Glycan 3D modeling & 3D Structures Displays

Description

Glycam: Online web that provides tools for 3D modelling carbohydrate-containing structures. It includes libraries and prediction tools together with useful drawing, scripting and building tools. (http://glycam.org/tools/molecular-dynamics/oligosaccharide-builder/build-glycan?id=1)

GLYCAM-web (Carbohydrate Builder): Online tool for carbohydrate building through three different options: manual building, using templates or in text format for structures that do not exist in the library. Easy to use allows downloading a sketch of the generated structure and the 3D structure in .pdb format. Really useful to prepare ligand for MD simulations as it can also solvate and generate the topology and coordinate files. (https://dev.glycam.org/cb/)

Glycosciences.de: a web portal unifying in a unique place different databases and bioinformatics tools. (http://glycosciences.de/index.php)

Sweet II: Inside the glycosciences.de webpage, Sweet II is a 3D modelling tool that allows other possibilities to generate a .pdb file from the generated sequence using standard nomenclature. It also offers the possibility to minimise the structures using MM2 and MM3 methods. (http://glycosciences.de/modeling/sweet2/doc/index.php)

doGlycans: Set of tools for carbohydrate generation using GROMACS. Different python scripts are constituted using GLYCAM naming and force fields, making the files compatible with AMBER. This tool allows for generating 3D models for later simulations. (https://bitbucket.org/biophys-uh/doglycans/src/master/)

PolysGlycanBuilder: Online tool to generate glycan structures. It is possible to drag the SNFG symbols directly in the canvas and define the monosaccharidesâ?? linkages. It is also possible to define the dihedral angles manually or to use values extracted from a database. It is possible to download the sketch of the glycan apart from obtaining the PDB file. (http://glycan-builder.cermav.cnrs.fr/)

CHARMM-GUI (Glycan Reader and Modeler): Online tool integrated inside CHARMM GUI web platform. Inside the input generator, a Glycan reader and modeller can be found, where it is possible to generate the glycan structure and perform molecular dynamics simulations to it. (http://www.charmm-gui.org/?doc=input/glycan)

Glyco3D: Online database encompassing other databases and tools for mono, di, oligo and polysaccharides and carbohydrate recognising proteins. It is also possible to build structures through Polys Glycan builder or other family-specific builders. (http://glyco3d.cermav.cnrs.fr/home.php)

3D- SNFG: Once the script is integrated into visual molecular dynamics (VMD) software, visualise 3D SNFG structures for the monosaccharides. It is a way to generate an image useful for quick

assessment of 3D models. (http://glycam.org/docs/othertoolsservice/2016/06/03/3d-symbol-nomenclature-for-glycans-3d-snfg/)

LiteMol: Online web viewer that, thanks to additional plugins, can be used in all modern web browsers. The viewer gets the PDB fileâ??s information to display a 3d carbohydrate representation in the form of SNFG symbols. However, some problems in the representation can appear due to mismatches with the annotation. Moreover, the representation does not provide any information about the linkages. (https://www.litemol.org/Viewer/)

PyMOL- Azahar plugin: Python-based tool in the form of a plugin for PyMOL environment suit. It is a useful tool to simplify glycans representation in a 3D way where the rings in sugars are represented as non-flat polygons or spheres depending on the representation mode. (https://pymolwiki.org/index.php/Azahar)

UnityMol/SweetUnityMol: Software used locally for molecular structure views compatible with Windows, macOS and Linux. It is possible to use a wide range of input files format and is also possible to open potential maps and trajectory files. It has different options to depict primary structures. However, the most curious thing is the recently developed version with Virtual Reality implemented. (https://sourceforge.net/projects/unitymol/files/)

RosettaCarbohydrate: Available for academia and commercial research, Rosetta Commons is a software suite that should be download and compiled to be used locally in a Linux or a macOS system. However, this tool fits better researchers with basic knowledge and skills to work with a command-line. (https://www.rosettacommons.org/software/license-and-download)

SugarbindDB: Interesting web database collects known carbohydrate sequences recognised by lectins or adhesins from pathogenic organisms. It offers other search options as the above mentioned Original GlycanBuilder. (https://sugarbind.expasy.org/)

GlycoEpitope: that provides information about glycan epitopes and antibodies presented as a compact encyclopaedia. (https://www.glycoepitope.jp/)

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