

SUGARDB: USER-CENTRED DESIGN OF A CARBOHYDRATE STRUCTURAL DATABASE FOR *KLEBSIELLA PNEUMONIAE* AND OTHER PATHOGENS

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
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With the increase in anti-microbial resistance (AMR), vaccination is becoming the first line of defense against bacterial pathogens. For example, *Klebsiella pneumoniae* (*Kp*) is a leading cause of neonatal sepsis and hence a major killer of newborns globally, with 87% of deaths AMR-related [1,2]. Two surface carbohydrates are potential vaccine targets: capsular polysaccharides (K-Ags) and O-antigens (O-Ags). The characterization of a large collection of emerging *Kp* strains has identified 32 distinct K-Ag and 8 O-Ag types [3]. Detailed structural elucidation (chemotyping) of the K-Ags recognised may enable identification of common structural features for potential cross-reactivity and thus the development of a simplified multivalent vaccine against neonatal *Kp* infections.

Validation and comparison of K-Ags across *Kp* strains could be facilitated by an effective database of *Kp* structures. Several web-based carbohydrate structure databases have been developed, including the Carbohydrate Structure Database curated collection of glycomics data [4], and the more focussed K-PAM (exclusively *Kp*) [5] and ECODAB (primarily *Escherichia coli* some *Streptococcus pneumoniae*) [6]. However, in the design and development of these tools, typically little attention has been to important software development principles such as usability (the ease with which users can interact with software to accomplish tasks) and extensibility (the ability to extend a system and the level of effort required to implement the extension).

We developed SugarDB (<https://sugardb.cs.uct.ac.za/>) as a prototype repository for the



SugarDB

SugarDB currently stores

- Metabolic pathways: 74
- Metabolic Reactions: 20
- 1 Exchangeable cofactor structure



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Search by specific field: For special characters, use \a for a, \b for b, ... etc. →

Antigen Structure

Showing all results

Serotype	2D Representation	Antigen Structure	Repeated Units	DOI
K9		--3 a e-4 b-Wap (1) --3B-D-GlypA (1) --4 e-4 b-Wap (1) --2 a e-4 b-Wap (1) --3 a D-Glyp (1) --	5	https://doi.org/10.1016/j.1016-0006-0210089-00009-0
K11		--3 B-D-Glyp (1) --3 (A-A-Par) D-Glyp (1) --4B-D-GlypA (1) --3 a D-Glyp (1) --	4	https://doi.org/10.1016-0006-0210089-00009-0

primary structure of Kp K-Ags using an iterative user-centred design process with user evaluation. SugarDB has a carbohydrate-specific query system for rapid searches, an intuitive interface to provide an instant overview of the contents of the database and to facilitate data access, automatic generation of Symbol

Nomenclature for Glycans primary structure graphs from CASPER text and the ability to rapidly add new structures. SugarDB adheres to standardised usability principles and evaluation heuristics, with novel features to support research into bacterial carbohydrates. The SugarDB prototype can be extended to cover a wide range of other pathogens.

References:

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3. F. Nonne, *Biology* **2024**, 13, 256
4. P. Toukach, *Analytical and Bioanalytical Chemistry* **2025**, 417, 1025–1034
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6. M. A. Rojas-Macias, et al., *Glycobiology* **2014**, 25, 3, 341–347.