# STEROIDS

**TABLE OF CONTENTS**

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

## DESCRIPTION

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**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 $^1$H 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.

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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.

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