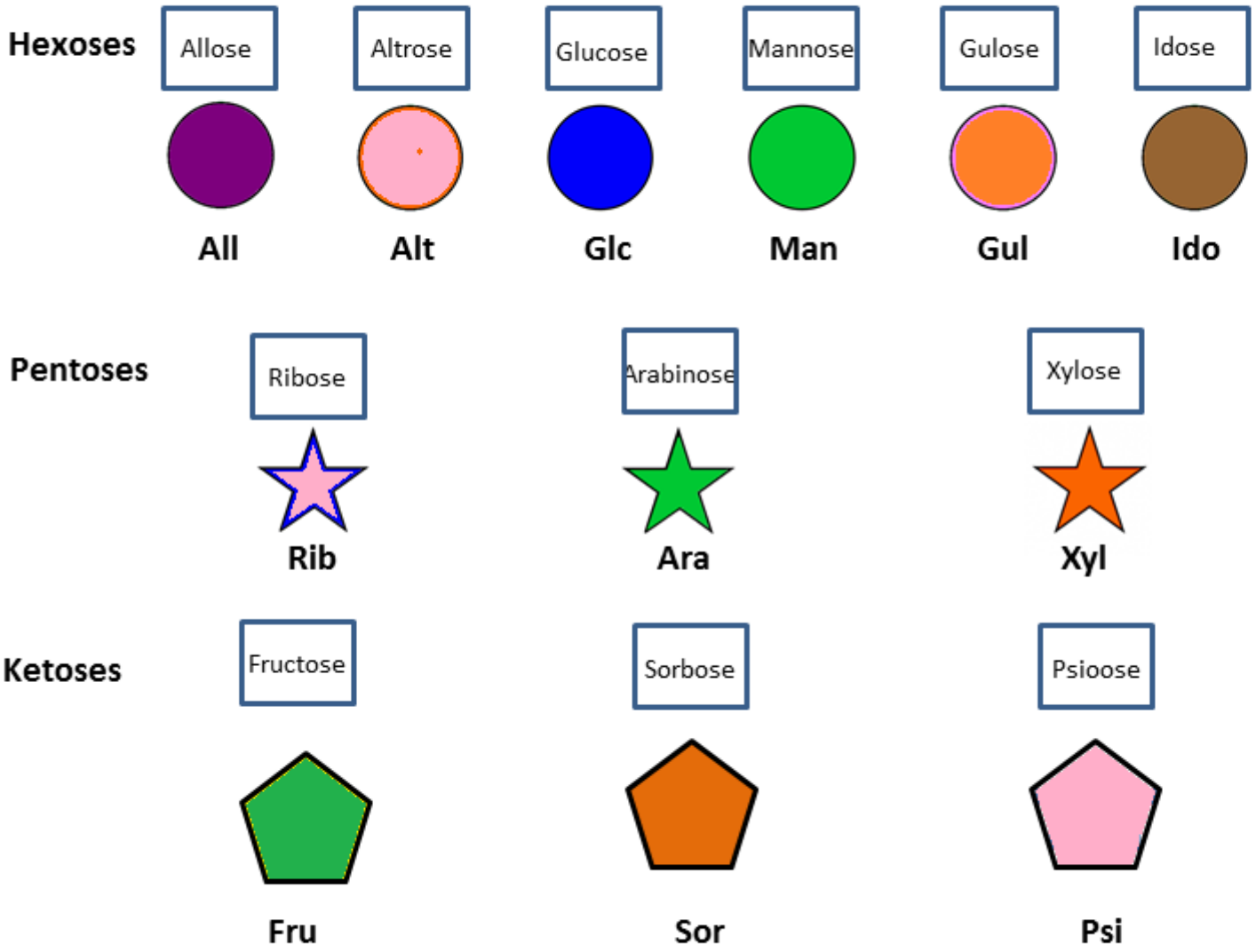
Presentation

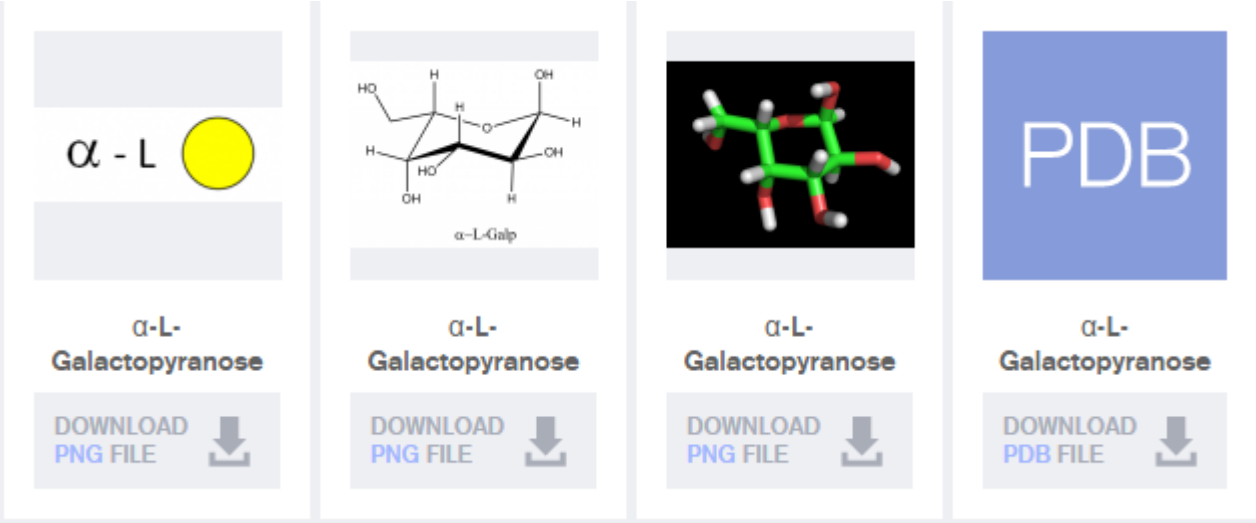
Description

This chapter offers a library of 128 monosaccharides which are presented throughout several levels of structural depiction, i.e. one dimension, two-dimension and three-dimension. The following three different families of monosaccharides are considered : hexoses, pentoses, ketoses.



For a given configuration (D) or (L) monosaccharide can occur as Î±-pyranose, Î²-pyranose, Î±-furanose, Î²-furanose, i.e under eight different 3-Dimensional structures. Irrespective of the fact that many of these combinations correspond to structures that occur in rare occasions or have not been identified yet, all possible combinations were generated. Complementary to its 3-Dimensional structure, each monosaccharide is presented in the form of a symbolic representation, in accordance with the rules set-forward in â??*The Symbolic Representation of Monosaccharides in the Age of Glycobiology*â?•, along with a drawing of the molecular structure. As such, each monosaccharide is depicted in the form of a mosaic comprising four vignettes, which are associated to pictures and coordinates file, each

of them being downloadable.



In its present release, the library covers 128 different monosaccharides which can be considered as templates to derivatives such as N-acetylhexoseamine, Hexoseamine, Hexuronate, Deoxyhexose, Deoxy-N-acetylthexosamine, Deoxypentose,â?¦ The atomic files follow the PDB record format for coordinate data and can be used in the most popular molecular modeling software to set up a consistent and annotated library of monosaccharides). [1]
An atom type specification has been added to each atom ; this is a compound number (atomic number in the periodic table ; specific functional group (i.e. carboxyl, ketone, â?¦) ; the atom valency) which may be used for further molecular mechanics computations.

Category

1. News