PHYTOCHEMISTRY

AUTHOR INFORMATION PACK

TABLE OF CONTENTS

- Description p.1
- Audience p.2
- Impact Factor p.2
- Abstracting and Indexing p.3
- Editorial Board p.3
- Guide for Authors p.4

DESCRIPTION

*Phytochemistry* is a leading international journal publishing studies of plant chemistry, biochemistry, molecular biology and genetics, structure and bioactivities of phytochemicals, including 'omics' and bioinformatics/computational biology approaches. *Phytochemistry* is a primary source for papers dealing with phytochemicals, especially reports concerning their biosynthesis, regulation, and biological properties both *in planta* and as bioactive principles. Articles are published online as soon as possible as Articles-in-Press and in 12 volumes per year. Occasional topic-focussed special issues are published composed of papers from invited authors.

**Article types**

Full papers are original research papers reporting new discoveries that lead to a deeper understanding of any aspect of plants covered by the journal. Full papers are invited in the following sections, but these are not exclusive.

**Molecular Genetics and Genomics** contains papers which demonstrate novelty and/or biological significance in relation to all aspects of gene structure and expression, and their role in plant function, regulation, comparative genomics, and reconstitution of biochemical pathways. This section may also contain studies of genetically modified plants that have been analysed for changes in their profiles of phytochemical production.

**Protein Biochemistry and Proteomics** contains reports on plant proteins, including their purification directly from the organism or as a result of heterologous expression. This section includes studies of the macromolecular structure of proteins, protein function, enzyme mechanism, and proteomics, including in relation to changed genetics, environment or metabolism.

**Metabolism and Metabolomics** contains papers reporting new discoveries in all aspects of plant metabolism, both primary and specialized (secondary). Contributions are encouraged that report the elucidation of metabolic pathways, metabolic regulation, or the biosynthesis and roles of macromolecules. Reports improving our understanding of how phytochemicals act in planta are particularly welcomed, as are studies of transgenic organisms or of metabolic variation.

**Ecological Biochemistry and Chemistry** contains papers on how plants interact with their environment, including adaptation to environmental stress, symbiosis, interactions with other
organisms, phytoalexins, phytotoxins, pollination (bio)chemistry, and the use of phytochemicals by other organisms.

**Chemistry and Bioactive Products** contains papers on structural elucidation and in planta and in vitro activities of newly identified phytochemicals, including studies that elucidate their role and mode of action in nutritional, pharmacological, medical or therapeutic use. Studies of the biological activity of known compounds will only be considered when they add significant insight to the way in which the biological action of the phytochemical(s) is manifest.

**Chemotaxonomy** contains papers on the comparative phytochemistry of plants, in particular their role as a taxonomic tool.

**Reviews** are an authoritative and timely overview in a defined area and are intended to catch the interest of the general reader. A Review is a critical analysis of the current state of knowledge, pointing out strengths and weaknesses, weighing the significance of the studies conducted, how these fit into the more general subject area, and what are the key areas for further work. Authors should consult the Editor-in-Chief before preparing such articles.

**Molecules of Interest** are short, focussed reviews (3-5 printed pages) of individual compounds or macromolecules that are currently attracting significant applied, commercial or biological interest. Authors should consult the Editor-in-Chief before preparing such articles.

**Viewpoints** are articles that advance new ideas and conclusions concerning any area of plant biology and phytochemistry pertinent to the journal. Examples include the re-analysis of data using a new mathematical model, the reassessment of a pathway, or a new hypothesis to explain existing data. Authors should consult the Editor-in-Chief before preparing such articles. Examples include nomenclature issues, ways of expressing data, suggestions for standardising experimental procedures or any other topic that should stimulate debate.

Further details of these categories are given in the Guide for Authors.

**Preparation of papers**

Authors are advised to prepare their paper directly into the *Phytochemistry* format. Details of this are given in the Guide to Authors and can be seen in recently published papers. Submissions must be in good quality scientific English.

**Submission:** papers must be submitted online at www.ees.elsevier.com/phytochem to the Editor-in-Chief. The Editor-in-Chief will designate an Associate Editor to handle the paper depending on the subject area in which the work reported was conducted. The author may propose a preferred Associate Editor in their cover letter.

*Phytochemistry* is an official journal of The Phytochemical Society of Europe (PSE), The Phytochemical Society of North America (PSNA), and The Phytochemical Society of Asia (PSA). Society announcements are published at the discretion of the Publisher.

**AUDIENCE**

Organic Chemists, Plant Chemists, Plant Biochemists, Plant Molecular Biologists, Chemical Ecologists and Natural Product Chemists.

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GUIDE FOR AUTHORS

INTRODUCTION

*Phytochemistry* invites research articles on all aspects of pure and applied plant chemistry, plant biochemistry, plant molecular biology and chemical ecology. The Journal is currently divided up into the following sections:

Editorial Comment, Molecules of Interest, Review Articles, Structural Elucidation and Full Papers.

*Editorial Comment* will be an occasional series where Regional Editors, Board Members or other scientists will be invited to comment on phytochemistry topics of global interest and debate.

*Molecules of Interest* will consist of invited short reviews (3-4) printed pages of individual compounds or macromolecules of plant, fungal or algal origin. These can be novel compounds or newly discovered properties of familiar compounds. Please contact Dr Richard J Robins if you wish to prepare a Molecules of Interest paper.

*Review Articles* are published at regular intervals, ranging in scope from primary metabolism and regulation of plant growth, through plant enzymology to natural product chemistry and the biological activity of plant products. They deal with significant new areas of research and are intended to command the interest of the general reader. Authors should consult their Regional Editors with an outline of their proposed Review before preparing such articles. Published Reviews include a biography and picture of each author.

*Structure Elucidation* papers, accepted as full papers in the Chemistry section, should include either a substantial description of several new compounds without any conclusion as to their significance, or a description of the study of new compounds with expected structures incorporating conclusions. These papers with a minimum of 16 pages of double-spaced manuscript should follow the general style of Full Papers although the Introduction, Results and Discussion may be combined as a single narrative. Brief abstracts must be included, containing significant facts derived from the work. Reports of known compounds, however rare, from new plant sources will not generally be accepted unless they have real chemotaxonomic or other biological significance. Authors are specifically discouraged from submitting papers as fragmented analyses of particular plant constituents.

*Full Papers*: Full journal articles will be drawn from areas described in the Aims and Scope: Bioactive Products, Chemotaxonomy, Chemistry, Ecological Biochemistry, Metabolism, Molecular Genetics & Genomics, Protein Biochemistry & Proteomics, Update in Bioinformatics. They are comprehensive papers, typically 6-8 printed pages in length (a minimum of 20 pages of double-spaced manuscript). Papers on plant chemistry must be substantial and contain convincing justification for undertaking the study, as well as having conclusions (e.g. on the biology, chemotaxonomy, new biosynthetic pathways etc.). Papers submitted under the Bioactive Products area are unlikely to be accepted if the bioactivity is measured on a mixture of compounds without further resolution.

*Submission checklist*

You can use this list to carry out a final check of your submission before you send it to the journal for review. Please check the relevant section in this Guide for Authors for more details.

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One author has been designated as the corresponding author with contact details:
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**BEFORE YOU BEGIN**

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**PREPARATION**

**Peer review**

This journal operates a single blind review process. All contributions will be initially assessed by the editor for suitability for the journal. Papers deemed suitable are then typically sent to a minimum of two independent expert reviewers to assess the scientific quality of the paper. The Editor is responsible for the final decision regarding acceptance or rejection of articles. The Editor's decision is final. More information on types of peer review.

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It is important that the file be saved in the native format of the word processor used. The text should be in single-column format. Keep the layout of the text as simple as possible. Most formatting codes will be removed and replaced on processing the article. In particular, do not use the word processor’s options to justify text or to hyphenate words. However, do use bold face, italics, subscripts, superscripts etc. When preparing tables, if you are using a table grid, use only one grid for each individual table and not a grid for each row. If no grid is used, use tabs, not spaces, to align columns. The electronic text should be prepared in a way very similar to that of conventional manuscripts (see also the Guide to Publishing with Elsevier). Note that source files of figures, tables and text graphics will be required whether or not you embed your figures in the text. See also the section on Electronic artwork.

To avoid unnecessary errors you are strongly advised to use the 'spell-check' and 'grammar-check' functions of your word processor.

**Article Structure**

The content of manuscripts must be arranged as follows: (1) a Graphical Abstract; (2) a Title Page with authors name(s) and address(es); (3) and Abstract, in which contents are briefly stated; (4) Keywords; (5) Introduction, and (6) the Results and Discussion (preferably combined). Although each section may be separated by headings, they should form one continuous narrative and only include details essential to the arguments presented. If a discussion is separately provided, it should not include a repetition of the results, but only indicate conclusions reached on the basis of them, and those from other referred works; (7) Conclusions or Concluding Remarks; (8) the Experimental should include brief details of the methods used such that a competent researcher in the field may be able to repeat the work; (9) Acknowledgments; (10) Figures and Legends, Formulae, Tables and References. Authors have to include pagination.

**Subdivision - numbered sections**

Divide your article into clearly defined and numbered sections. Subsections should be numbered 1.1. (then 1.1.1., 1.1.2., ...), 1.2., etc. (the abstract is not included in section numbering). Use this numbering also for internal cross-referencing: do not just refer to "the text". Any subsection may be given a brief heading. Each heading should appear on its own separate line.

**Introduction**

State the objectives of the work and provide an adequate background, avoiding a detailed literature survey or a summary of the results.


**Theory/calculation**

A Theory section should extend, not repeat, the background to the article already dealt with in the Introduction and lay the foundation for further work. In contrast, a Calculation section represents a practical development from a theoretical basis.
Results
Results should be clear and concise.

Discussion
This should explore the significance of the results of the work, not repeat them. A combined Results and Discussion section is often appropriate. Avoid extensive citations and discussion of published literature.

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Provide sufficient detail to allow the work to be reproduced. Methods already published should be indicated by a reference: only relevant modifications should be described.
Subsections on the Experimental Procedures should be italicized and inserted as part of the first line of the text to which they apply. Phytochemistry encourages an extensive use of abbreviations (these are listed at the back of the Instructions to Authors, or the reader is referred to other sources). The Experimental should begin with a subsection entitled General Experimental Procedures. This subsection will typically contain brief details of instruments used, and identification of sources of specialized chemicals, biochemistry and molecular biology kits.
The next subsection describes the source(s) and documentation of biological materials used, whether in reference to whole plants or parts therefrom, crude drugs, or any other plant material from which identifiable chemical substances are obtained for the first time. Documentation must also include a reference to voucher specimen(s) and voucher number(s) of the plants or other material examined. If available, authors should quote the name and address of the authority who identified each non-cultivated plant investigated. Specimens should preferentially be deposited in a major regional herbarium where the collection is maintained by state or private institution and which permits loan of such materials.
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Compound characterization: Physical and spectroscopic data for new compounds must be comprehensive, and follow the order shown below: compound name (and assigned number in text); physical state of compound (e.g. oil, crystal, liquid, etc.), melting and/or boiling point; optical rotation and/or circular dichroism measurements, if optically active; UV; IR, \(^1\)H NMR; \(^{13}\)C NMR; MS. For all new compounds, either high-resolution mass spectral or elemental analysis data are required.

Conclusions
The main conclusions of the study may be presented in a short Conclusions section, which may stand alone or form a subsection of a Discussion or Results and Discussion section.

Essential title page information
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A concise and factual abstract is required. The abstract should state briefly the purpose of the research, the principal results and major conclusions. An abstract is often presented separately from the article, so it must be able to stand alone. For this reason, References should be avoided, but if essential, then cite the author(s) and year(s). Also, non-standard or uncommon abbreviations should be avoided, but if essential they must be defined at their first mention in the abstract itself.

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Highlights are mandatory for this journal. They consist of a short collection of bullet points that convey the core findings of the article and should be submitted in a separate editable file in the online submission system. Please use 'Highlights' in the file name and include 3 to 5 bullet points (maximum 85 characters, including spaces, per bullet point). You can view example Highlights on our information site.

Keywords
Authors must give 3-10 keywords or phrases, which identify the most important subjects covered by the paper. They should be placed at the beginning of the manuscript in the following order: name of plant species examined (Latin binomial); plant family; common epithet (where applicable); type of investigation; class of compound; protein or gene; name of compound(s); protein(s) and gene(s).

Abbreviations
About, approximately: ca.
Anhydrous: dry (not anhyd.)
Aqueous: aq.
Circular dichroism: CD
Concentrated (or mineral acids): conc.
Concentrations: ppm (never ppb!), μM, mM, M, %
Dry weight: dry wt; fresh weight: fr. wt
Electricity: V, mA, eV
Force due to gravity (centrifugation): g; rpm (revolutions/min)
Gas chromatography: GC
Gas chromatography-mass spectrometry: GC-MS
trimethylsilyl derivative: TMSi (TMS cannot be used as this refers to the internal standard tetramethylsilane used in 1H NMR)
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Length: nm, μm, mm, cm, m
Literature: lit.
Mass: pg, ng, μg, mg, g, kg
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Melting points: uncorr. (uncorrected)
Molecular mass: Da (daltons), kDa
Molecular weight: Mr
Nuclear magnetic resonance: 1H NMR, 13C NMR, Hz, δ
Numbers: e.g. 1, 10, 100, 1000, 10,000: per or -1
Optical rotatory dispersion: ORD
Paper chromatography: PC
Precipitate: ppt.
Preparative thin-layer chromatography: prep. TLC
Radioactivity: dpm (disintegrations per min), Ci (curie), sp. act (specific activity), Bq (1 becquerel = 1 nuclear transformation/sec)
Repetitive manipulations: once, twice, \( \times 3, \times 4 \), etc.

**RR**\( t \) (relative retention time), **R**\( t \) (Kovat's retention index), **ECL** (equivalent chain length - term frequently used in fatty acid work)

**Saturated:** satd.

**Solution:** soln.

Solvent mixtures including chromatographic solvents: abbreviate as follows \( n\)-BuOH–HOAc–H\( \text{H}_2\text{O} \) (4:1:5)

**Statistics:** LSD (least significant difference), s.d. (standard deviation), s.e. (standard error)

**Temperature:** (with centigrade), mp, mps, mmp, bp

**Time:** s, min, h, day, week, month, year

Ultraviolet spectrophotometry: UV, \( A \) (absorbance, not OD - optical density)

**Volume:** l (litre), \( \mu l \), ml

**Weight:** wt

For preparation of Inorganics and Organics please see the full instructions to authors, including all special characters, available for download as a pdf file. [pdf link](#)

For further terms used in biochemistry and molecular biology the authors should see the websites of the nomenclature committees. [http://www.chem.qmul.ac.uk/iubmb/](http://www.chem.qmul.ac.uk/iubmb/).

**Acknowledgements**

Collate acknowledgements in a separate section at the end of the article before the references and do not, therefore, include them on the title page, as a footnote to the title or otherwise. List here those individuals who provided help during the research (e.g., providing language help, writing assistance or proof reading the article, etc.).

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**Nomenclature and Units**

Chemical nomenclature, abbreviations and symbols must follow IUPAC rules. Whenever possible, avoid coining new trivial names; every effort should be made to modify an existing name. For example, when a new compound is described, it should be given a full systematic name according to IUPAC nomenclature and this should be cited in the Abstract or in the Experimental section. Isotopically-labeled substances should be written with the correct chemical name of the compound. The symbol for the isotope should be placed in square brackets and should precede that part of the name to which it refers, e.g. sodium \([14C]\)formate.

In Table headings and legends on graph axes numerical data should be identified in the form data name/units.

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Mass spectral data should be presented in full as Supplementary Information for all newly identified compounds. If the data are already published elsewhere then relevant references should be quoted. Presentation of mass spectral data should in general follow the recommendations given in Int. J. Mass
Spectrom. Ion Processes, 142, 211-240 (1995), and must indicate the method used (EIMS, CIMS, GC-MS, TOFMS, FABMS, SIMS, APCI etc.) and the relevant experimental details (ionizing energy, voltages etc). The data should give only diagnostically important ions, the character of the fragmentation ions in relation to the molecular ion and the intensity relative to the major ion. For example-EIMS (probe) 70 eV, m/z (rel. int.): 386 [M]+ (36), 368 [M - H2O]+ (100), 353 [M - H2O - Me] + (23), 275 [M - 111] + (35), etc. CIMS (iso-butane, probe), 200 eV, m/z (rel. int.): 387 [M + H]+ (100), 369 [(M + H) - H2O] + (23), etc. High-resolution spectra can be given in more detail if necessary for [M] + and the more important fragment ions.

X-ray crystallography
Only essential data (e.g. a three-dimensional structural drawing with bond distances) should be included in manuscripts. A complete list of data in CIF (Crystallographic Information File) format should be prepared separately and deposited with the Cambridge Crystallographic Data Centre (see http://www.ccdc.cam.ac.uk for further information) before the paper is submitted. A footnote indicating this fact is to be included in the manuscript. "CCDC...contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html (or from the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk). Please submit a copy of the CIF data when you submit your manuscript.

Elemental analysis results for compounds which have been adequately described in the literature must be given in the form: (Found: C, 62.9; H, 5.4. Calc. for C13H13O4N: C, 63.2; H, 5.3%). New compounds must be indicated by giving analytical results in the form: (Found: C, 62.9; H, 5.4. C13H13O4N requires: C, 63.2; H, 5.3%).

Thin-layer chromatography
(a) For analytical TLC, dimensions of the plates can be deleted if layer thickness is 0.25 mm.
(b) Abbreviate common adsorbents: (but use silica gel, not SiO2 as this does not describe the material accurately), Al2O3 (alumina).
(c) Preparative forms of the technique should include details of (i) layer thickness (preparative TLC only), (ii) amount of sample applied to the layer, (iii) method of detection used to locate the bands and (iv) the solvent used to recover the compounds from the adsorbent after development.
(d) Special forms of TLC on impregnated adsorbents can be abbreviated, e.g. AgNO3-silica gel (1:9), by wt can be assumed.
(e) Solvent mixtures should be specified as under Abbreviations above.

Gas chromatography
(a) Detector used should be specified, e.g. dual FID, EC, etc.
(b) Carrier gas and flow rate or inlet pressure should be given, e.g. N2 at 3 ml min-1/10 psi.
(c) Operating conditions, such as injector and detector heater temperatures, oven temperature programme, should be included.
(d) Packed columns, e.g. 6 m x 3 mm (i.d. measurement only) packed with 1% SE-30 (support material and mesh size can be omitted unless unusual).
(e) Capillary columns the type (e.g. WCOT, SCOT), manufacturer's designation (e.g. DB5) and dimensions (length, internal/external diameter, film thickness) should be specified.

High performance liquid chromatography
(a) Solvent or solvent gradients used together with flow rate should be given.
(b) Column dimensions (length x i.d. only) and packing used.
(c) Method of detection employed, e.g. UV or refractive index.

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Enzyme characterization
(a) Enzyme activity is expressed in units of katals (symbol kat), the conversion of one mol of substrate per sec. It should be made clear that the measurements were made under specified optimum conditions and were not seriously affected by losses during extraction and analysis.
(b) pH optima should be given together with pH values for half maximal activity.
(c) Kinetic parameters should be expressed as $V_{\text{max}}$, $K_m$ etc.
(d) Enzyme inhibitors-effectiveness should be expressed as $K_i$ or concentration for half-maximal activity.
(e) Optimal temperature of enzymes should not be given. This should be expressed in terms of "Energy of Activation" and "Energy of Activation for Denaturation".
(g) Labeling of proteins and nucleic acids-use of labeled precursors in assessing the rate of synthesis of macromolecules must be validated by evidence of real, direct incorporation. The possibility of occlusion or adsorption of isotopic material should be noted and it should be shown that the labeled precursor is incorporated without prior catabolism.

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