

Introduction

Current topics in carbohydrate modelling: diverse questions, diverse methods

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We are currently moving beyond the stage of where carbohydrate modelling solely consisted of a set of molecular mechanics calculations. Recent developments in computational science provide a broad range of methods which may be harnessed for application to different and diverse aspects of carbohydrate structural analysis.

Classical stereoelectronic effects such as the anomeric and exo-anomeric effects can be studied with improved accuracy with quantum mechanical methods applied to systems of the size of a monosaccharide or disaccharide and which may also include certain environmental effects. Solvation effects, which remain difficult to treat, can be explored with extensive but expensive molecular dynamics calculations which are increasingly being used to understand the important consequences of solvent structure in the neighbourhood of the surfaces of carbohydrates and their receptors and in the study of phase-dependent behaviour. Exploration of the conformational space of oligosaccharides demands the use of methods such as Monte Carlo and Genetic Algorithm-based conformational searching and generation techniques. The treatment of the physical properties of large complex

polysaccharide systems often necessitates the use of non-molecular-based modelling, and reduced representations or hydrodynamic theory need to be invoked for these problems.

Comparisons of modelling with experimental data such as obtained from NMR remain a vital and active but challenging area of research. Basic hypotheses, such as the glycosidic linkage flexibility hypothesis, remain open to examination.

The recent generation of large numbers of biologically relevant oligosaccharide sequences is opening up a very promising new area of carbohydrate modelling based on bioinformatics methods aimed at discovering sequence-function relationships. The combination of this new informatics modelling with structural modelling will be particularly interesting. The growth of World Wide Web-based resources offers the opportunity for the integration of glycoscience-related sequence, structure, and property data which may act as a profitable springboard for international carbohydrate-related scientific progress, particularly if performed within the context of a collaborative community-based environment.