

Rick's metabolomics papers of interest

Reviews

- Bedair M and Sumner L W 2008 Current and emerging mass-spectrometry technologies for metabolomics *Trac-Trends in Analytical Chemistry* **27** 238-50
- Bino R J, Hall R D, Fiehn O, Kopka J, Saito K, Draper J, Nikolau B J, Mendes P, Roessner-Tunali U, Beale M H, Trethewey R N, Lange B M, Wurtele E S and Sumner L W 2004 Potential of metabolomics as a functional genomics tool *Trends Plant Sci.* **9** 418-25
- Brown S C, Kruppa G and Dasseux J L 2005 Metabolomics applications of FT-ICR mass spectrometry *Mass Spectrom. Rev.* **24** 223-31
- Ellis D I and Goodacre R 2006 Metabolic fingerprinting in disease diagnosis: biomedical applications of infrared and Raman spectroscopy *Analyst* **131** 875-85
- Fiehn O 2001 Combining genomics, metabolome analysis, and biochemical modelling to understand metabolic networks *Compar. Funct. Genom.* **2** 155-68
- Fiehn O 2002 Metabolomics - the link between genotypes and phenotypes *Plant Mol.Biol.* **48** 155-71
- German J B, Gillies L A, Smilowitz J T, Zivkovic A M and Watkins S M 2007 Lipidomics and lipid profiling in metabolomics *Curr. Opin. Lipidology* **18** 66-71
- Gibney M and Brennan L 2007 What can we expect from metabolomics and system biology? *Int. J. Obes.* **31** S1-S
- Glinski M and Weckwerth W 2006 The role of mass spectrometry in plant systems biology *Mass Spectrom. Rev.* **25** 173-214
- Goodacre R 2005 Making sense of the metabolome using evolutionary computation: seeing the wood with the trees *J. Exp. Bot.* **56** 245-54
- Goodacre R 2007 Metabolomics of a superorganism *J. Nutr.* **137** 259S-66S
- Griffin J L 2004 Metabolic profiles to define the genome: can we hear the phenotypes? *Philosophical Transactions of the Royal Society of London Series B-Biological Sciences* **359** 857-71
- Griffin J L 2006a The Cinderella story of metabolic profiling: does metabolomics get to go to the functional genomics ball? *Philos. Trans. R. Soc. B-Biol. Sci.* **361** 147-61
- Griffiths W J, Karua K, Hornshaw M, Woffending G and Wanga Y 2007 Metabolomics and metabolite profiling: past heroes and future developments *Eur. J. Mass Spectrom.* **13** 45-50
- Hollywood K, Brison D R and Goodacre R 2006 Metabolomics: Current technologies and future trends *Proteomics* **6** 4716-23
- Kell D B 2004 Metabolomics and systems biology: making sense of the soup *Current Opinion in Microbiology* **7** 296-307
- Kell D B 2005b Metabolomics, machine learning and modelling: towards an understanding of the language of cells *Biochem. Soc. Trans.* **33** 520-4
- Kell D B 2006a Metabolomics, modelling and machine learning in systems biology - towards an understanding of the languages of cells *Febs J.* **273** 873-94
- Kell D B 2006b Metabolomics: The new science of metabolic integration *J. Mol. Cell. Cardiol.* **40** 935-
- Kell D B 2006c Systems biology, metabolic modelling and metabolomics in drug discovery and development *Drug Discov. Today* **11** 1085-92
- Kell D B 2007 The virtual human: Towards a global systems biology of multiscale, distributed biochemical network models *IUBMB Life* **59** 689-95
- Kopka J, Fernie A, Weckwerth W, Gibon Y and Stitt M 2004 Metabolite profiling in plant biology: platforms and destinations *Genome Biol.* **5**
- Nobeli I and Thornton J M 2006 A bioinformatician's view of the metabolome *Bioessays* **28** 534-45
- ogr. A* **1184** 341-52
- Quackenbush J 2007 Extracting biology from high-dimensional biological data *J. Exp. Biol.* **210** 1507-17
- Metzger R P 2006 Thoughts on the teaching of metabolism *Biochem. Mol. Biol. Educ.* **34** 78-87
- Mendes P, Camacho D and de la Fuente A 2005 Modelling and simulation for metabolomics data analysis *Biochem. Soc. Trans.* **33** 1427-9
- Shulaev V 2006 Metabolomics technology and bioinformatics *Brief. Bioinform.* **7** 128-39
- Siuzdak G 2008 A metabolomics platform for discovery and diagnosis *Eur. J. Pharm. Sci.* **34** S22-S

- Steuer R, Kurths J, Fiehn O and Weckwerth W 2003 Interpreting correlations in metabolomic networks *Biochem. Soc. Trans.* **31** 1476-8
- Sweetlove L J, Fell D and Fernie A R 2008 Getting to grips with the plant metabolic network *Biochem. J.* **409** 27-41
- Viant M R 2007 Metabolomics of aquatic organisms: the new 'omics' on the block *Mar. Ecol.-Prog. Ser.* **332** 301-6
- Want E J, Nordstrom A, Morita H and Siuzdak G 2007 From exogenous to endogenous: The inevitable imprint of mass spectrometry in metabolomics *J. Proteome Res.* **6** 459-68
- Weckwerth W 2008 Integration of metabolomics and proteomics in molecular plant physiology - coping with the complexity by data-dimensionality reduction *Physiol. Plant.* **132** 176-89
- Weckwerth W and Morgenthal K 2005 Metabolomics: from pattern recognition to biological interpretation *Drug Discov. Today* **10** 1551-8

Instrument and Methodology Development

- Beckmann M, Parker D, Enot D P, Duval E and Draper J 2008 High-throughput, nontargeted metabolite fingerprinting using nominal mass flow injection electrospray mass spectrometry *Nat. Protoc.* **3** 486-504
- Bottcher C, von Roepenack-Lahaye E, Willscher E, Scheel D and Clemens S 2007 Evaluation of matrix effects in metabolite profiling based on capillary liquid chromatography electrospray ionization quadrupole time-of-flight mass spectrometry *Anal. Chem.* **79** 1507-13
- Breitling R, Ritchie S, Goodenowe D, Stewart M L and Barrett M P 2006 Ab initio prediction of metabolic networks using Fourier transform mass spectrometry data *Metabolomics* **2** 155-64
- Chen H W, Wortmann A and Zenobi R 2007 Neutral desorption sampling coupled to extractive electrospray ionization mass spectrometry for rapid differentiation of biosamples by metabolomic fingerprinting *J. Mass Spectrom.* **42** 1123-35
- Coulier L, Bas R, Jespersen S, Verheij E, van der Werf M J and Hankemeier T 2006 Simultaneous quantitative analysis of metabolites using ion-pair liquid chromatography - Electrospray ionization mass spectrometry *Anal. Chem.* **78** 6573-82
- Cubbon S, Bradbury T, Wilson J and Thomas-Oates J 2007 Hydrophilic interaction chromatography for mass spectrometric metabolomic studies of urine *Anal. Chem.* **79** 8911-8
- Deport C, Ratel J, Berdague J L and Engel E 2006 Comprehensive combinatorial standard correction: A calibration method for handling instrumental drifts of gas chromatography-mass spectrometry systems *J. Chromatogr. A* **1116** 248-58
- Dettmer K, Aronov P A and Hammock B D 2007 Mass spectrometry-based metabolomics *Mass Spectrom. Rev.* **26** 51-78
- Dwivedi P, Wu P, Klopsch S J, Puzon G J, Xun L and Hill H H 2008 Metabolic profiling by ion mobility mass spectrometry (IMMS) *Metabolomics* **4** 63-80
- Fiehn O 2008 Extending the breadth of metabolite profiling by gas chromatography coupled to mass spectrometry *Trac-Trends in Analytical Chemistry* **27** 261-9
- Gika H G, Theodoridis G A, Wingate J E and Wilson I D 2007 Within-day reproducibility of an HPLC-MS-Based method for metabolomic analysis: Application to human urine *J. Proteome Res.* **6** 3291-303
- Gipson G T, Tatsuoka K S, Sokhansanj B A, Ball R J and Connor S C 2008 Assignment of MS-based metabolomic datasets via compound interaction pair mapping *Metabolomics* **4** 94-103
- Han J, Danell R M, Patel J R, Gumerov D R, Scarlett C O, Speir J P, Parker C E, Rusyn I, Zeisel S and Borchers C H 2008 Towards high-throughput metabolomics using ultrahigh-field Fourier transform ion cyclotron resonance mass spectrometry *Metabolomics* **4** 128-40
- Hansen M A E and Smedsgaard J 2007 Automated work-flow for processing high-resolution direct infusion electrospray ionization mass spectral fingerprints *Metabolomics* **3** 41-54
- Hegeman A D, Schulte C F, Cui Q, Lewis I A, Huttlin E L, Eghbalnia H, Harms A C, Ulrich E L, Markley J L and Sussman M R 2007 Stable isotope assisted assignment of elemental compositions for metabolomics *Anal. Chem.* **79** 6912-21
- Hu Q Z, Noll R J, Li H Y, Makarov A, Hardman M and Cooks R G 2005 The Orbitrap: a new mass spectrometer *J. Mass Spectrom.* **40** 430-43

- Huang X D and Regnier F E 2008 Differential metabolomics using stable isotope labeling and two-dimensional gas chromatography, with time-of-flight mass spectrometry *Anal. Chem.* **80** 107-14
- Idborg H, Zamani L, Edlund P O, Schuppe-Koistinen I and Jacobsson S P 2005 Metabolic fingerprinting of rat urine by LC/MS Part 1. Analysis by hydrophilic interaction liquid chromatography-electrospray ionization mass spectrometry *J. Chromatogr. B* **828** 9-13
- Jonsson P, Johansson E S, Wuolikainen A, Lindberg J, Schuppe-Koistinen I, Kusano M, Sjoström M, Trygg J, Moritz T and Antti H 2006a Predictive metabolite profiling applying hierarchical multivariate curve resolution to GC-MS data - A potential tool for multi-parametric diagnosis *J. Proteome Res.* **5** 1407-14
- Jonsson P, Stenlund H, Moritz T, Trygg J, Sjoström M, Verheij E R, Lindberg J, Schuppe-Koistinen I and Antti H 2006b A strategy for modelling dynamic responses in metabolic samples characterized by GC/MS *Metabolomics* **2** 135-43
- Kind T and Fiehn O 2006 Metabolomic database annotations via query of elemental compositions: Mass accuracy is insufficient even at less than 1 ppm *BMC Bioinformatics* **7**
- Kind T, Tolstikov V, Fiehn O and Weiss R H 2007 A comprehensive urinary metabolomic approach for identifying kidney cancer *Anal. Biochem.* **363** 185-95
- Koek M M, Muilwijk B, van Stee L L P and Hankemeier T 2008 Higher mass loadability in comprehensive two-dimensional gas chromatography-mass spectrometry for improved analytical performance in metabolomics analysis *J. Chromatogr. A* **1186** 420-9
- Kopka J, Schauer N, Krueger S, Birkemeyer C, Usadel B, Bergmüller E, Dormann P, Weckwerth W, Gibon Y, Stitt M, Willmitzer L, Fernie A R and Steinhauser D 2005 GMD@CSB.DB: the Golm Metabolome Database *Bioinformatics* **21** 1635-8
- Kopka J 2006 Current challenges and developments in GC-MS based metabolite profiling technology *J. Biotechnol.* **124** 312-22
- Koulman A, Tapper B A, Fraser K, Cao M S, Lane G A and Rasmussen S 2007 High-throughput direct-infusion ion trap mass spectrometry: a new method for metabolomics *Rapid Commun. Mass Spectrom.* **21** 421-8
- Lenz E M and Wilson I D 2007 Analytical strategies in metabolomics *J. Proteome Res.* **6** 443-58
- Lu X, Zhao X J, Bai C M, Zhao C X, Lu G and Xu G M 2008 LC-MS-based metabolomics analysis *J. Chromatogr. B* **866** 64-76
- Luedemann A, Strassburg K, Erban A and Kopka J 2008 TagFinder for the quantitative analysis of gas chromatography - mass spectrometry (GC-MS)-based metabolite profiling experiments *Bioinformatics* **24** 732-7
- Mas S, Villas-Boas S G, Hansen M E, Akesson M and Nielsen J 2007 A comparison of direct infusion MS and GC-MS for metabolic footprinting of yeast mutants *Biotechnol. Bioeng.* **96** 1014-22
- Metz T O, Page J S, Baker E S, Tang K Q, Ding J, Shen Y F and Smith R D 2008 High-resolution separations and improved ion production and transmission in metabolomics *Trac-Trends in Analytical Chemistry* **27** 205-14
- Metz T O, Zhang Q B, Page J S, Shen Y F, Callister S J, Jacobs J M and Smith R D 2007 Future of liquid chromatography-mass spectrometry in metabolic profiling and metabolomic studies for biomarker discovery *Biomark. Med.* **1** 159-85
- Mihaleva V V, Vorst O, Maliepaard C, Verhoeven H A, de Vos R C H, Hall R D and van Ham R 2008 Accurate mass error correction in liquid chromatography time-of-flight mass spectrometry based metabolomics *Metabolomics* **4** 171-82
- Moco S, Bino R J, De Vos R C H and Vervoort J 2007 Metabolomics technologies and metabolite identification *Trac-Trends in Analytical Chemistry* **26** 855-66
- Mohler R E, Tu B P, Dombek K M, Hoggard J C, Young E T and Synovec R E 2008 Identification and evaluation of cycling yeast metabolites in two-dimensional comprehensive gas chromatography-time-of-flight-mass spectrometry data *J. Chromatogr. A* **1186** 401-11
- Nordstrom A, Want E, Northen T, Lehtio J and Siuzdak G 2008 Multiple ionization mass spectrometry strategy used to reveal the complexity of metabolomics *Anal. Chem.* **80** 421-9
- Overy D P, Enot D P, Tailliant K, Jenkins H, Parker D, Beckmann M and Draper J 2008 Explanatory signal interpretation and metabolite identification strategies for nominal mass FIE-MS metabolite fingerprints *Nat. Protoc.* **3** 471-85
- Pierce K M, Hoggard J C, Mohler R E and Synovec R E 2008 Recent advancements in comprehensive two-dimensional separations with chemometrics *J. Chromatogr. A*

- Schauer N, Steinhauser D, Strelkov S, Schomburg D, Allison G, Moritz T, Lundgren K, Roessner-Tunali U, Forbes M G, Willmitzer L, Fernie A R and Kopka J 2005 GC-MS libraries for the rapid identification of metabolites in complex biological samples *Febs Letters* **579** 1332-7
- Shellie R A 2005 Comprehensive two-dimensional gas chromatography-mass spectrometry and its use in high-resolution metabolomics *Aust. J. Chem.* **58** 619-
- Southam A D, Payne T G, Cooper H J, Arvanitis T N and Viant M R 2007 Dynamic range and mass accuracy of wide-scan direct infusion nanoelectrospray Fourier transform ion cyclotron resonance mass spectrometry-based metabolomics increased by the spectral stitching method *Anal. Chem.* **79** 4595-602
- Strelkov S, von Elstermann M and Schomburg D 2004 Comprehensive analysis of metabolites in *Corynebacterium glutamicum* by gas chromatography/mass spectrometry *Biol. Chem.* **385** 853-61
- Sturm M, Bertsch A, Gropl C, Hildebrandt A, Hussong R, Lange E, Pfeifer N, Schulz-Trieglaff O, Zerck A, Reinert K and Kohlbacher O 2008 OpenMS-An open-source software framework for mass spectrometry *BMC Bioinformatics* **9**
- t'Kindt R, Alaerts G, Heyden Y V, Deforce D and Bocxlaer J 2007 Broad-spectrum separations in metabolomics using enhanced polar LC stationary phases: A dedicated evaluation using plant metabolites *J. Sep. Sci.* **30** 2002-11
- t'Kindt R, Storme M, Deforce D and Van Bocxlaer J 2008 Evaluation of hydrophilic interaction chromatography versus reversed-phase chromatography in a plant metabolomics perspective *J. Sep. Sci.* **31** 1609-14
- Takats Z, Wiseman J M and Cooks R G 2005 Ambient mass spectrometry using desorption electrospray ionization (DESI): instrumentation, mechanisms and applications in forensics, chemistry, and biology *J. Mass Spectrom.* **40** 1261-75
- Theodoridis G, Gika H G and Wilson I D 2008 LC-MS-based methodology for global metabolite profiling in metabonomics/metabolomics *Trac-Trends in Analytical Chemistry* **27** 251-60
- Vaidyanathan S and Goodacre R 2007 Quantitative detection of metabolites using matrix-assisted laser desorption/ionization mass spectrometry with 9-aminoacridine as the matrix *Rapid Commun. Mass Spectrom.* **21** 2072-8
- Wilson I D, Plumb R, Granger J, Major H, Williams R and Lenz E A 2005 HPLC-MS-based methods for the study of metabonomics *J. Chromatogr. B* **817** 67-76

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- Atherton H J, Bailey N J, Zhang W, Taylor J, Major H, Shockcor J, Clarke K and Griffin J L 2006 A combined H-1-NMR spectroscopy- and mass spectrometry-based metabolomic study of the PPAR-alpha null mutant mouse defines profound systemic changes in metabolism linked to the metabolic syndrome *Physiol. Genomics* **27** 178-86
- Beger R D, Holland R D, Sun J, Schnackenberg L K, Moore P C, Dent C L, Devarajan P and Portilla D 2008 Metabonomics of acute kidney injury in children after cardiac surgery *Pediatr. Nephrol.* **23** 977-84
- Boernsen K O, Gatzek S and Imbert G 2005 Controlled protein precipitation in combination with chip-based nanospray infusion mass spectrometry. An approach for metabolomics profiling of plasma *Anal. Chem.* **77** 7255-64
- Bogdanov M, Matson W R, Wang L, Matson T, Saunders-Pullman R, Bressman S S and Beal M F 2008 Metabolomic profiling to develop blood biomarkers for Parkinson's disease *Brain* **131** 389-96
- Brisson D R, Hollywood K, Arnesen R and Goodacre R 2007 Predicting human embryo viability: the road to non-invasive analysis of the secretome using metabolic footprinting *Reprod. Biomed. Online* **15** 296-302
- Cezar G G, Quam J A, Smith A M, Rosa G J M, Piekarczyk M S, Brown J F, Gage F H and Muotri A R 2007 Identification of small molecules from human embryonic stem cells using metabolomics *Stem Cells Dev.* **16** 869-82
- Costello L C and Franklin R B 2005 'Why do tumour cells glycolyse?': From glycolysis through citrate to lipogenesis *Mol. Cell. Biochem.* **280** 1-8
- Collings F B and Vaidya V S 2008 Novel technologies for the discovery and quantitation of biomarkers of toxicity *Toxicology* **245** 167-74

- Davis C D and Milner J A 2007 Biomarkers for diet and cancer prevention research: potentials and challenges *Acta Pharmacol. Sin.* **28** 1262-73
- Denkert C, Budczies J, Kind T, Weichert W, Tablack P, Sehouli J, Niesporek S, Konsgen D, Diemel M and Fiehn O 2006 Mass spectrometry-based metabolic profiling reveals different metabolite patterns in invasive ovarian carcinomas and ovarian borderline tumors *Cancer Res.* **66** 10795-804
- Dixon S J, Xu Y, Brereton R G, Soini H A, Novotny M V, Oberzaucher E, Grammer K and Penn D J 2007 Pattern recognition of gas chromatography mass spectrometry of human volatiles in sweat to distinguish the sex of subjects and determine potential discriminatory marker peaks *Chemometrics Intell. Lab. Syst.* **87** 161-72
- Draisma H H M, Reijmers T H, Bobeldijk-Pastorova I, Meulman J J, Burk G, Bartels M, Ramaker R, Van der Greef J, Boomsma D I and Hankemeier T 2008 Similarities and differences in lipidomics profiles among healthy monozygotic twin pairs *Omics* **12** 17-31
- Fan T W M, Higashi R M and Lane A N 2006 Integrating metabolomics and transcriptomics for probing Ser anticancer mechanisms *Drug Metab. Rev.* **38** 707-32
- Feala J D, Coquin L, Paternostro G and McCulloch A D 2008 Integrating metabolomics and phenomics with systems models of cardiac hypoxia *Prog. Biophys. Mol. Biol.* **96** 209-25
- German J B, Watkins S M and Fay L B 2005 Metabolomics in practice: Emerging knowledge to guide future dietetic advice toward individualized health *J. Am. Diet. Assoc.* **105** 1425-32
- Griffin J L 2006b Understanding mouse models of disease through metabolomics *Curr. Opin. Chem. Biol.* **10** 309-15
- Griffin J L 2008 Following the role of PPARs in controlling systemic metabolism by metabolomics *Eur. J. Pharm. Sci.* **34** S22-S
- Griffin J L and Kauppinen R A 2007 A metabolomics perspective of human brain tumours *Febs J.* **274** 1132-9
- Gu H W, Chen H W, Pan Z Z, Jackson A U, Talaty N, Xi B W, Kissinger C, Duda C, Mann D, Raftery D and Cooks R G 2007 Monitoring diet effects via biofluids and their implications for metabolomics studies *Anal. Chem.* **79** 89-97
- Harrigan G G and Yates L A 2006 High-throughput screening, metabolomics and drug discovery *IDrugs* **9** 188-92
- Kaddurah-Daouk R, Kristal B S and Weinshilboum R M 2008 Metabolomics: A global biochemical approach to drug response and disease *Annu. Rev. Pharmacol. Toxicol.* **48** 653-83
- Kaddurah-Daouk R, McEvoy J, Baillie R A, Lee D, Yao J K, Doraiswamy P M and Krishnan K R R 2007 Metabolomic mapping of atypical antipsychotic effects in schizophrenia *Mol. Psychiatr.* **12** 934-45
- Keun H C and Athersuch T J 2007 Application of metabolomics in drug development *Pharmacogenomics* **8** 731-41
- Knopf C, Baruch O, Eden E, Yakhini Z and Hochberg Z 2006 Steroid metabolomics using GC-MS *Horm. Res.* **65** 12-
- Lin C Y, Wu H F, Tjeerdema R S and Viant M R 2007 Evaluation of metabolite extraction strategies from tissue samples using NMR metabolomics *Metabolomics* **3** 55-67
- Lindon J C, Holmes E and Nicholson J K 2007 Metabolomics in pharmaceutical R & D *Febs J.* **274** 1140-51
- Lindon J C and Nicholson J K 2008 Analytical technologies for metabolomics and metabolomics, and multi-omic information recovery *Trac-Trends in Analytical Chemistry* **27** 194-204
- Mao Y Y, Bai J Q, Chen J H, Shou Z F, He Q, Wu J Y, Chen Y and Cheng Y Y 2008 A pilot study of GC/MS-based serum metabolic profiling of acute rejection in renal transplantation *Transpl. Immunol.* **19** 74-80
- Martin F P J, Dumas M E, Wang Y L, Legido-Quigley C, Yap I K S, Tang H R, Zirah S, Murphy G M, Cloarec O, Lindon J C, Sprenger N, Fay L B, Kochhar S, van Bladeren P, Holmes E and Nicholson J K 2007 A top-down systems biology view of microbiome-mammalian metabolic interactions in a mouse model *Mol. Syst. Biol.* **3**
- Nordstrom A, O'Maille G, Qin C and Siuzdak G 2006 Nonlinear data alignment for UPLC-MS and HPLC-MS based metabolomics: Quantitative analysis of endogenous and exogenous metabolites in human serum *Anal. Chem.* **78** 3289-95
- Oresic M, Seppanen-Laakso T, Simell S, Suortti T, Parikka V, Nanto-Salonen K, Lahde J, Sysi-Aho M, Reinikainen A, Simell T, Ilonen J, Hyoty H, Knip M, Veijola R and Simell O 2006a Serum

- metabolite patterns between birth and development of autoantibodies and overt type 1 diabetes: application of large-scale metabolomics to the Type 1 Diabetes Prediction and Prevention study (DIPP) *Diabetologia* **49** 147-
- Oresic M, Vidal-Puig A and Hanninen V 2006b Metabolomic approaches to phenotype characterization and applications to complex diseases *Expert Rev. Mol. Diagn.* **6** 575-85
- Paige L A, Mitchell M W, Krishnan K R R, Kaddurah-Daouk R and Steffens D C 2007 A preliminary metabolomic analysis of older adults with and without depression *Int. J. Geriatr. Psychiatr.* **22** 418-23
- Pears M R, Cooper J D, Mitchison H M, Mortishire-Smith R J, Pearce D A and Griffin J L 2005 High resolution H-1 NMR-based metabolomics indicates a neurotransmitter cycling deficit in cerebral tissue from a mouse model of Batten disease *J. Biol. Chem.* **280** 42508-14
- Pohjanen E, Thysell E, Jonsson P, Eklund C, Silfver A, Carlsson I B, Lundgren K, Moritz T, Svensson M B and Antti H 2007 A multivariate screening strategy for investigating metabolic effects of strenuous physical exercise in human serum *J. Proteome Res.* **6** 2113-20
- Price K E, Lunte C E and Larive C K 2008 Development of tissue-targeted metabolomics. Part 1. Analytical considerations *J. Pharm. Biomed. Anal.* **46** 737-47
- Robertson D G 2005 Metabolomics in toxicology: A review *Toxicol. Sci.* **85** 809-22
- Sabatine M S, Liu E, Morrow D A, Heller E, McCarroll R, Wiegand R, Berriz G F, Roth F P and Gerszten R E 2005 Metabolomic identification of novel biomarkers of myocardial ischemia *Circulation* **112** 3868-75
- Sanders M, Shipkova P A, Zhang H Y and Warrack B M 2006 Utility of the hybrid LTQ-FTMS for drug metabolism applications *Curr. Drug Metab.* **7** 547-55
- Saric J, Wang Y, Li J, Coen M, Utzinger J, Marchesi J R, Keiser J, Veselkov K, Lindon J C, Nicholson J K and Holmes E 2008 Species variation in the fecal metabolome gives insight into differential gastrointestinal function *J. Proteome Res.* **7** 352-60
- Schnackenberg L K and Beger R D 2008 The role of metabolic biomarkers in drug toxicity studies *Toxicol. Mech. Methods* **18** 301-11
- Serkova N J, Jackman M, Brown J L, Liu T, Hirose R, Roberts J P, Maher J J and Niemann C U 2006 Metabolic profiling of livers and blood from obese Zucker rats *J. Hepatol.* **44** 956-62
- Van der Greef J, Hankemeier T and McBurney R N 2006 Metabolomics-based systems biology and personalized medicine: moving towards n=1 clinical trials? *Pharmacogenomics* **7** 1087-94
- van der Greef J, Martin S, Juhasz P, Adourian A, Plasterer T, Verheij E R and McBurney R N 2007 The art and practice of systems biology in medicine: Mapping patterns of relationships *J. Proteome Res.* **6** 1540-59
- van der Greef J, Stroobant P and van der Heijden R 2004 The role of analytical sciences medical systems biology *Curr. Opin. Chem. Biol.* **8** 559-65
- Viant M R, Ludwig C, Rhodes S, Guenther U L and Allaway D 2007 Validation of a urine metabolome fingerprint in dog for phenotypic classification *Metabolomics* **3** 453-63
- Viant M R, Lyeth B G, Miller M G and Berman R F 2005 An NMR metabolomic investigation of early metabolic disturbances following traumatic brain injury in a mammalian model *NMR Biomed.* **18** 507-16
- Walsh M C, Brennan L, Malthouse J P G, Roche H M and Gibney M J 2006 Effect of acute dietary standardization on the urinary, plasma, and salivary metabolomic profiles of healthy humans *Am. J. Clin. Nutr.* **84** 531-9
- Wang Y and Griffiths W J 2007 Modern methods of bile acid analysis by mass spectrometry: A view into the metabolome *Curr. Anal. Chem.* **3** 103-26
- Want E J, O'Maille G, Smith C A, Brandon T R, Uritboonthai W, Qin C, Trauger S A and Siuzdak G 2006a Solvent-dependent metabolite distribution, clustering, and protein extraction for serum profiling with mass spectrometry *Anal. Chem.* **78** 743-52
- Want E J, Smith C A, Qin C A, VanHorne K C and Siuzdak G 2006b Phospholipid capture combined with non-linear chromatographic correction for improved serum metabolite profiling *Metabolomics* **2** 145-54
- Waybright T J, Van Q N, Muschik G M, Conrads T P, Veenstra T D and Issaq H J 2006 LC-MS in metabolomics: Optimization of experimental conditions for the analysis of metabolites in human urine *J. Liq. Chromatogr. Relat. Technol.* **29** 2475-97

- Wishart D S, Tzur D, Knox C, Eisner R, Guo A C, Young N, Cheng D, Jewell K, Arndt D, Sawhney S, Fung C, Nikolai L, Lewis M, Coutouly M A, Forsythe I, Tang P, Shrivastava S, Jeroncic K, Stothard P, Amegbey G, Block D, Hau D D, Wagner J, Miniaci J, Clements M, Gebremedhin M, Guo N, Zhang Y, Duggan G E, MacInnis G D, Weljie A M, Dowlatabadi R, Bamforth F, Clive D, Greiner R, Li L, Marrie T, Sykes B D, Vogel H J and Querengesser L 2007 HMDB: the human metabolome database *Nucleic Acids Res.* **35** D521-D6
- Wu H F, Southam A D, Hines A and Viant M R 2008 High-throughput tissue extraction protocol for NMR and MS-based metabolomics *Anal. Biochem.* **372** 204-12

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- Bolten C J, Kiefer P, Letisse F, Portais J C and Wittmann C 2007 Sampling for metabolome analysis of microorganisms *Anal. Chem.* **79** 3843-9
- Cakir T, Patil K R, Onsan Z I, Ulgen K O, Kirdar B and Nielsen J 2006 Integration of metabolome data with metabolic networks reveals reporter reactions *Mol. Syst. Biol.*
- Castrillo J I, Hayes A, Mohammed S, Gaskell S J and Oliver S G 2003 An optimized protocol for metabolome analysis in yeast using direct infusion electrospray mass spectrometry *Phytochemistry* **62** 929-37
- Dalluge J J, Smith S, Sanchez-Riera F, McGuire C and Hobson R 2004 Potential of fermentation profiling via rapid measurement of amino acid metabolism by liquid chromatography-tandem mass spectrometry *J. Chromatogr. A* **1043** 3-7
- Faijes M, Mars A E and Smid E J 2007 Comparison of quenching and extraction methodologies for metabolome analysis of *Lactobacillus plantarum* *Microb. Cell. Fact.* **6**
- Gao P, Shi C Y, Tian J, Shi X Z, Yuan K L, Lu X and Xu G W 2007 Investigation on response of the metabolites in tricarboxylic acid cycle of *Escherichia coli* and *Pseudomonas aeruginosa* to antibiotic perturbation by capillary electrophoresis *J. Pharm. Biomed. Anal.* **44** 180-7
- Hoskisson P A and Hobbs G 2005 Continuous culture - making a comeback? *Microbiology-(UK)* **151** 3153-9
- Kaderbhai N N, Broadhurst D I, Ellis D I, Goodacre R and Kell D B 2003 Functional genomics via metabolic footprinting: monitoring metabolite secretion by *Escherichia coli* tryptophan metabolism mutants using FT-IR and direct injection electrospray mass spectrometry *Compar. Funct. Genom.* **4** 376-91
- Kern A, Tilley E, Hunter I S, Legisa M and Glieder A 2007 Engineering primary metabolic pathways of industrial micro-organisms *J. Biotechnol.* **129** 6-29
- Kilstrup M, Hammer K, Jensen P R and Martinussen J 2005 Nucleotide metabolism and its control in lactic acid bacteria *Fems Microbiol. Rev.* **29** 555-90
- Khoo S H G and Al-Rubeai M 2007 Metabolomics as a complementary tool in cell culture *Biotechnol. Appl. Biochem.* **47** 71-84
- Koek M M, Muilwijk B, van der Werf M J and Hankemeier T 2006 Microbial metabolomics with gas chromatography/mass spectrometry *Anal. Chem.* **78** 1272-81
- Lafaye A, Junot C, Pereira Y, Lagniel G, Tabet J C, Ezan E and Labarre J 2005 Combined proteome and metabolite-profiling analyses reveal surprising insights into yeast sulfur metabolism *J. Biol. Chem.* **280** 24723-30
- Larsen T O, Smedsgaard J, Nielsen K F, Hansen M E and Frisvad J C 2005 Phenotypic taxonomy and metabolite profiling in microbial drug discovery *Nat. Prod. Rep.* **22** 672-95
- Lu P, Rangan A, Chan S Y, Appling D R, Hoffman D W and Marcotte E M 2007 Global metabolic changes following loss of a feedback loop reveal dynamic steady states of the yeast metabolome *Metab. Eng.* **9** 8-20
- Maharjan R P, Seeto S and Ferenci T 2007 Divergence and redundancy of transport and metabolic rate-yield strategies in a single *Escherichia coli* population *J. Bacteriol.* **189** 2350-8
- Martins A M, Camacho D, Shuman J, Sha W, Mendes P and Shulaev V 2004 A systems biology study of two distinct growth phases of *Saccharomyces cerevisiae* cultures *Current Genomics* **5** 649-63
- Mashego M R, Gulik W M and Heijnen J J 2007a Metabolome dynamic responses of *Saccharomyces cerevisiae* to simultaneous rapid perturbations in external electron acceptor and electron donor *FEMS Yeast Res.* **7** 48-66

- Mashego M R, Rumbold K, De Mey M, Vandamme E, Soetaert W and Heijnen J J 2007b Microbial metabolomics: past, present and future methodologies *Biotechnol. Lett.* **29** 1-16
- Noh K, Gronke K, Luo B, Takors R, Oldiges M and Wiechert W 2007 Metabolic flux analysis at ultra short time scale: Isotopically non-stationary C-13 labeling experiments *J. Biotechnol.* **129** 249-67
- Smedsgaard J and Nielsen J 2005 Metabolite profiling of fungi and yeast: from phenotype to metabolome by MS and informatics *J. Exp. Bot.* **56** 273-86
- Wittmann C, Kromer J O, Kiefer P, Binz T and Heinzle E 2004 Impact of the cold shock phenomenon on quantification of intracellular metabolites in bacteria *Anal. Biochem.* **327** 135-9
- Wang Q Z, Yang Y D, Chen X and Zhao X M 2006 Comparisons of different extraction methods in *Escherichia coli* metabolome analysis *Chin. J. Anal. Chem.* **34** 1295-8
- Villas-Boas S G, Hojer-Pedersen J, Akesson M, Smedsgaard J and Nielsen J 2005b Global metabolite analysis of yeast: evaluation of sample preparation methods *Yeast* **22** 1155-69
- Villas-Boas S G, Akesson M and Nielsen J 2005a Biosynthesis of glyoxylate from glycine in *Saccharomyces cerevisiae* *FEMS Yeast Res.* **5** 703-9
- Villas-Boas S G and Bruheim P 2007 Cold glycerol-saline: The promising quenching solution for accurate intracellular metabolite analysis of microbial cells *Anal. Biochem.* **370** 87-97
- van der Werf M J, Jellema R H and Hankemeier T 2005 Microbial metabolomics: replacing trial-and-error by the unbiased selection and ranking of targets *J. Ind. Microbiol. Biotechnol.* **32** 234-52
- van der Werf M J, Overkamp K M, Muilwijk B, Coulier L and Hankemeier T 2007 Microbial metabolomics: Toward a platform with full metabolome coverage *Anal. Biochem.* **370** 17-25
- van der Werf M J, Overkamp K M, Muilwijk B, Koek M M, van der Werff-van der Vat B J C, Jellema R H, Coulier L and Hankemeier T 2008 Comprehensive analysis of the metabolome of *Pseudomonas putida* S12 grown on different carbon sources *Mol. Biosyst.* **4** 315-27
- van der Werf M 2006 New tools improve bioprocess operations - Applying metabolomics and multivariate data analysis tools for strain improvement and medium optimization *Genet. Eng. News* **26** 44-5
- Rabinowitz J D 2007 Cellular metabolomics of *Escherichia coli* *Expert Rev. Proteomics* **4** 187-98

Plant Metabolomics

- De Vos R C H, Moco S, Lommen A, Keurentjes J J B, Bino R J and Hall R D 2007 Untargeted large-scale plant metabolomics using liquid chromatography coupled to mass spectrometry *Nat. Protoc.* **2** 778-91
- Catchpole G S, Beckmann M, Enot D P, Mondhe M, Zywicki B, Taylor J, Hardy N, Smith A, King R D, Kell D B, Fiehn O and Draper J 2005 Hierarchical metabolomics demonstrates substantial compositional similarity between genetically modified and conventional potato crops *Proc. Natl. Acad. Sci. U. S. A.* **102** 14458-62
- Colebatch G, Desbrosses G, Ott T, Krusell L, Montanari O, Kloska S, Kopka J and Udvardi M K 2004 Global changes in transcription orchestrate metabolic differentiation during symbiotic nitrogen fixation in *Lotus japonicus* *Plant J.* **39** 487-512
- Davey M P, Burrell M M, Woodward F I and Quick W P 2008 Population-specific metabolic phenotypes of *Arabidopsis lyrata* ssp *petraea* *New Phytol.* **177** 380-8
- Gibon Y, Usadel B, Blaesing O E, Kamlage B, Hoehne M, Trethewey R and Stitt M 2006 Integration of metabolite with transcript and enzyme activity profiling during diurnal cycles in *Arabidopsis* rosettes *Genome Biol.* **7**
- Hall R D 2007 Food metabolomics: META-PHOR - A new European research initiative *Agro Food Ind. Hi-Tech* **18** 14-6
- Hall R D, Brouwer I D and Fitzgerald M A 2008 Plant metabolomics and its potential application for human nutrition *Physiol. Plant.* **132** 162-75

Data processing in metabolomics

- Adourian A, Jennings E, Balasubramanian R, Hines W M, Damian D, Plasterer T N, Clish C B, Stroobant P, McBurney R, Verheij E R, Bobeldijk I, Van der Greef J, Lindberg J, Kenne K, Andersson U, Hellmold H, Nilsson K, Salter H and Schuppe-Koistinen I 2008 Correlation network analysis for data integration and biomarker selection *Mol. Biosyst.* **4** 249-59
- Baran R, Kochi H, Saito N, Suematsu M, Soga T, Nishioka T, Robert M and Tomita M 2006 MathDAMP: a package for differential analysis of metabolite profiles *BMC Bioinformatics* **7**
- Broadhurst D I and Kell D B 2006 Statistical strategies for avoiding false discoveries in metabolomics and related experiments *Metabolomics* **2** 171-96
- Broeckling C D, Reddy I R, Duran A L, Zhao X C and Sumner L W 2006 MET-IDEA: Data extraction tool for mass spectrometry-based metabolomics *Anal. Chem.* **78** 4334-41
- Bruschi S, Calzolari D, Coquin L and Paternostro G 2008 HORA suite: a database and software for human metabolomics *Metabolomics* **4** 90-3
- Damian D, Oresic M, Verheij E, Meulman J, Friedman J, Adourian A, Morel N, Smilde A and van der Greef J 2007 Applications of a new subspace clustering algorithm (COSY) in medical systems biology *Metabolomics* **3** 69-77
- Jansen J J, Bro R, Hoefsloot H C J, van den Berg F W J, Westerhuis J A and Smilde A K 2008 PARAFASCA: ASCA combined with PARAFAC for the analysis of metabolic fingerprinting data *J. Chemometr.* **22** 114-21
- Jarvis R M and Goodacre R 2005 Genetic algorithm optimization for pre-processing and variable selection of spectroscopic data *Bioinformatics* **21** 860-8
- Katajamaa M and Oresic M 2007 Data processing for mass spectrometry-based metabolomics *J. Chromatogr. A* **1158** 318-28
- Smith C A, Want E J, O'Maille G, Abagyan R and Siuzdak G 2006 XCMS: Processing mass spectrometry data for metabolite profiling using Nonlinear peak alignment, matching, and identification *Analytical Chemistry* **78** 779-87

Others

- Ananiadou S, Kell D B and Tsujii J 2006 Text mining and its potential applications in systems biology *Trends Biotechnol.* **24** 571-9
- De Haro L and Panda S 2006 Systems biology of circadian rhythms: An outlook *J. Biol. Rhythms* **21** 507-18
- Doerr A 2007 Systems biology - Annotating the unannotated *Nat. Methods* **4** 8-9
- Fiehn O, Robertson D, Griffin J, van der Werf M, Nikolau B, Morrison N, Sumner L W, Goodacre R, Hardy N W, Taylor C, Fostel J, Kristal B, Kaddurah-Daouk R, Mendes P, van Ommen B, Lindon J C and Sansone S A 2007 The metabolomics standards initiative (MSI) *Metabolomics* **3** 175-8
- Lee J A 2003 Another load of metabolomics *Lancet Oncology* **4** 644-
- Li P, Oinn T, Soiland S and Kell D B 2008 Automated manipulation of systems biology models using libSBML within Taverna workflows *Bioinformatics* **24** 287-9
- Michaud M R, Benoit J B, Lopez-Martinez G, Elnitsky M A, Lee R E and Denlinger D L 2008 Metabolomics reveals unique and shared metabolic changes in response to heat shock, freezing and desiccation in the Antarctic midge, *Belgica antarctica* *J. Insect Physiol.* **54** 645-55
- Reynolds T 2007 The evolution of chemosystematics *Phytochemistry* **68** 2887-95
- Saito N, Robert M, Kitamura S, Baran R, Soga T, Mori H, Nishioka T and Tomita M 2006 Metabolomics approach for enzyme discovery *J. Proteome Res.* **5** 1979-87
- Sanchez-Ponce R and Guengerich F P 2007 Untargeted analysis of mass spectrometry data for elucidation of metabolites and function of enzymes *Anal. Chem.* **79** 3355-62
- Sansone S A, Fan T, Goodacre R, Griffin J L, Hardy N W, Kaddurah-Daouk R, Kristal B S, Lindon J, Mendes P, Morrison N, Nikolau B, Robertson D, Sumner L W, Taylor C, van der Werf M, van Ommen B and Fiehn O 2007 The metabolomics standards initiative *Nat. Biotechnol.* **25** 844-8