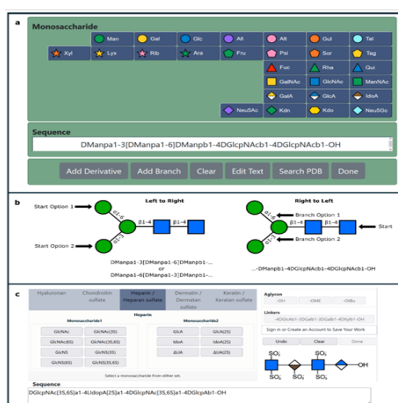




Generating 3D Models of Carbohydrates with GLYCAM-Web

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	Alt	Alt	Gul	Tal
Xyl	Lyx	Rib	Ara	Fru	Psi	Sor
					Fuc	Rha
					GalNAc	GlcNAc
					GalA	GlcA
					Neu5Ac	Kdn
						Kdo
						Neu5Gc

Sequence

DManpa1-3[DManpa1-6]DManpb1-4DGlcNac1-4DGlcNac1-OH

Add Derivative Add Branch Clear Edit Text Search PDB Done

b

Left to Right

Start Option 1 →

Start Option 2 →

β1-6

β1-4

β1-4

DManpa1-3[DManpa1-6]DManpb1-...
or
DManpa1-6[DManpa1-3]DManpb1-...

Right to Left

Branch Option 1

Branch Option 2

Start

β1-6

β1-4

β1-4

...-DManpb1-4DGlcNac1-4DGlcNac1-OH

c

Hyaluronan Chondroitin sulfate Heparin / Heparan sulfate Dermatan / Dermatan sulfate Keratin / Keratan sulfate

Heparin

Monosaccharide1

GlcNAc	GlcNAc(3S)
GlcNAc(6S)	GlcNAc(3S,6S)
GlcNS	GlcNS(3S)
GlcNS(6S)	GlcNS(3S,6S)

Monosaccharide2

GlcA	GlcA(2S)
IdoA	IdoA(2S)
ΔUA	ΔUA(2S)

Select a monosaccharide from either set.

Sequence

DGlcNac[3S,6S]a1-4IdopA[2S]a1-4DGlcNac[3S,6S]a1-4DGlcAb1-OH

Aglycon

-OH -OME -OtBu

Linkers

-4DGlcAb1-3DGal1-3DGal1-4Oxyb1-OH

Sign in or Create an Account to Save Your Work

Undo Clear Done

SO₃⁻ SO₃⁻ SO₃⁻ SO₃⁻ OH

Category

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