POLYS-GLYCAN-BUILDER

A user friendly tool to build 3D structures of complex glycan and polysaccharides

Before reading the following make sure that Javascript is installed on your computer.

The POLYS-Glycan-Builder is a user-friendly graphical interface that sets up the input file to the POLYS software, for which the syntax was generally considered too complex to set up and manipulate. The monosaccharide units are depicted in the form of simple pictograms in agreement with the most accepted in glycoscience, to which have been encapsulated key 3D information (configuration, furanose/pyranose shape, anomery, and ring conformation (as in the case of idoses or 5 membered rings). At the present time, about 150 of such monosaccharides of biological relevance are available; they all have been subjected to geometry optimization throughout molecular mechanics. Depending upon their origin or types, these monosaccharides are arranged in several classes (Plant, Bacteria, Algea, Bacteria, N- O- Lipid linked, GAG, …..).

Selecting one such family, will display in the upper part of the screen the corresponding whole subset of monosaccharides, from which the user can drag with the mouse the needed unit for the construction, either in the intermediate screen or in the main screen. This operation can be repeated several times, allowing the selection of monosaccharides from different subsets.

The graphical construction of the complete oligosaccharide or polysaccharide can then proceed, by a simple game of mouse select and drag operations which take place on the main screen. The monosaccharides are placed on a grid (12x8) (which can be displayed or not). The proximity two monosaccharides which are likely to be linked by a glycosidic junction, generates a small menu inviting the user to define the nature of the glycosidic linkage (1-1, 1-2, 1-3, 1-4, 1- 6, 2-1, ….. 2-6, 2-8) and specifiy the value of the glycosidic linkages: PHI, PSI and OME these being referred to the so-caled heavy atoms conventions. The relative orientation of two contiguous monosaccharides linked by a glycosidic bond in a disaccharide is characterized by the Φ and Ψ torsion angles. In the so called "Heavy Atom Definition" commonly used in crystallography, Φ is the torsion angle Φ= O5-C1-O-Cx and Ψ is the torsion angle Ψ=C1-O1-Cx-Cx+1, where x is the number of the carbon atom of the second monosaccharide with which the 1→ x glycosidic bond is formed. For two monosaccharides linked by a 1→ 6 linkage, another parameter (ω) is required describing the orientation about the exo-cyclic bond C5-C6. Its orientation is customarily described by the torsion angles O5-C5-C6-O6 and C4-C5-C6-O6, which combination defines the so called *gauche-trans* (gt), *gauche-gauche* (gg) and *trans-gauche* (tg) conformations.

The construction can proceeds in a step wise manner, with the possibility to make corrections at any time of the process. An option is also given to display the constructed sequence either with the pictorial representation or with the abbreviated letter codes of the monosaccharides.

The only constraint lies in the way to process, i.e. always constructing the longest branch (displayed horizontally) to which side chains are attached.

The builder offers the unique opportunity to generate repeating motifs (as in any stereoregular polysaccharides) by selecting the number of times a given construction is to be duplicated by clicking on “repetition” and input the required information.

At the same time the structure is being graphically constructed, the proper POLYS syntax is generated, and appears in the window SYNTAX at the bottom left corner of the screen. This provides the expert user to control the building process for the growing molecules which is relatively simple and based on fundamental Euclidian geometry. The whole input file to POLYS which is so generated can be saved (Click on: Save POLYS session). By clicking on Build, the POLYS software automatically generates the 3D structure with the atomic coordinates at a PDB format. This actions is accompanied by a display of the molecular structure (generated by JsMol), which can be send to DOWLOADS of your computer.