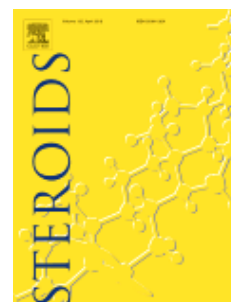




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Guidelines Concerning Identification, Characterization, and Purity of Compounds

Compound identity and purity

Evidence must be presented establishing the identity and purity of all new compounds, and of all compounds subjected to biochemical or biological assays. High quality reproductions of ^1H and ^{13}C NMR spectra must accompany the manuscript, in a Supporting Information Section, which will not appear in the journal, but will be used by reviewers and be available on the web (see below). A structure drawing and structure number should be placed on each NMR spectrum, along with the solvent and field strength. The contents of the Supporting Information Section should be summarized in a brief statement at the end of the manuscript, and a complete Table of Contents should appear at the beginning of the Supporting Information Section. When single-crystal X-ray diffraction structures are reported, CIF files need to be furnished as separate supporting information files, even if text tables of crystallographic data are included, and even if the data have been deposited in a crystallographic database.

Identification of structure: Sufficient spectroscopic information must be presented to establish the structural identity of all new compounds, whether isolated as naturally occurring steroids or newly synthesized ones. These data should appear in the Experimental Section and be adequate for unambiguous structure elucidation. A list of proton or ^1H and ^{13}C NMR peaks is generally sufficient, but if structural identification was based on NMR data, peak assignments should also be given. Chemical shift data should be given only to two decimal places. Infrared absorptions, diagnostic for key functional groups, are also helpful, and high resolution mass spectroscopic data can provide an additional criterion of compound identity. When a series of closely related compounds is reported, spectroscopic data can be presented in a table, or full spectroscopic data for a representative member can be presented, with comments made on the spectral features unique to other members of the series. For known compounds, the source or literature reference(s) to the previous isolation or to the previous method of preparation and characterization must be provided.

For known compounds, indicate the observed and literature melting points for crystalline solids, and/or the observed and literature optical rotations, in the following formats: mp xx °C (lit [ref] xx °C) and/or $[\text{D}]^{\text{C}}_{\text{xx}^{\circ}}$ (c, xx g/100 mL; solvent) (lit [ref] $[\text{D}]^{\text{C}}_{\text{xx}^{\circ}}$ (c, xx g/100 mL; solvent). Provide comments (either in general or for individual compounds) comparing the observed ^1H and ^{13}C NMR data of known compounds with the literature values, e.g., The ^1H and ^{13}C NMR data (xx MHz, solvent) agreed well with the literature values [ref]. It is not necessary to report complete data sets for known compounds. However, significantly different or improved data (e.g., different chemical shifts, data in different solvents, data taken at higher field, improved coupling analyses, etc.) should be reported in the Experimental Section or in a Table of NMR data and assignments.

Many naturally occurring steroids are isolated as glycoside derivatives. In such cases, the structures and absolute configuration of the individual sugar residues should be determined after hydrolysis. The absolute configuration of an individual sugar can be determined by comparing its optical rotation with the literature value for sugars of well-established absolute configuration. Another approach is direct comparison with authentic samples of the D and L sugars, or their derivatives, by high-pressure liquid chromatography (HPLC) or by gas chromatography (GC) on columns containing suitable chiral adsorbents, provided it is demonstrated that the enantiomeric compounds give separate peaks on the chiral columns.

Criteria for the purity of all compounds and of compounds with biological data: All new compounds need to be pure. Evidence of high purity is essential where biochemical or biological assay data are presented and related to compound structures; these compounds are termed "SAR compounds." The purity of SAR compounds should be more than 98 percent; the purity of other compounds should be more than 95 percent. Any questions regarding the purity of SAR compounds should appear in the Results.

The methods used to establish the purity of steroids subjected to biochemical or biological assays must be described in the Experimental Section. Most steroids obtained in pure form will be crystalline. Thus, there should be an attempt to purify and crystallize all products of chemical reactions or compounds isolated from plant extracts. Melting points should be recorded and reported for all crystalline compounds. It is strongly recommended that optical rotations be reported for new compounds. The weights and % yields should be reported for products isolated from chemical transformations.

Evidence for purity can take many forms: Combustion analyses for carbon, hydrogen and nitrogen are adequate. These data should appear in the Experimental Section and should agree with the calculated data within 0.4 percent. A recommended form for presentation is: C₁₈H₂₃NO₄: calcd. C, 68.12; H, 7.30; N, 4.41. Found. C, 68.50; H, 7.18; N, 4.26. When satisfactory combustion analyses are not available, evidence of purity should be provided by HPLC chromatograms run in two divergent solvent systems (typically normal and reversed phase) or by high quality proton NMR spectra obtained at high signal-to-noise. These chromatograms or spectra should be included as supplementary data.

Footnotes

Footnotes should be used sparingly. Number them consecutively throughout the article. Many word processors can build footnotes into the text, and this feature may be used. Otherwise, please indicate the position of footnotes in the text and list the footnotes themselves separately at the end of the article. Do not include footnotes in the Reference list.

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Electronic artwork

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Provide a title for each table. If a table must be continued to a second page, repeat all headings.

References

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Text: Indicate references by number(s) in square brackets in line with the text. The actual authors can be referred to, but the reference number(s) must always be given.

Example: '..... as demonstrated [3,6]. Barnaby and Jones [8] obtained a different result'

List: Number the references (numbers in square brackets) in the list in the order in which they appear in the text.

Examples:

Reference to a journal publication:

[1] J. van der Geer, J.A.J. Hanraads, R.A. Lupton, The art of writing a scientific article, *J. Sci. Commun.* 163 (2010) 51–59.

Reference to a book:

[2] W. Strunk Jr., E.B. White, *The Elements of Style*, fourth ed., Longman, New York, 2000.

Reference to a chapter in an edited book:

[3] G.R. Mettam, L.B. Adams, How to prepare an electronic version of your article, in: B.S. Jones, R.Z. Smith (Eds.), *Introduction to the Electronic Age*, E-Publishing Inc., New York, 2009, pp. 281–304.

Reference to a website:

[4] Cancer Research UK, Cancer statistics reports for the UK. <http://www.cancerresearchuk.org/aboutcancer/statistics/cancerstatsreport/>, 2003 (accessed 13 March 2003).

Reference to a dataset:

[dataset] [5] M. Oguro, S. Imahiro, S. Saito, T. Nakashizuka, Mortality data for Japanese oak wilt disease and surrounding forest compositions, *Mendeley Data*, v1, 2015. <https://doi.org/10.17632/xwj98nb39r.1>.

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Example 2: "(GenBank accession nos. AI631510, AI631511, AI632198, and BF223228), a B-cell tumor from a chronic lymphatic leukemia (GenBank accession no. BE675048), and a T-cell lymphoma (GenBank accession no. AA361117)". In the final version of the electronic copy, the accession number text will be linked to the appropriate source in the NCBI databases, enabling readers to go directly to that source from the article (see Example 3 below).

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Style

Note that Steroids uses the serial comma, e.g., Jones, Smith, and Brown (comma before 'and' in a series of three or more items). American-style spelling is required. For example: color, not colour; hydrolyze, not hydrolyse; estrogen, not oestrogen; labeled, not labelled. End-of-line hyphenation should be according to American-style word division (based on pronunciation, not word derivation). Leave a space between number and unit (50 mg, 3.5 M). For solvent proportions use the following style: ethanol/methanol (70:30 v/v) or ethyl acetate/isooctane (1:1).

Letters to the Editor

There is no specific format but there should be a short abstract of no more than 2 sentences; and no more than 5 references. There is word limit of 2, 500 words, not to exceed 2 -3 published pages including figures, tables, abstract and references. A maximum of any combination of 2 tables or figures is allowed.

AFTER ACCEPTANCE

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