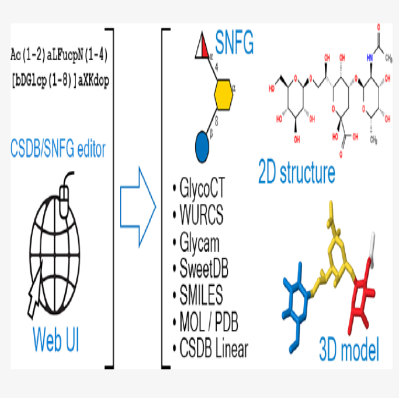
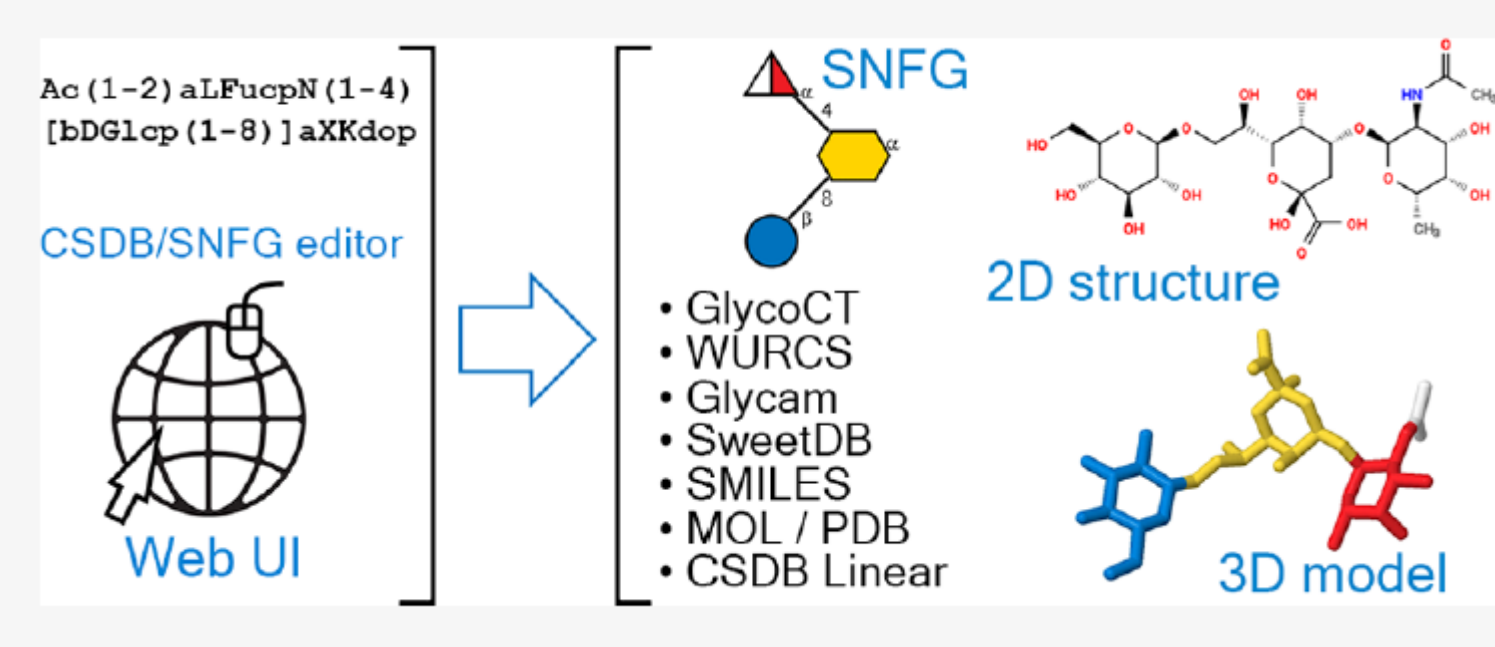


CSDB/SNFG Structure Editor: An Online Glycan Builder with 2D and 3D Structure Visualization

Description

This article describes the features, usage, and application of a CSDB/SNFG Structure Editor, a new online tool for quick and intuitive input of carbohydrate and derivative structures using Symbol Nomenclature for Glycans (SNFG). The Editor is built on the Carbohydrate Structure Database (CSDB) platform and relies on its online services via the dedicated web API. The Editor allows the building of oligo- and polymeric glycan structures and supports most features of natural glycans, such as underdetermined structures, alternative branches, repeating subunits, SMILES specification of atypical monomers, and others.



The vocabulary of building blocks contains 600+ monomeric residues, including 327 monosaccharides. Support for SMILES allows input and visualization of chemical structures of virtually unlimited complexity. On the other hand, the interface follows the recognized GlycanBuilder style accessible to novice users. The export feature includes support for CSDB Linear, GlycoCT, WURCS, SweetDB,

Glycam notations, SMILES codes, MOL/PDB atomic coordinate formats, raster and vector SNFG images, and on-the-fly visualization as 2D structural formulas and 3D molecular models. Integration of the Editor into any web-based glycoinformatics project is straightforward, similarly to any other modern JavaScript application.

Category

1. News