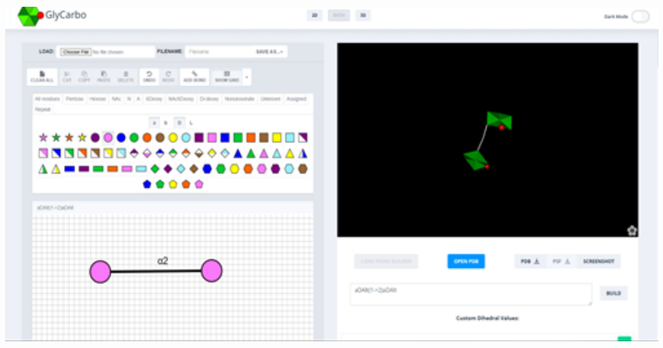
★SugarToo▲

Design and Implementation of **Carbohydrate Web-Tools**

VISUALISATION TOOLS

Research into the structural properties of carbohydrates (glycans) is vital for the development of vaccines. Such research relies on the use of software tools in order to **visualise** and understand the 2D and 3D **structure** of molecules. UCT's Glycarbo is a tool built for this purpose and this part of the project demonstrates the inspection, editing and user- testing of Glycarbo. The focus of the project the user experience and maintainability of Glycabo's 2D builder.

This included documenting its codebase, user-testing and code refactoring.



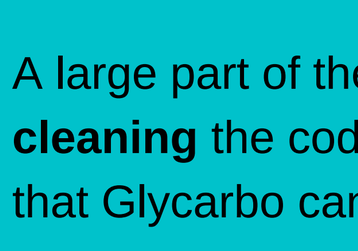
GLYCARBO

Glycarbo comprises of a 2D sketcher (Glycano) and a 3D builder that generates a 3D molecule. Glycarbo faced issues generating these 3D molecules as many of the naming conventions in Glycano were incorrect. Changes were made to ensure all names and visual representations were correct according to the SNFG convention.

GLYCANO

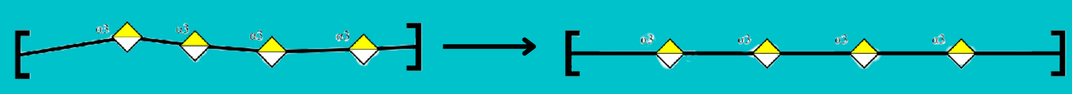
Glycano forms the 2D sketcher part of Glycarbo and allows users to **build 2D glycans** by placing saccharides (from the **SNFG** symbol set) on to the canvas and bonding them together.

BONDING



In the previous version of Glycano, bonding was automatic, and users would need to move residues until the correct bond location was found. Now users can place saccharides wherever, click the "Add Bond" button and **select** the bond location they desire.

STRAIGHTEN



In order for the 2D molcules generated by Glycano to be of use in academic papers and institutions, a "straighten" feature was added to make the bonds and sacchairdes **uniform**.

MAINTAINABILITY

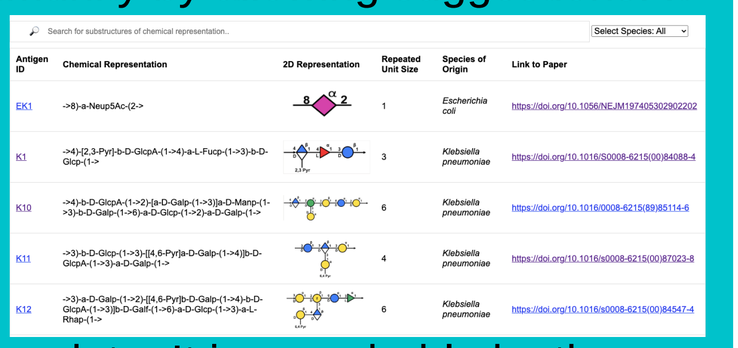
A large part of the project was **documenting** and **cleaning** the codebase from previous project iterations so that Glycarbo can be maintained and edited for future use.

MICROBIAL CARBOHYDRATES

For the database stage of this project, we focused on populating the database with *Klebsiella pneumoniae* and *Escherichia coli* data. These two bacterium cause many diseases and are becoming more antibiotic resistant. Developing a store of their carbohydrate structures is vital in helping the development of carbohydrate based vaccines.

GLYCAN3DB HOME PAGE

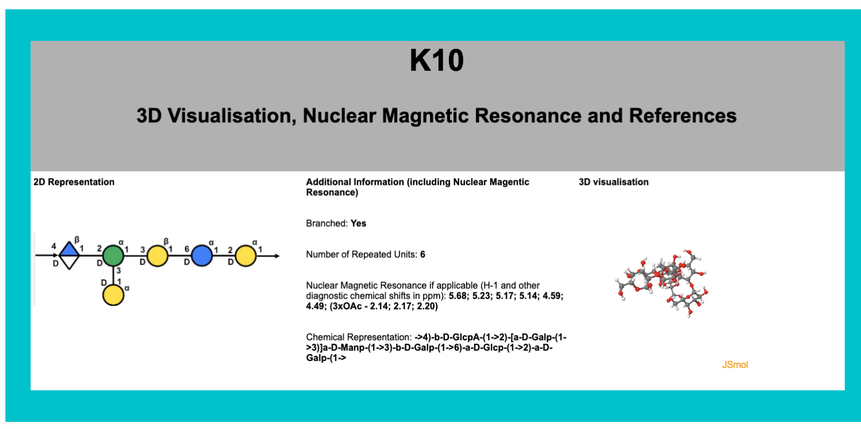
Glycan3DB was developed as a general, extensible and usable database. It has explanations of the data hosted in the database to give it a usable overview. It was also able to be extended through the community by allowing suggestions. It was built to have data on potentially any carbohydrate and is easily maintainable and navigable It has string, 2D representation and other data. It is searchable by the chemical representation sub-structures and filterable by the species origin.



3D VISUALISATION AND INFOCARD

The infocard section of Glycan3DB is critical. It houses the Nuclear Magentic Resonance data along with the 3D visualisation. There is one page for each of the 83 antigens housed in the database. It also hosts a larger image of the 2D SNFG symbol representation, along with all other data related to the antigen that was not able to fit in the home page of Glycan3DB. The .pdb 3D coordinate file for each antigen is downloadable. This page is seen as the detail on demand page for the database, and is crucial for full understanding of the carbohydrate, where the main page is crucial for getting an overview of the carbohydrate's physical structure.

The 3D visualisation was implemented using JSmol, a 3D molecule viewing package for JavaScript.



Team:
Joseph Sidley (sdljos001@myuct.ac.za)
Lauren Paton (ptnlau002@myuct.ac.za)
Supervisor: Prof. Michelle Kuttel