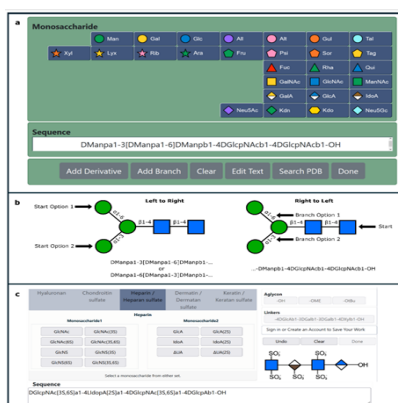




Generating 3D Models of Carbohydrates with GLYCAM-Web

Description

The carbohydrate 3D structure-prediction tools (builders) at GLYCAM-Web (glycam.org) are widely used for generating experimentally-consistent 3D structures of oligosaccharides suitable for data interpretation, hypothesis generation, simple visualization, and subsequent molecular dynamics (MD) simulation. The graphical user interface (GUI) enables users to create carbohydrate sequences (e.g. DGalpb1-4DGlcpb1-OH) that are converted to 3D models of the carbohydrate structures in multiple formats, including PDB and OFF (AMBER software format). The resulting structures are energy minimized before download and online visualization. There are advanced options for selecting which shapes (rotamers) of the oligosaccharide to generate, and for creating explicitly solvated structures for subsequent MD simulation. The GLYCAM-Web builders integrate known conformational preferences of oligosaccharides and employ the GLYCAM forcefield for energy minimization with algorithms tailored for speed and scalability. Even for large oligosaccharides (100 residues, ~2100 atoms), a 3D structure is typically returned to the user in less than a minute.

a

Monosaccharide

Man	Gal	Glc	All	Alt	Gul	Tal	
Xyl	Lyx	Rib	Ara	Fru	Pal	Sor	
					Fuc	Rha	Qui
					GalNAc	GlcNAc	ManNAc
					GalA	GlcA	IdoA
					Neu5Ac	Kdn	Kdo
						Neu5Gc	

Sequence

b

Left to Right

DManp1-3[DManp1-6]DManpb1-4DGlcNacp1-4DGlcNacp1-OH
or
DManp1-6[DManp1-3]DManpb1-4DGlcNacp1-4DGlcNacp1-OH

Right to Left

...DManpb1-4DGlcNacp1-4DGlcNacp1-OH

c

Hyaluronan	Chondroitin sulfate	Heparin / Heparan sulfate	Dermatan / Dermatan sulfate	Keratan / Keratan sulfate								
Monosaccharide1 <table border="1"> <tr> <td> GlcNAc</td> <td> GlcNAc(3S)</td> </tr> <tr> <td> GlcNAc(6S)</td> <td> GlcNAc(3S,6S)</td> </tr> <tr> <td> GlcNS</td> <td> GlcNS(3S)</td> </tr> <tr> <td> GlcNS(6S)</td> <td> GlcNS(3S,6S)</td> </tr> </table> Select a monosaccharide from either set.					GlcNAc	GlcNAc(3S)	GlcNAc(6S)	GlcNAc(3S,6S)	GlcNS	GlcNS(3S)	GlcNS(6S)	GlcNS(3S,6S)
GlcNAc	GlcNAc(3S)											
GlcNAc(6S)	GlcNAc(3S,6S)											
GlcNS	GlcNS(3S)											
GlcNS(6S)	GlcNS(3S,6S)											
Monosaccharide2 <table border="1"> <tr> <td> GlcA</td> <td> GlcA(2S)</td> </tr> <tr> <td> IdoA</td> <td> IdoA(2S)</td> </tr> <tr> <td> ΔUA</td> <td> ΔUA(2S)</td> </tr> </table>					GlcA	GlcA(2S)	IdoA	IdoA(2S)	ΔUA	ΔUA(2S)		
GlcA	GlcA(2S)											
IdoA	IdoA(2S)											
ΔUA	ΔUA(2S)											

Aglycon

Links

Sequence

Category

1. News