Chen, P Yin, X Lu, G Xu](#) - *Metabolomics*, 2008 - Springer

A metabonomics technique based on ultra-performance liquid chromatography (UPLC) coupled with Q-TOF mass spectrometry was employed to investigate the sera from 32 patients with chronic renal failure (CRF) without renal replacement therapy and 30 healthy ...

Cited by 79

### [Future of liquid chromatography–mass spectrometry in metabolic profiling and metabolomic studies for biomarker discovery](#)

[TO Metz, Q Zhang, JS Page, Y Shen, SJ Callister...](#) - 2007 - *Future Medicine*

The future utility of liquid chromatography–mass spectrometry (LC–MS) in metabolic profiling and metabolomic studies for biomarker discovery is discussed, beginning with a brief description of the evolution of metabolomics and the utilization of the three most ...

Cited by 73

### [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 ...

Cited by 61

### [Metabolic profiling of infant urine using comprehensive two-dimensional gas chromatography: application to the diagnosis of organic acidurias and biomarker ...](#)

[KA Kouremenos, J Pitt, PJ Marriott](#) - *Journal of Chromatography A*, 2010 - Elsevier

Comprehensive two-dimensional gas chromatography (GC $\times$  GC) time-of-flight mass spectrometry (ToFMS) was applied to the analysis of urinary organic acids from patients with inborn errors of metabolism. Abnormal profiles were obtained from all five patients studied ...

Cited by 62

### [Serum metabonomics study of adenine-induced chronic renal failure in rats by ultra performance liquid chromatography coupled with quadrupole time-of-flight mass ...](#)

[YY Zhao, XL Cheng, F Wei, XY Xiao, WJ Sun...](#) - *Biomarkers*, 2012 - Taylor & Francis

An ultra performance liquid chromatography coupled with quadrupole time-of-flight mass spectrometry (UPLC Q-TOF MS) metabonomics approach was employed to study the serum metabolic profiling of adenine-induced chronic renal failure (CRF) rats. Acquired data were ...

Cited by 63

## 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 ...

Cited by 60

## Mass spectrometry-based technologies for high-throughput metabolomics

J Han, R Datla, S Chan, CH Borchers - *Bioanalysis*, 2009 - Future Science

The metabolome is composed of a vast number of small-molecule metabolites that exhibit a diversity of physical and chemical properties and exist over a wide dynamic range in biological samples. Multiple analytical techniques, used in a complementary manner, are ...

Cited by 58

## Selective screening for inborn errors of metabolism and secondary methylmalonic aciduria in pregnancy at high risk district of neural tube defects: a human ...

YZ Song, BX Li, H Hao, RL Xin, T Zhang, CH Zhang... - *Clinical ...*, 2008 - Elsevier

Objective Urease pretreatment-gas chromatography-mass spectrometry (UP-GC-MS) has become a valuable tool in the field of metabolome research, including analysis of inborn errors of metabolism (IEMs) and acquired metabolic disturbances secondary to nutrition or ...

Cited by 57

## An automated method for peak detection and matching in large gas chromatography- mass spectrometry data sets

SJ Dixon, RG Brereton, HA Soini... - *Journal of ...*, 2006 - Wiley Online Library

A new approach for peak detection and matching has been developed and applied to two data sets. The first consisted of the Gas Chromatography-Mass Spectrometry (GC-MS) samples of 965 human sweat samples obtained from a population of 197 individuals. The ...

Cited by 57

## Influences of methamphetamine-induced acute intoxication on urinary and plasma metabolic profiles in the rat

N Shima, I Miyawaki, K Bando, H Horie, K Zaitso... - *Toxicology*, 2011 - Elsevier

Methamphetamine (MA) is an illicit psychostimulant, and its abuse has become an international public health problem. MA intoxication can cause life-threatening hyperthermia, renal and liver failure, cardiac arrhythmias, and neurological damage. To investigate the ...

Cited by 45

## Global metabolic profiling and its role in systems biology to advance personalized medicine in the 21st century

LK Schnackenberg - *Expert Review of Molecular Diagnostics*, 2007 - Taylor & Francis

Systems biology attempts to elucidate the complex interaction between genes, proteins and metabolites to provide a mechanistic understanding of cellular function and how this function is affected by disease processes, drug toxicity or drug efficacy effects. Global metabolic ...

Cited by 42

## [HTML] Untargeted metabolomic analysis for the clinical screening of inborn errors of metabolism

MJ Miller, AD Kennedy, AD Eckhart, LC Burrage... - *Journal of inherited ...*, 2015 - Springer

Global metabolic profiling currently achievable by untargeted mass spectrometry-based metabolomic platforms has great potential to advance our understanding of human disease states, including potential utility in the detection of novel and known inborn errors of ...

Cited by 55

## Multiwell plates loaded with fluorescent hydrogel sensors for measuring pH and glucose concentration

B Vilozny, A Schiller, RA Wessling... - *Journal of Materials ...*, 2011 - pubs.rsc.org

Fluorescent hydrogels were polymerized directly in multi-well plates at ambient temperature and in the presence of air, producing sensors for measuring pH and glucose concentration. The plates were rapidly analyzed using a fluorescence plate reader. Multiwell pH sensors ...

Cited by 35

## The application of mass spectrometry to proteomics and metabolomics in biomarker discovery and drug development

T Mikami, M Aoki, T Kimura - *Current molecular pharmacology*, 2012 - [ingentaconnect.com](http://ingentaconnect.com)

Drugs are launched to market after the lengthy process of development. Despite careful preclinical assessment, there is still a significant risk that a drug candidate may elicit adverse effects or display a low level of efficacy during clinical trials. If a drug candidate fails in the ...

Cited by 39

## Direct sample injection for capillary electrophoretic determination of organic acids in cerebrospinal fluid

R Ramautar, GW Somsen, GJ de Jong - *Analytical and bioanalytical ...*, 2007 - Springer

Organic acids in cerebrospinal fluid (CSF) are potential diagnostic markers for neurological diseases and metabolic disorders. A capillary electrophoretic (CE) method for the direct analysis, ie, without any sample preparation, of six organic acids in CSF was developed. A...

Cited by 30

## Biomarkers for neuroAIDS: the widening scope of metabolomics

G Pendyala, EJ Want, W Webb, G Siuzdak... - *Journal of Neuroimmune ...*, 2007 - Springer

Abstract "Metabolomics", the measurement of metabolite concentrations and fluxes in cell systems, is an emerging science that has enormous potential and several unique characteristics. The current applications for this field are, primarily, toxicological profiling and ...

Cited by 30

## Metabolomic biomarkers: their role in the critical path

LK Schnackenberg, RD Beger - *Drug Discovery Today: Technologies*, 2007 - Elsevier

Global metabolic profiling is being applied to identify biomarkers of health. Some small molecules are exquisitely sensitive indicators of health status. Metabolic profiling analyses are being used to determine biomarkers of drug safety and effectiveness as well as disease ...

Cited by 29

## Application of supercritical fluid chromatography to the analysis of hydrophobic metabolites

T Bamba - *Journal of separation science*, 2008 - Wiley Online Library

This review describes the usefulness of supercritical fluid chromatography (SFC) in the analysis of hydrophobic metabolites. The use of SFC for the analysis of naturally occurring polyprenols markedly improves the chromatographic resolution of polyprenol homologues ...

Cited by 26