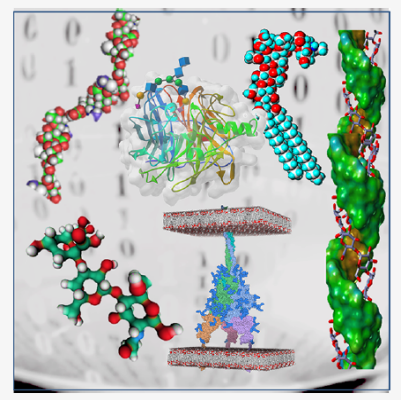
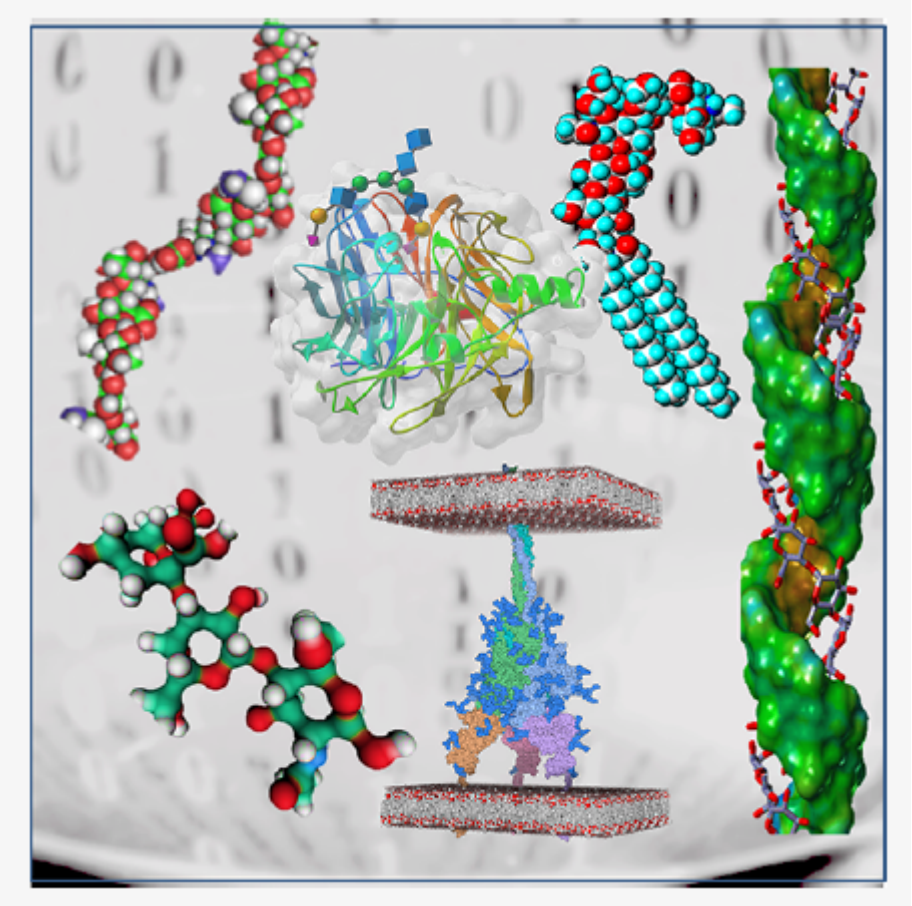


Multifaceted Computational Modeling in Glycoscience

Description

https://hal.archives-ouvertes.fr/hal-03841124/document
Glycoscience assembles all the scientific disciplines involved in studying various molecules and macromolecules containing carbohydrates and complex glycans. Such an ensemble involves one of the most extensive sets of molecules in quantity and occurrence since they occur in all microorganisms and higher organisms. Once the compositions and sequences of these molecules are established, the determination of their three-dimensional structural and dynamical features is a step toward understanding the molecular basis underlying their properties and functions.



The range of the relevant computational methods capable of addressing such issues is anchored by the specificity of stereoelectronic effects from quantum chemistry to mesoscale modeling throughout molecular dynamics and mechanics and coarse-grained and docking calculations. The Review leads the reader through detailed presentations of the applications of computational modeling. The illustrations cover carbohydrateÃ¢Ë?â??carbohydrate interactions, glycolipids, and N- and O-linked glycans, emphasizing their role in SARS-CoV-2. The presentation continues with the structure of polysaccharides in solution and solid-state and lipopolysaccharides in membranes. The full range of protein-carbohydrate interactions is presented, as exemplified by carbohydrate-active enzymes, transporters, lectins, antibodies, and glycosaminoglycan binding proteins. A final section features a list of 150 tools and databases to help address the many issues of structural glycobioinformatics.

Category

1. News