CARBOHYDRATE RESEARCH
An International Journal of Molecular Glycoscience

AUTHOR INFORMATION PACK

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DESCRIPTION

Carbohydrate Research publishes reports of original research in the following areas of carbohydrate science: action of enzymes, analytical chemistry, biochemistry (biosynthesis, degradation, structural and functional biochemistry, conformation, molecular recognition, enzyme mechanisms, carbohydrate-processing enzymes, including glycosidases and glycosyltransferases), chemical synthesis, isolation of natural products, physicochemical studies, reactions and their mechanisms, the study of structures and stereochemistry, and technological aspects.

Papers on polysaccharides should have a "molecular" component; that is a paper on new or modified polysaccharides should include structural information and characterization in addition to the usual studies of rheological properties and the like. A paper on a new, naturally occurring polysaccharide should include structural information, defining monosaccharide components and linkage sequence.

Papers devoted wholly or partly to X-ray crystallographic studies, or to computational aspects (molecular mechanics or molecular orbital calculations, simulations via molecular dynamics), will be considered if they meet certain criteria. For computational papers the requirements are that the methods used be specified in sufficient detail to permit replication of the results, and that the conclusions be shown to have relevance to experimental observations - the authors' own data or data from the literature. Specific directions for the presentation of X-ray data are given below under Results and "discussion".

AUDIENCE

Chemists, Biologists, Biochemists and Medical Researchers/Scientists involved in studies of molecular aspects of glycoscience.

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INTRODUCTION

Carbohydrate Research publishes reports of original research in the following areas of carbohydrate science: action of enzymes, analytical chemistry, biochemistry (biosynthesis, degradation, structural and functional biochemistry, conformation, molecular recognition, enzyme mechanisms, carbohydrate-processing enzymes, including glycosidases and glycosyltransferases), chemical synthesis, isolation of natural products, physicochemical studies, reactions and their mechanisms, the study of structures and stereochemistry, and technological aspects.

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Types of paper
Contributions to Carbohydrate Research may be in the form of the following article types:

**Full Papers** - these should be substantial completed pieces of original research that are of significance and which, in addition, are presented clearly and concisely.

**Notes** - these are concise but complete descriptions of an investigation of a limited scope that will not be included in a later paper.

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Title Compounds
3.1.1. Methyl 6-O-tert-butyldimethylsilyl-β-D-allopyranoside (4).

Note that the (numbered) compound is an example of a title compound, which should satisfy certain criteria if it is to be listed this way. Convincing evidence for identity and purity must be presented for all new carbohydrate derivatives listed as title compounds. Ordinarily, identity is established by NMR and mass spectral data. As evidence of purity authors are required to include an elemental (combustion) analysis (minimally C and H), with values deviating from the theoretical not more than 0.4% absolute. When a C and H analysis is not feasible (e.g., very small amounts of material available), the criteria used to assess purity should be specified; these should include NMR observations (absence of extraneous lines in a spectrum run at high sensitivity) and chromatographic data (GLC, HPLC, or TLC at high sensitivity). Also desirable are m/z values from mass spectra.

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Nomenclature

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If there are published physical constants (mp, [α]D, λmax, etc.) for the compound these should be cited, using the following format:

...allyl 2-acetamido-2-deoxy-[α]-L-glucopyranoside (1α): mp 175176 C, lit.6 172174 C; [α]D25 +155 (c 1.43, water), lit.6 +149; 1H NMR...

NMR data. NMR data may be presented in either tables or in the text. Tables are preferred for complex NMR assignments and for series of compounds with full assignments. Full assignments are encouraged using 2D NMR techniques, especially for large, complex structures. For listings as running text please adhere strictly to a uniform style. The following is the preferred format:

1H NMR (CDCl3): δ 7.35 (d, 1H, J3,4 2.0 Hz, H-3), 5.10 (dd, 1H, J4,5 4.0 Hz, H-4), 4.40 (ddd, 1H,J5,6a 6.5, J5,6b 5.5 Hz, H-5),...

Additional conventions used in describing higher order data include, for example, the designation of peaks in COSY spectra: Man H-1,2; HOHAHA tracking: GlcNAc H-2,3,4,5,6a,6b etc.; NOE contacts: Glc H-1, Xyl H-4,5e, etc. For designating resonances in oligosaccharides, the sugar units should be numbered with Roman numerals I, II, III, etc. beginning at the reducing (upstream) end of the molecule. (See IUPAC Nomenclature for Carbohydrates, 2-CARB-37.2.) The individual resonances are numbered with Roman numeral superscripts as, for example, the following: H-3I, H-3II, H-3III.

1H (signals and coupling constants assigned) and 13C NMR data are required for all synthetic compounds and must be included as electronic supporting information. A minimum of three pieces of analytical data are required for all known compounds, while five pieces of data are required for all new compounds. The latter must include either C and H analysis or high resolution mass spectrometry data.
Elemental analysis data. Elemental analysis results follow the last spectral data, in the same paragraph. Use the following format: "Anal. Calcd for C_{13}H_{17}BrO_{8}S: C, 37.78; H, 4.15; Br, 19.34; S, 7.76. Found: C, 37.86; H, 4.13; Br, 19.45; S, 7.84". Note the arrangement of element symbols in the molecular formula: C, H, then the remaining symbols (including metals in salts and complexes) in alphabetical order (standard Hill system).

Elemental analysis data

X-ray crystallographic data. Before submission of the paper, the X-ray data must be filed with and accepted by the Cambridge Crystallographic Data Centre in the usual CIF (Crystallographic Information File) file format. Under a section, "Supplementary Data," that is placed just after the Experimental section, a statement is made as follows:

"Complete crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, CCDC no. 000000. Copies of this information may be obtained free of charge from the Director, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, CB2 1EZ, UK. (fax: +44-1223-336033, e-mail: deposit@ccdc.cam.ac.uk or via: www.ccdc.cam.ac.uk)."

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For cases where X-ray crystallography is used to support the structural identification of a synthetic or natural product in a paper devoted largely to synthetic or isolation chemistry, the authors may wish to report only the ORTEP or similar depiction of the molecule(s). At a minimum, a description of the experimental methods and a tabulation of crystal data should be provided as Supplementary Data to appear with the electronic version of the paper (in addition to filing the data with CCDC, above.)

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