Webtools For the Study and Development of Novel Glycomaterials

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Introduction

As part of GlycoMIP, the team at Glycam-Web (glycam.org) are developing web tools that enable glycomaterial researchers to discover structure-function relationships in polysaccharides with the goal of accelerating rational material design.

With our current generation of webtools, users can generate representative 3D structures for their polysaccharides, and are also able to download input files to perform molecular dynamics (MD) simulations. As part of GlycoMIP we wish to expand the possibilities using feedback from the glycomaterials community.

Carbohydrate Builder

Build Sequence Via Point-and-Click:
Build a sequence representation of a polysaccharide in a point-and-click interface, as shown in Figure 1. The interface will disable residues and linkages that are not viable, keeping track of positions that are either not possible, or already used.

When the sequence is complete, the Carbohydrate Builder provides the files needed for performing MD simulations, visualization, and further analysis.

Enter Sequence Via Text
Users who know the modified condensed IUPAC input format can type or copy and paste that in, rather than using the point-and-click interface for each residue.

A polymeric repeating unit syntax is fully supported in this interface, and is shown for a 9-mer repeat of Manα1-2Manα in Figure 2.

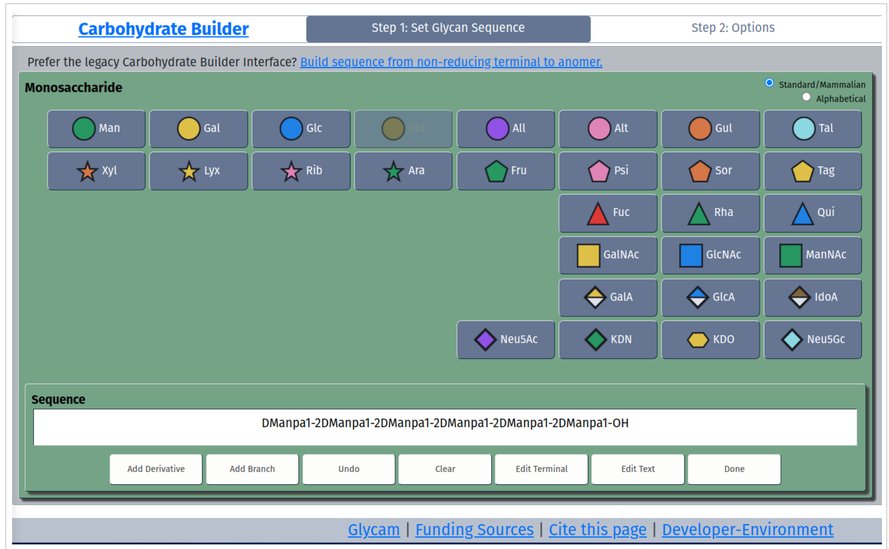


Figure 1: Our point-and-click interface guides users through the generation of a valid carbohydrate sequence.

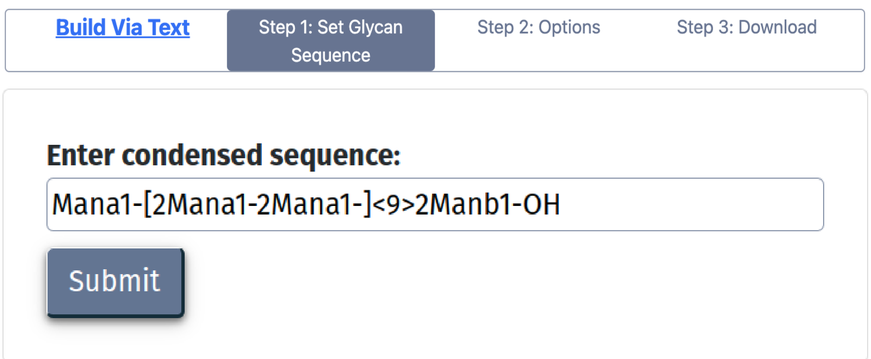
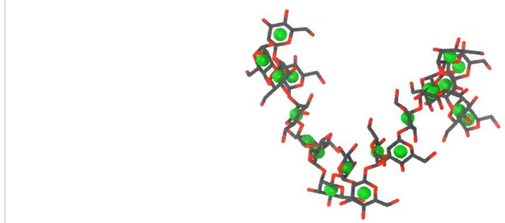
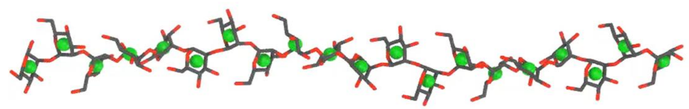


Figure 2: Our Build Via Text tool allows users to enter full sequences or, as shown above, sequences with **repeating units** useful for polysaccharide generation. The repeat unit may contain branches and even nested repeating units.



Mana1-[2Man**b**1-2Mana1-]<9>2Manb1-OH



Mana1-[2Man**a**1-2Mana1-]<9>2Manb1-OH

Figure 3: The 3D shapes of the polysaccharides can be extremely different given only small changes to the sequence of the monosaccharides.

Future Directions (Feedback Welcome)

Potential Analyses Performed for the User by the Website:

- Automated MD simulations.
- Radius of gyration and hydrodynamic radius.
- Viscosity prediction.
- NMR properties prediction.
- Predict a polysaccharide's ability to form double or triple helices.
- Relative solubilities.

Acknowledgement

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