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PHYTOCHEMISTRY

INSTRUCTIONS TO AUTHORS--1987

1. INTRODUCTION

1.1 PHYTOCHEMISTRY is intended to cover research on all aspects of pure and applied plant biochemistry, especially that which leads to a deeper understanding of the factors underlying the growth, development and differentiation of plants and the chemistry of plant products. The Journal is divided into seven sections, *Growth and Metabolism*, *Ecological Biochemistry*, *Biosynthesis*, *Cell Culture and Biotechnology*, *Chemotaxonomy*, *Plant Chemistry* and *Short Reports*.

2. SUBMISSION OF CONTRIBUTIONS

2.1 Contributions must be original and **must not** have been submitted elsewhere. If part of the results has been reported previously in any form whatsoever, a copy of that publication **must** accompany the manuscript on submission. Papers will only be accepted if they fall within the scope of the Journal as outlined in paragraph 1.1; those which deal only with either analytical methods or the synthesis of organic compounds will be rejected. Preliminary communications are not published in the Journal.

2.2 Contributions must be in the English language and submitted either as Full Papers, or as Short Reports. Reviews which survey important areas of plant biochemistry will also be considered, but Authors must consult the Editors before preparing such articles. The contents of papers are the sole responsibility of the Authors, and publication does not imply the concurrence of Editors or Publishers.

2.3 All manuscripts and contributions should be submitted to Prof. J. B. HARBORNE, Department of Botany, The University of Reading, Whiteknights, P.O. Box 221, Reading RG6 2AS, Berkshire, U.K. Authors in North America may send their manuscripts to Prof. G. CORDELL, Program for Collaborative Research in the Pharmaceutical Sciences, College of Pharmacy, University of Illinois at Chicago, IL 60612, U.S.A. for onward transmission.

3. EDITORIAL AUTHORITY

3.1 The Editors reserve the right to make alterations in manuscripts submitted for publication. Such alterations will be made if manuscripts do not conform with accepted scientific standards or if they contain matter which in the opinion of the Editors is unnecessarily verbose or repetitive. If Authors wish to see such alterations before their paper is accepted for press, they **must** so indicate when their manuscript is submitted. Alterations may be queried at the proof stage, but this will inevitably delay publication and **should only be done if the scientific meaning has been seriously upset.** Where papers need extensive alteration, they will be returned to the Authors for checking and re-typing. Such papers must be returned to the Editors within one month. Otherwise they will be deemed to be new and will be subject to further review.

4. FORM OF CONTRIBUTIONS

4.1 All manuscripts intended for publication must be submitted *in duplicate* on good quality paper typed throughout with double-spacing between lines, with adequate margins (4 cm) and liberal space at the top and bottom of each page.

4.2.1 If authors are unfamiliar with the Journal, they should consult a recent copy to see the conventions followed in both Full Papers and Short Reports. Note especially that Experimental Methods are placed at the end and that References are numbered sequentially.

4.2.2 The content of manuscripts must be arranged as follows: (1) a *Title*; (2) authors name(s) and address(es); (3) a *Key Word Index*; (4) an *Abstract*, in which the contents are briefly stated; (5) the *Introduction*, the *Results* and the *Discussion*. Although these three sections may be separated by headings, they should, as far as possible, form one continuous narrative and only include such details which are essential to the argument presented. *Discussions* should not include a repetition of results but only indicate conclusions reached on the basis of them and those from other works referred to. (6) The *Experimental* which should include brief details of the methods used such that a competent operator may repeat the work; (7) *Acknowledgements*; (8) *Figures*, *Formulae*, *Tables* and *References*.

4.2.3 Titles must be as brief as possible, consistent with clarity, and should not exceed ten words in length. Uninformative phrases such as "Chemical examination of", "Studies on", etc., will be deleted. The taxonomic authority after a plant name must be omitted from the title. If a paper is part of a series, this must not be given in the heading, but referred to in a footnote in the form: *Part 9 in the series "The Alkaloids of *Papaver somniferum*" followed by a numbered reference to the previous part.

4.2.4 *Authors' names*. Each author should identify himself or herself with one forename, initials of other forenames and surname. This is to enable more exact computerized indexing and information retrieval.

4.2.5 *Key Word Index*. Authors must give from three to ten "key words" 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; compound(s). For example; **Key Word Index**—*Musa sapientum*; Musaceae; banana; biosynthesis; phytosterols; cycloeucalenol.

4.2.6 *Abstracts.* Abstracts should briefly describe the results obtained and conclusions reached, *not* the methods used, or speculations on any other matter. They are not expected to be a complete summary but only an outline of the main findings.

4.2.7 *Introductions* should give the **minimum** historical data needed to set the scene for the author's own investigation. Only results essential to the arguments should be presented. Much data can be taken for granted or quoted in abbreviated form. Authors are encouraged to combine the *Results* and *Discussion* sections wherever possible and are asked to avoid undue speculation.

4.2.8 *Figures, diagrams, formulae,* and *tables* of the following type generally will **not** be accepted for publication: (1) diagrams of photographs of chromatograms (PC and TLC), electrophoretic separations, or recorder traces of GC and HPLC data wich are given *merely* to prove indentification; (2) straight-line graphs; (3) generalized pH and temperature–denaturation curves of enzymes; (4) illustrations of IR, UV, NMR or MS (values can be quoted in the text or Experimental); (5) flow sheets illustrating isolation of compounds, (6) expectable MS fragmentation patterns; (7) formulae of well-known compounds or reaction schemes; (8) tables either giving single values for each parameter which could be easily quoted in the text or repeating data shown elsewhere.

4.2.9 *Figures, schemes and chemical formulae* for publication should first be drawn on separate sheets of good quality paper using black waterproof ink. They should be drawn twice the size finally required; that is not more than 12 cm wide and 30 cm high. Lettering should be in initial capital—small *sans serif* style and drawn using any suitable stencil or added from a transfer sheet. The letters should be 3–4 mm high with a line thickness of 0.3–0.5 mm. Lines on graphs should be 0.5–0.6 mm thick and should not pass through the symbols used as datum points. The symbols used and their size for half reduction are ○ ● △ □ ■ × +. All graphs must have a border all around 0.3–0.4 mm thick, and the scales, which must be clearly shown, should be marked outside this. Each curve in a graph must be clearly identified, either by a caption within the border or in the descriptive legend. Each scheme and graph must be clearly identified with the author's name, abbreviated title of the paper and the figure number. Descriptive legends, which must include a title, should be collected together on a separate sheet. Chemical formulae must be made absolutely clear; printers are not chemists and much delay is caused by sloppy drawing. Aromatic rings must be drawn with alternate double bonds and conformation of single bonds shown by thickened (▶) or dashed (||||) lines according to convention. Formulae should be numbered consecutively in *arabic* numerals.

4.2.10 *Half-tone photographs* can only be submitted by prior arrangement with the Editors. They must have good contrast and not be more than 25 cm wide and not more than 30 cm high.

4.2.11 *Tables* must be typed on separate sheets and arranged to be viewed vertically. They must be so constructed as to be intelligible without reference to the text. Every table must have an arabic number, a title and each column must be provided with an explanatory reading. Footnotes may be used to expand column headings, etc. and should be used in the order: *, †, ‡, §, ¶, , **, etc. Results should be cited only to the degree of accuracy justified on the basis of the errors of the method and **usually** only to three significant figures. Units must always be clearly indicated and chosen so as to avoid excessively high (> 100) or low (< 0.01) values. The figure zero should precede the decimal point for all numbers below one (e.g. 0.1).

4.2.12 *References* must be numbered consecutively in the text (one reference per number) and should be typed in order on a separate sheet. Only essential references should be included. These should be given in the correct format, i.e. the names of the Authors, followed by their initials in sequence; the year of publication in parentheses; the title of the journal (abbreviated in accordance with *Chemical Abstracts*) and underlined once; the volume number, squiggly line underneath; and the first page number. Personal communications or unpublished results should be referred to *only* in the body of the text (e.g. as Synge, R. L. M., personal communication) without any reference number. Any footnote must be presented separately from the references.

4.2.13 *Experimental.* The Experimental must be concise and extensive use of abbreviations is essential (see below). Experimental details which must be omitted are: (1) method of preparation of common chemical derivatives, such as acetates, methyl ethers, etc; (2) excessive details of separation of compounds, e.g. preparation of columns, TLC plates, column and fraction size; (3) commercial source of instruments, chemicals and biochemicals.

Subtitles in the Experimental should be italicized (underlined) and inserted as *part* of the first line of the text to which they apply.

4.2.14 *Documentations of plant materials.* In **all cases** when papers contain references to whole plants or parts therefrom, to crude drugs, or to any other plant material from which identifiable chemical substances have been obtained for the first time, they must also include, when at all possible, reference to voucher specimen(s) of the plants or other material examined. If available, authors should quote the name and address of the authority who undertook the identification of each non-cultivated plant investigated. Such specimens should be deposited in a major regional herbarium where the collection is maintained by state or private institution and which permits the loan of such materials.

4.2.15 *Short reports* are those which can be adequately presented in up to two printed pages (i.e. six to eight pages of manuscript). They should be well documented and should generally follow the 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.**

5. OTHER MATTERS

Proofs and reprints

5.1.1 *Proofs* will be sent to Authors for checking before publication normally to the first-named Author at the address given at the head of the manuscript. Corrections to the Proof must be marked clearly. Any substantial alterations other than printer's errors will be charged to the Author(s). A reprint order form will accompany the proofs and should be returned, with the proofs, to the Publisher. It should be noted that proof corrections are subject to Editorial control.

5.1.2 *Errata and addenda* to published articles will, **at the discretion of the Editors**, be incorporated in the June and December issues of the Journal.

Nomenclature

5.2.1 *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. 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 labelled 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.

For further details of the 'square-brackets-preceding' system see the Instructions to Authors of the Biochemical Journal, the Chemical Society or the American Chemical Society.

5.2.2 *Terms in biological chemistry* should follow: (a) the *Instructions to Authors of the Biochemical Journal* (revised annually), or the notes given at the beginning of each number of the *Journal of Biological Chemistry*; (b) the IUPAC rules on biological chemistry nomenclature. Where there is any difference in recommendations, the Editors will follow the latest publication.

5.2.3 *Specific names* (genus, species, authority for the binomial) of all experimental plants must be given at first mention according to the *Index Kewensis* or similar authority, and preferably be in the form recommended by the *International Code of Botanical Nomenclature*. Named varieties of cultivars are given as, e.g. *Lactuca sativa* cv Grand Rapids.

5.2.4 *Analytical 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%).

5.2.5 *NMR 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 data should specify the carbon concerned, using the recommended IUPAC numbering (e.g. C-1, C-2). ^{1}H NMR 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 (25.15 MHz, $CDCl_3$): δ 30.09 (*t*, C-5), 74.07 (*d*, C-6), 121.73 (*d*, C-3), 144.15 (*s*, C-4), etc. ^{1}H NMR (100 MHz, $CDCl_3$): δ 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).

5.2.6 *Mass spectral data* should only be presented in full if they have not been published separately elsewhere in which case only the relevant references should be quoted. Presentation of mass spectral data should in general follow the recommendations given in *Org. Mass Spectrom.* **14**, 1–2 (1979) and must indicate the method used (EIMS, CIMS, GC-MS, etc.) and the ionizing energy. The data should give only the 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 $[M - H_2O]^+$ (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.

5.2.7 *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 refined co-ordinates (as the computer print-out), together with any other relevant data not included in the manuscript should be prepared separately in a form suitable for deposit at the Cambridge Crystallographic Data Centre. These data should be submitted with the manuscript and the Authors should also deposit the material at Cambridge at the time the paper is published. A note indicating this fact should be included in the manuscript.

Abbreviations

5.3.1 Trivial names for enzymes can be used provided that reference is made at the beginning of the manuscript to the Enzyme Commission (EC) number when one has been allocated [see *Enzyme Nomenclature*, Academic Press, New York (1978)].

5.3.2 *Examples of accepted abbreviations* are given separately below. All other abbrevations must be defined when first mentioned in the text.

ABBREVIATIONS

Weight: wt, pg, ng, μg, mg, g, kg
Molecular weight: M_r
Dry weight: dry wt; fresh weight: fr. wt
Volume: l, (litre), μl, ml
Length: nm, μm, mm, cm, m
Time: sec, min, hr, day, week, month, year
Temperature: ° (without centrigrade), mp, mps, mmp, bp
Force due to gravity (centrifugation): *g*; rpm (revolutions/min)
Electricity: V, mA, eV

Concentrations: ppm (never ppb!), μM, mM, M, %, mol
Numbers: e.g. 1, 10, 100, 1000, 10000; per or /, not ⁻¹
About, approximately: *ca*
Paper chromatography: PC
Thin-layer chromatography: TLC, R_f
Preparative-layer chromatography: prep. TLC
High pressure liquid chromatography: HPLC
Gas chromatography: GC, prep. GC/MS
RR_t (relative retention time), R_t (Kovat's retention index), ECL (equivalent chain length - -term frequently used in fatty acid work)
Ultraviolet spectrophotometry: UV, *A* (absorbance not OD—optical density)
Infrared spectrophotometry: IR
Optical rotatory dispersion: ORD
Circular dichroism: CD
Nuclear magnetic resonance: ^{1}H NMR, ^{13}C NMR, Hz, δ
Mass spectrometry: *m/z*, M⁺ (molecular ion, parent ion)
Gas chromatography mass spectrometry: GC/MS
Trimethylsilyl derivative: TMSi (TMS cannot be used as this refers to internal standard tetramethylsilane used in ^{1}H NMR)
Solution: soln
Concentrated (or mineral acids): conc
Anhydrous: dry (not anhyd)
Saturated: satd
Aqueous: aq.
Temperature: temp.
Precipitate: ppt.
Repetitive manipulations: once, twice, ×3, ×4, etc.
Radioactivity: cpm (counts per min), dpm (disintegrations per min), Ci (curie), sp. act. (specific activity), Bq (1 becquerel = 1 nuclear transformation/sec)
Statistics: LSD (least significant differences), s.d. (standard deviation), s.e. (standard error)
Solvent mixtures including chromatographic solvents: abbreviate as follows *n*-BuOH–HOAc–H_2O (4:1:5)
Melting points: uncorr. (uncorrected), lit. (literature)

Inorganics e.g.

CO_2, N_2, O_2, H_2, He, H_2O, H_2O_2, NH_3, HCl, H_2SO_4, HNO_3, H_3BO_3 (boric acid), NaCl, $(NH_4)_2SO_4$, NaOH, KOH, $NaIO_4$ (sodium periodate), $KMnO_4$ (potassium permanganate), $MgCl_2$, $Na_2S_2O_3$ (sodium thiosulphate), Na_2SO_3 (sodium sulphite), Na_2SO_4 (sodium sulphate), $KHCO_3$ (potassium bicarbonate), $HClO_4$ (perchloric acid), $AlCl_3$ (aluminium chloride), Na^+, Mg^{2+}, Cl^-, SO_4^{2-}, Pi, PPi (inorganic phosphate), BF_3 (boron trifluoride), Tris (buffer), etc., K-Pi buffer (potassium phosphate buffer), $LiAlH_4$ (lithium aluminium hydride), $NaBH_4$ (sodium borohydride).

Organics e.g.

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

^{1}H NMR solvents and standards: $CDCl_3$ (deuterochloroform), DMSO-d_6 [deuterodimethylsulphoxide not $(CD_3)_2SO$], pyridine-d_5 (deuteropyridine), D_2O, TMS (tetramethylsilane).

Biochemicals: consult *Biochemical Journal*.

ATP (etc), DNA, RNA, *t*RNA, etc., RNase, NAD, NADP, FAD, FMN, GSH, CoA, Ala (alanine), etc., Glc (glucose), etc.

Thin-layer chromatography

(a) For analytical TLC, dimensions of the plates can be deleted and it can be assumed that layer thickness is 0.25 mm.

(b) Abbreviate common adsorbents: (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 (prep. 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) Omit manufacturer's name.

(b) Detector used should be specified, e.g. dual FID, EC, etc.

(c) Carrier gas and flow rate should be given, e.g. N_2 at 30 ml/min.

(d) Operating conditions, e.g. isothermal 250°, temp. programmed 100° to 300° at 2°/min. Details such as injector and detector heater temps. should be included.

(e) Packed columns, e.g. 6 m × 3 mm (i.d. measurement only) packed with 1% SE-30 (support material and mesh size can be omitted unless unusual).

(f) 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 vol. for the sample should also be included.

High pressure liquid chromatography

(a) Pressure and solvent or solvent gradients used should be given.

(b) Column dimensions (length × i.d. only) and packing used.

(c) Method of detection employed, e.g. UV, refractive index.

Visible and ultraviolet spectra

Data should be presented in the established form viz.

$$\lambda_{max}^{EtOH}\ \text{nm}: \ldots 203, \text{ etc.}$$

ϵ values are given as log values in brackets, e.g. λ_{max}^{EtOH} nm ($\log \epsilon$): 203 (4.17), etc.

Optical rotation, optical rotary dispersion, circular dichroism. Data should be presented in the established form, viz.

$[\alpha]_D^{temp.}$/Value + or − in° (solvent used; c {wt. of compound in / 100 ml solvent})

Example: $[\alpha]_D^{23}$ + 32° (EtOH; c 0.3210).

ORD curves are usually described as a series of values based on [α] or (ϕ] (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. $\Delta\epsilon_{253}$ − 1.0 (MeOH; c 0.164).

Infrared spectra

(a) Data should be presented in the established form, viz.

$$\nu_{max}^{CHCl_3}\ \text{cm}^{-1}: \ldots 1740, \text{ etc.}$$

Absorptions should be expressed only as wave-numbers and structural assignments should be indicated whenever possible in brackets after the relevant wave-number, e.g. 1740 (>C=O) etc.

(b) 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.

Biochemistry

(a) *Enzyme activity* is now 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 killing, extraction and analysis.

(b) *pH optima* should be given together with pH values for half maximal activity.

(c) *Enzyme inhibitors*—effectiveness should be expressed as K_i or concentration for half maximal activity.

(d) *Optimal temperature* of enzymes should not be given. This should be expressed in terms of "Energy of Activation" and "Energy of Activation for Denaturation".

(e) *Enzyme nomenclature* is now given in the Recommendations (1978) of the IUPAC and I.U.B., Elsevier (1979).

(f) *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.

A CHECK LIST FOR AUTHORS BEFORE SUBMISSION

1. Is the subject matter really appropriate to this journal?
2. Is the work described both new and significant?
3. Is the title both *short* and *informative?*
4. Have you remembered to include *Key Word Index* and *Running Title*?
5. Does the *Abstract* fully represent your scientific contribution? It is self-contained? (Avoid formulae numbers and abbreviations given in the text.)
6. Is your manuscript typed clearly on good quality paper, double spaced throughout with adequate margins?
7. Have you avoided repeating yourself? Have you avoided presenting the same data more than once? Can you really justify writing separate 'Results' and 'Discussion' sections?
8. Have you numbered the references *sequentially* in the text in square brackets and allotted a separate number for each reference?
9. Have you checked plant names? Are you sure of the identity of the plants examined? Have you indicated the *part* of the plant you extracted?
10. Have you remembered to add the accepted IUPAC systematic names for new plant products?
11. Have you used all the suggested abbreviations in the Experimental?

(Copies of these instructions can be obtained from the Editors.)