Phytochemistry Letters - Guide for Authors

Introduction

Phytochemistry Letters invites rapid communications on all aspects of natural product research including: structural elucidation of natural products, biotechnology, pharmacology of natural products, ethnobotany and traditional usage, genetics of natural products, analytical evaluation of herbal medicines, clinical efficacy, safety and pharmacovigilance of herbal medicines, bioassay-guided isolation, natural product synthesis and chemical modification, natural product biosynthesis, metabolomics, natural product metabolism and chemical ecology.

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- Structural elucidation of natural products
- Analytical evaluation of herbal medicines
- Clinical efficacy, safety and pharmacovigilance of herbal medicines
- Natural product biosynthesis
- Natural product synthesis and semi-synthesis
- Chemical ecology
- Biotechnology
- Bioassay-guided isolation
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- Pharmacology of natural products
- Metabolomics
- Ethnobotany and traditional usage
- Natural product metabolism
- Genetics of natural products

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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.

Specific names (genus, species, authority for the binomial) of all experimental plants must be given at first mention according to the Index Kewensis (searchable online at http://www.ipni.org or similar authority. (The Plant-Book: A Portable Dictionary of the Vascular Plants, by D. J. Mabberley, 2nd ed., June 1997, Cambridge University Press; ISBN:0521414210), and preferably be in the form recommended by the International Code of Botanical Nomenclature (http://www.bgbm.fu-berlin.de/iapt/nomenclature/code/tokyo-e/default.htm. Named varieties of cultivars are given e.g. *Lactuca sativa cv.* Grand Rapids. (The official printed version of the International Code of Botanical Nomenclature has been published as International Code of Botanical Nomenclature {Tokyo Code}. Regnum Vegetabile 131. Koeltz Scientific Books, Konigstein. ISBN: 3-87429-367-X or 1-878762-66-4 or 80-901699-I-0.)

Material and methods
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Experimental
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 Letters encourages an extensive use of abbreviations (these are below, 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, biochemicals and molecular biology kits.

This subsection describes the source(s) and documentation of biological materials used, whether in reference to whole plants or parts there from, crude drugs, or any other 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 that 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.

With micro-organisms, the culture collection from which they were either accessed and/or deposited should be included, together with identification of the strain designation code.

The Experimental Procedures employed should be concise but sufficiently detailed that a qualified researcher will be able to repeat the studies undertaken, and these should emphasize either truly new procedures or essential modifications of existing procedures. Experimental details normally omitted include: (1) method of preparation of common chemical and biochemical derivatives, (2) excessive details of separation of compounds, proteins and enzymes, e.g. preparation of columns, TLC plates, column and fraction size.

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. See later section for method of data presentation.

Nomenclature: 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 [^{14}C]formate.

Optical rotation, optical rotary dispersion, circular dichroism: Data should be presented in the established form, e.g. [α] value (+ or -) in ° (c {wt of compound in 100 ml of solvent}, solvent used) temp. Example: [α] +32 ° (c 0.3210, EtOH). ORD curves usually described as a series of values based on [α] or [Θ] (molecular rotation) at various wavelengths. CD values may be expressed as molecular ellipticity values [Θ], e.g., $[\Theta]_{256}$ +21 780, $[\Theta]_{307}$ - 16 113 or as differential dichroic absorption, e.g. $\delta_{\varepsilon 253}$ - 1.0 (MeOH; *c* 0.164). Ultraviolet–visible spectra: ε values are given as log values in parentheses, e.g. λ nm (log ε): 203 (4.7), etc. $EtOH_{max}$

Infrared spectra: Data should be presented in the established form, e.g. v cm^{-1}: 1740, etc. 3CHClmax. Absorption should be expressed only in wave-numbers and structural assignments should be indicated when possible in parentheses after the relevant wave-number, e.g. 1740(>C=O), etc. The following abbreviations should be used if the intensity of absorption bands are included: w-weak intensity, m-medium intensity, v-variable intensity, s-strong intensity, vs-very strong intensity.

NMR spectral data should only be presented in full if they have not been published separately elsewhere, in which case only relevant references should be quoted. Data must be specified as ^{1}H NMR or ^{13}C NMR and should indicate the frequency of the instrument, the solvent used and the internal standard. Chemical shifts should be quoted in δ units relative to TMS with indication of whether the signal is a singlet *s*, doublet *d*, doublet of doublets *dd*, triplet *t*, multiplet *m*, etc. ^{13}C NMR spectral data should specify the carbon concerned, using the recommended IUPAC numbering (e.g. C-1, C-2), and should be given to one decimal place. ^{1}H NMR spectral data should indicate the

number of hydrogens involved and their position of attachment based on the numbering of the carbon atoms, preferably according to IUPAC rules. For example - ^{13}C NMR spectral data (25.15 MHz, $CDCl_3$): ð 30.1 (*t*, C-5), 74.1 (*d*, C-6), 121.7 (*d*, C-3), 144.2 (*s*, C-4), etc. ^{1}H NMR spectral data (100 MHz, $CDCl_3$): ð 0.68 (3H, *s*, H-18), 0.88 (6H, *d*, *J*=6 Hz, H-26 and H-27), 0.90 (3H, *d*, *J*=5 Hz, H-21), 4.34 (1H,*q*, $J_{6\alpha,7\alpha}$=4.5 Hz, $J_{6\alpha,7\beta}$ =2 Hz, H-6), 4.21 (1H, *m*, $W_{1/2}$ 18 Hz, H-3α).

Mass spectral data should only be presented in full if they have not been published separately elsewhere, in which case only 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, etc.) and the ionizing energy. 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) eV, *m/z* (rel. int.): 386[M]+ (36), 368 [M - H_2O]+ (100), 353 [M - H_2O - Me] + (23), 275 [M - 111] + (35), etc. CIMS (*iso*-butane, probe), 200 eV, *m/z* (rel. int.): 387 [M + H] + (100), 369 [(M + H) - H_2O] + (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)". Crystal structures of proteins should be submitted to the Protein Data Bank (see http://www.rcsb.org/pdb e-mail: info@rcsb.org). 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 $C_{13}H_{13}O_4N$: 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. $C_{13}H_{13}O_4N$ 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 SiO_2 as this does not describe the material accurately), Al_2O_3 (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. $AgNO_3$-silica gel (1:9), by wt can be assumed.

Gas chromatography
(a) Detector used should be specified, e.g. dual FID, EC, etc.
(b) Carrier gas and flow rate should be given, e.g. N_2 at 3 ml min^{-1}.
(c) Operating conditions, such as injector and detector heater temperatures etc., 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 should be specified, e.g. WCOT (wall coated open tubular), SCOT (support

coated open tubular). The split ratio used in the injection system and the injection volume for the sample should also be included.

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.

Biochemical conventions

Unless a common biochemical term (e.g. ATP, NADH), biochemicals that are abbreviated should be spelled out in full (in brackets) immediately following their first usage in the text.

Enzyme names are typically not abbreviated, unless there are accepted abbreviations, such as ATPase. Where possible, E.C. numbers should be used for enzymes, and the recommendations of the Nomenclature Committee of the International Union of Biochemistry and Molecular Biology (IUBMB) should be used (see below).

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_{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".
(f) Enzyme nomenclature is now given in "Enzyme Nomenclature, Recommendations", Academic Press (1992) (http://www.chem.qmul.ac.uk/iubmb).
(g) Labelling of proteins and nucleic acids-use of labelled 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 labelled precursor is incorporated without prior catabolism.

Protein and nucleotide sequences

The Experimental must contain explicit documentation of the ends of nucleotide probes used in the study if previously unpublished, or by appropriate reference to published nucleotide numbers and/or restriction map.

In manuscripts to be published in Phytochemistry Letters, any new protein and/or nucleotide sequence must have been submitted to EMBL, GenBank™ or DNA Data Bank of Japan databases, with designated accession number(s) obtained **prior** to paper acceptance by the Regional Editor. The Author(s) must ensure access to this database information by timely release of data prior to publication, as well as providing necessary documentation to those already in the databases.

Nucleotide sequence data can be submitted either electronically (e-mail) or in computer-readable format, GenBank™ , EMBL and the DNA Data Bank of Japan addresses are: GenBank Submissions, National Center for Biotechnology Information, Building 38A, Room 8N-803, Bethesda, MD 20894.

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Acknowledgements
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Follow internationally accepted rules and conventions: use the international system of units (SI). If other units are mentioned, please give their equivalent in SI.

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Strunk Jr., W., White, E.B., 1979. The Elements of Style, third ed. Macmillan, New York.
Reference to a chapter in an edited book:
Mettam, G.R., Adams, L.B., 1999. How to prepare an electronic version of your article, in: Jones, B.S., Smith , R.Z. (Eds.), Introduction to the Electronic Age. E-Publishing Inc., New York, pp. 281–304.

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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, %, mol
Dry weight: dry wt; fresh weight: fr. wt
Electricity: V, mA, eV
Force due to gravity (centrifugation): *g*; rpm (revolutions min^{-1})
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 ^{1}H NMR)
High performance liquid chromatography: HPLC
Infrared spectrophotometry: IR
Length: nm, µm, mm, cm, m
Literature: lit.
Mass spectrometry: *m/z* [M]+ (molecular ion, parent ion)
Melting points: uncorr. (uncorrected)
Molecular mass: Da (daltons), kDa
Molecular weight: M_r
Nuclear magnetic resonance: ^{1}H NMR, ^{13}C NMR, Hz, ð
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^{-1})
Repetitive manipulations: once, twice, x3, x4, 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_2O (4:1:5)
Statistics: LSD (least significant difference), s.d. (standard deviation), s.e. (standard error)
Temperature: (with centigrade), mp, mps, mmp, bp
Temperature: temp.
Thin-layer chromatography: TLC, R_f
Time: s, min, h, day, week, month, year
Ultraviolet spectrophotometry: UV, *A* (absorbance, not OD—optical density)
Volume: l (litre), µl, ml
Weight: wt, pg, ng, µg, mg, g, kg

Inorganics, e.g. $AlCl_3$ (aluminum chloride), BF_3 (boron trifluoride), Cr^-, CO_2, H_2, HCl, $HClO_4$ (perchloric acid), HNO_3, H_2O, H_2O_2, H_2SO_4, H_3BO_3 (boric acid), He, $KHCO_3$ (potassium bicarbonate), $KMnO_4$ (potassium permanganate), KOH, K-Pi buffer (potassium phosphate buffer), $LiAlH_4$ (lithium aluminium hydride), Mg^{2+}, $MgCl_2$, N_2, NH_3, $(NH_4)_2SO_4$, Na^+, $NaBH_4$ (sodium borohydride), NaCl, $NaIO_4$ (sodium periodate), NaOH, Na_2SO_3 (sodium sulphite), Na_2SO_4 (sodium sulphate), $Na_2S_2O_3$ (sodium thiosulphate), O_2, PPi (inorganic phosphate), SO, Tris (buffer).

Organics, e.g. Ac_2O (acetic anhydride), *n*-BuOH (butanol), C_6H_6 (benzene), CCl_4 (carbon tetrachloride), CH_2Cl_2 (methylene chloride), $CHCl_3$ (chloroform), CH_2N_2 (diazo-methane), CM (carboxymethyl), DEAE (diethylaminoethyl), DMF (dimethylformamide), DMSO (dimethyl sulphoxide), EDTA (ethylene-diaminetetra-acetic acid), Et_2O (diethyl ether), EtOAc (ethyl acetate), EtOH (ethanol), HCO_2H (formic acid), HOAc (acetic acid), *iso*-PrOH (*iso*-propanol), Me_2CO (acetone), MeCOEt (methyl ethyl ketone), MeOH (methanol), NaOAc (sodium acetate), NaOMe (sodium methoxide), petrol (not light-petroleum or petroleum ether), PhOH (phenol), PrOH (propanol), PVP (polyvinylpyrrolidone), TCA (trichloroacetic acid), TFA (trifluoroacetic acid), THF (tetrahydrofuran).

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/).

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