Phytochemistry, 2003, **62**, 817

Plant metabolomics: large-scale phytochemistry in the functional genomics era

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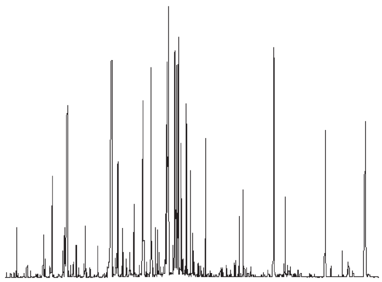
The critical role of metabolomics in functional genomics and systems biology of plants is reviewed. The development of metabolomics, current literature, technological approaches, bioinformatic tools and plant applications are discussed.



Phytochemistry, 2003, **62**, 837

Metabolome diversity: too few genes, too many metabolites?

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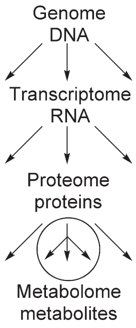
Lehrstuhl für Lebensmittelchemie, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The multitude of metabolites found in living organisms and the calculated small number of genes identified during genome sequencing projects discomfort biologists. Several processes on the transcription and translation level lead to the formation of isoenzymes and can therefore explain at least parts of this unexpected result. In this review it is assumed that metabolome diversity is governed by enzyme specificity and also by availability of suitable substrates as multifunctional enzymes are involved in various metabolic pathways.



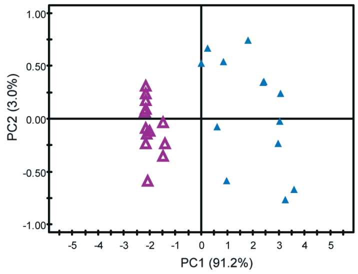
Phytochemistry, 2003, **62**, 851

Metabolomic analysis of the consequences of cadmium exposure in *Silene cucubalus* cell cultures via ^{1}H NMR spectroscopy and chemometrics

Nigel J.C. Bailey[a], Matjaz Oven[b], Elaine Holmes[a], Jeremy K. Nicholson[a], Meinhart H. Zenk[c]

[a]*Biological Chemistry, Biomedical Sciences Division, Imperial College of Science, Technology and Medicine, University of London, Sir Alexander Fleming Building, South Kensington, London SW7 2AZ, UK*
[b]*Leibniz-Institut für Pflanzenbiochemie, Weinberg 3, D-06120 Halle/Saale, Germany*
[c]*Biozentrum, Pharmazie, Universität Halle, Weinbergweg 22, D-06120 Halle/Saale, Germany*

Silene cucubalus plant cell cultures were exposed to cadmium chloride. By using a combination of NMR spectroscopy and principal components analysis, it was possible to discriminate between dosed (open triangles) and control (closed triangles) groups based on differences in their overall metabolic profile.



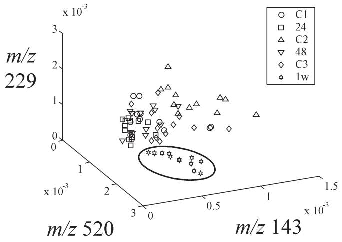
Phytochemistry, 2003, **62**, 859

Chemometric discrimination of unfractionated plant extracts analyzed by electrospray mass spectrometry

Royston Goodacre, Emma V. York, James K. Heald, Ian M. Scott

Institute of Biological Sciences, University of Wales Aberystwyth, Ceredigion SY23 3DA, UK

Chemometric methods including discriminant function analysis, artificial neural networks, and genetic programming, could discriminate the metabolic fingerprints obtained from unfractionated *Pharbitis nil* leaf sap by direct infusion into an electrospray ionization MS.



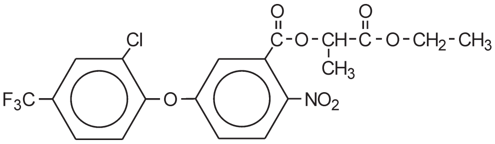
Phytochemistry, 2003, **62**, 865

Lactofen induces isoflavone accumulation and glyceollin elicitation competency in soybean

Serena Landini, Madge Y. Graham, Terrence L. Graham

Department of Plant Pathology, The Ohio State University, Columbus, OH 43210, USA

The disease protectant herbicide lactofen has several complementary effects on phenylpropanoid defense metabolism in soybean.



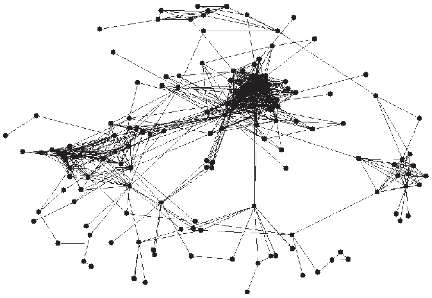
Phytochemistry, 2003, **62**, 875

Metabolic networks of *Cucurbita maxima* phloem

Oliver Fiehn

Max-Planck-Institute of Molecular Plant Physiology, D-14424 Potsdam/Golm, Germany

Co-regulatory networks comprising of 400 metabolites are shown to be robust compared to the large biological variation found for *Cucurbita maxima* vascular exudates.



Phytochemistry, 2003, **62**, 887

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

Cornelia Wagner[a], Michael Sefkow[b], Joachim Kopka[a]

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[b]*Division of Natural Product Chemistry, Institute for Chemistry, University of Potsdam, Karl-Liebknecht-Strasse 24-25, D-14467 Golm, Germany*

A mass spectral and retention time index library of 6205 mass spectral components was generated in a non-supervised manner from plant metabolic profiles covering major organs of potato, tobacco, and *Arabidopsis thaliana*. Using the two model compounds, 3-caffeoyl-quinic acid and galactonic acid, this database was employed to automated identification and classification of unknown components via mass spectral matching and hierarchical clustering.

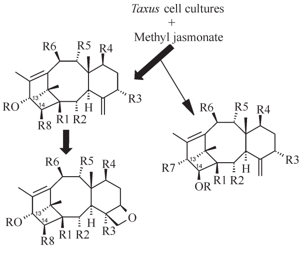
Phytochemistry, 2003, **62**, 901

Taxus metabolomics: methyl jasmonate preferentially induces production of taxoids oxygenated at C-13 in *Taxus* x *media* cell cultures

Raymond E.B. Ketchum[a], Christopher D. Rithner[b], Deyou Qiu[a], You Sun Kim[a], Robert M. Williams[b], Rodney B. Croteau[a]

[a]*Institute of Biological Chemistry, Washington State University, Pullman, WA 99164, USA*
[b]*Chemistry Department, Colorado State University, Ft. Collins, CO 80523, USA*

Methyl jasmonate elicitation of *Taxus* cell suspension cultures preferentially increased production of taxoids oxygenated at C-13, including paclitaxel (Taxol®).



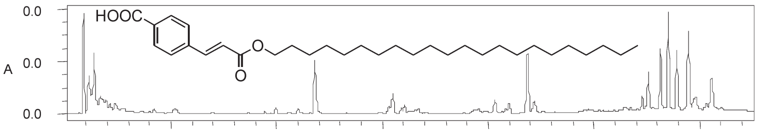
The role of chemical fingerprinting: application to *Ephedra*

Phytochemistry, 2003, **62**, 911

Brian T. Schaneberg[a], Sara Crockett[b], Erdal Bedir[a], Ikhlas A. Khan[a,b]

[a]*National Center for Natural Products Research, Research Institute of Pharmaceutical Sciences, School of Pharmacy,*
The University of Mississippi, University, MS 38677, USA
[b]*Department of Pharmacognosy, School of Pharmacy, The University of Mississippi, University, MS 38677, USA*

Ephedra sinica, known as *Ma Huang*, is one of the oldest medicinal herbs in traditional Chinese medicine. Reverse phase high performance liquid chromatography with photodiode array detection was applied for the chemical fingerprinting of the *Ephedra* species. Two compounds, 4-(2-eicosyl-oxycarbonyl-vinyl)-benzoic acid and 4-(2-docosyl-oxycarbonyl-vinyl)-benzoic acid, were isolated.



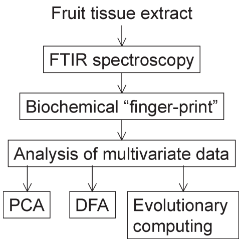
Metabolic fingerprinting of salt-stressed tomatoes

Phytochemistry, 2003, **62**, 919

Helen E. Johnson, David Broadhurst, Royston Goodacre, Aileen R. Smith

Institute of Biological Sciences, Cledwyn Building, University of Wales, Aberystwyth, Ceredigion, SY23 3DD, Wales, UK

The metabolic fingerprinting approach using Fourier transform infrared spectroscopy, chemometrics and evolutionary computing has been adopted to study the effect of salt stress on tomato fruit.



An optimized protocol for metabolome analysis in yeast using direct infusion electrospray mass spectrometry

Phytochemistry, 2003, **62**, 929

Juan I. Castrillo[a], Andrew Hayes[a], Shabaz Mohammed[b], Simon J. Gaskell[b], Stephen G. Oliver[a]

[a]*School of Biological Sciences, University of Manchester, 2.205 Stopford Building,*
Oxford Road, Manchester M13 9PT, UK
[b]*Michael Barber Centre for Mass Spectrometry, Department of Chemistry, UMIST,*
Manchester M60 1QD, UK

A method of quenching and extraction of cellular metabolites is optimized for direct analysis of samples by electrospray mass spectrometry (ES-MS) and application in functional genomics studies.

Cultivation →
Sampling (Quenching) →
Washing →
Extraction →
Concentration (Storage) →
ES-MS analysis (Direct Infusion) →
Metabolic Profiles →
Functional Genomics

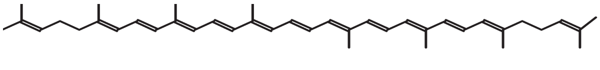
Identification and quantification of carotenoids, tocopherols and chlorophylls in commonly consumed fruits and vegetables

Phytochemistry, 2003, **62**, 939

Jennifer Burns, Paul D. Fraser, Peter M. Bramley

School of Biological Sciences, Royal Holloway, University of London, Egham, Surrey TW20 0EX, UK

The identity and levels of carotenoids, tocopherols and chlorophylls in fruits and vegetables have been achieved with on-line PDA detection.

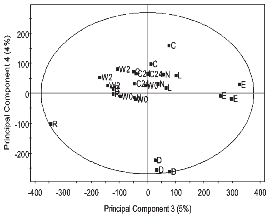


Phytochemistry, 2003, **62**, 949

Assessment of ^{1}H NMR spectroscopy and multivariate analysis as a technique for metabolite fingerprinting of *Arabidopsis thaliana*

Jane L. Ward, Cassandra Harris, Jennie Lewis, Michael H. Beale

IACR-Long Ashton Research Station, Department of Agricultural Sciences, University of Bristol, Long Ashton, Bristol BS41 9AF, UK



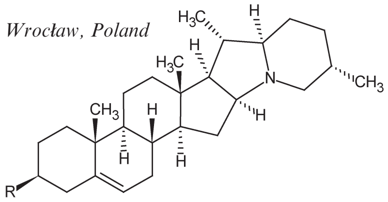
An approach to the metabolomic analysis of crude plant extracts has been developed using ^{1}H nuclear magnetic resonance spectroscopy and multivariate statistics. Using a set of ecotypes of *Arabidopsis thaliana*, a method has been developed for the rapid analysis of unfractionated polar plant extracts, enabling the creation of metabolite fingerprints. Comparison of datasets using chemometric methods led to conclusions regarding the structures of the compounds contributing to differences between spectra.

Phytochemistry, 2003, **62**, 959

Monitoring changes in anthocyanin and steroid alkaloid glycoside content in lines of transgenic potato plants using liquid chromatography/mass spectrometry

Maciej Stobiecki[a], Iwona Matysiak-Kata[b], Rafał Frański[c], Jacek Skała[d], Jan Szopa[b]

[a]*Institute of Bioorganic Chemistry PAS, Noskowskiego 12/14, 61-704 Poznań, Poland*
[b]*Institute of Biochemistry and Molecular Biology, University of Wrocław, Przybyszewskiego 63/77, 51-148 Wrocław, Poland*
[c]*Faculty of Chemistry, A. Mickiewicz University, Grunwaldzka 6, 60-708 Poznań, Poland*
[d]*Institute of Microbiology, University of Wrocław, Przybyszewskiego 63/77, 51-148 Wrocław, Poland*



Changes in qualitative and quantitative composition of steroid alkaloid glycosides in tubers of genetically modified plants (*Solanum tuberosum*) overexpressing and repressing enzymes of flavonoid synthesis are reported.

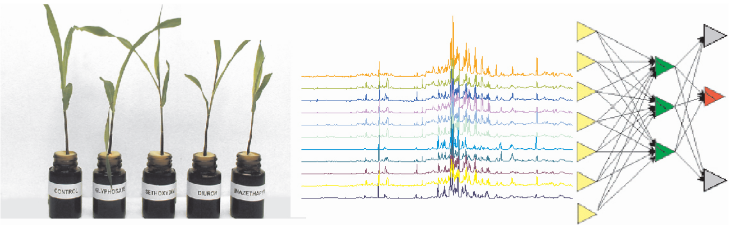
Phytochemistry, 2003, **62**, 971

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

Karl-Heinz Ott, Nelly Araníbar, Bijay Singh, Gerald W. Stockton

BASF Agro Research, Princeton, NJ 08543, USA

Neural network analysis of NMR spectra extracts from plants treated with different herbicides identifies biochemical mode-of-action.



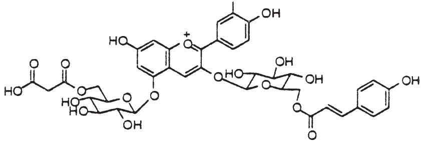
Phytochemistry, 2003, **62**, 987

Metabolomics and differential gene expression in anthocyanin chemo-varietal forms of *Perilla frutescens*

Mami Yamazaki[a], Jun-ichiro Nakajima[a], Mutsuki Yamanashi[a], Mitsuyo Sugiyama[a], Yukiko Makita[a], Karin Springob[a], Motoko Awazuhara[a], Kazuki Saito[a,b]

[a]*Graduate School of Pharmaceutical Sciences, Chiba University, Yayoi-cho 1-33, Inage-ku, Chiba 263-8522, Japan*
[b]*CREST of Japan Science and Technology Corporation, Yayoi-cho 1-33, Inage-ku, Chiba 263-8522, Japan*

The metabolites and gene expression in anthocyanin chemo-varietal forms of *Perilla frutescens* were profiled. The localization of anthocyanin accumulation and anthocyanidin synthase protein was also investigated. The linkage of metabolites and expression of genes and proteins are described.



Malonylshisonin

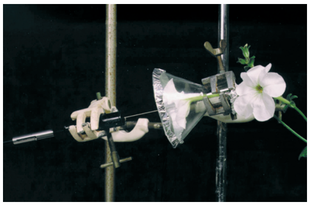
Phytochemistry, 2003, **62**, 997

Regulation of floral scent production in petunia revealed by targeted metabolomics

Julian C. Verdonk[a], C.H. Ric de Vos[b], Harrie A. Verhoeven[b], Michel A. Haring[a], Arjen J. van Tunen[a], Robert C. Schuurink[a]

[a]*Department of Plant Physiology, Swammerdam Institute for Life Sciences, University of Amsterdam, Kruislaan 318, 1098 SM Amsterdam, The Netherlands*
[b]*Plant Research International, PO Box 16, 6700 AA Wageningen, The Netherlands*

By applying solid phase micro extraction techniques, the composition and temporal emission of floral scent by petunia W115 was determined. The floral scent was dominated by volatile benzenoids. Microarray analysis showed that synthesis of the precursors of these benzenoids was regulated at the transcript level.



Phytochemistry, 2003, **62**, 1009

Factors affecting the robustness of metabolite fingerprinting using ^{1}H NMR spectra

Marianne Defernez, Ian J. Colquhoun

Institute of Food Research, Norwich Research Park, Colney, Norwich NR4 7UA, UK

The link between spectral quality and analysis by PCA is examined, highlighting the factors that may adversely affect the rigorousness of the approach.