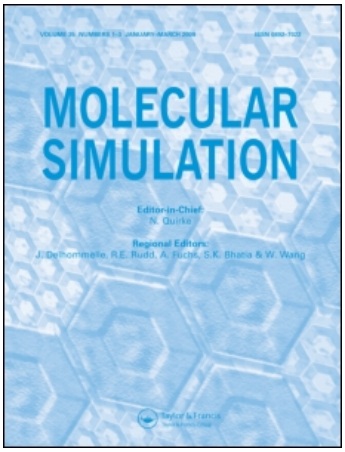

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Guest Editorial

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Guest Editorial

The biological importance of carbohydrates cannot be understated. Advances in the structural characterisation and synthesis of complex carbohydrates have allowed the investigation of these biomolecules in a wide range of contexts, from their possible use in carbohydrate-based drugs to their structural and functional roles in cell biology. Along with these exciting developments, the field of molecular modelling and computational chemistry has made substantial advances in recent years in order to be able to cope with the chemical diversity and structural complexity of carbohydrate molecules and their interactions with proteins and other biological components.

This special issue on *Molecular Modelling of Carbohydrates* marks a first for *Molecular Simulation* by expanding the scope of the journal into this growing area. The 10 papers in this issue make use of a variety of computational methods, from forcefield-based molecular dynamics simulations to quantum chemical calculations and ligand–protein docking. These papers provide a representative sample of the wide range of problems involving carbohydrates being researched today and illustrate the level of complexity that molecular modelling methods are now able to tackle. Hopefully, the quality of the work described in this special issue will motivate many other researchers in the field of carbohydrates to consider *Molecular Simulation* when publishing their future work.

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