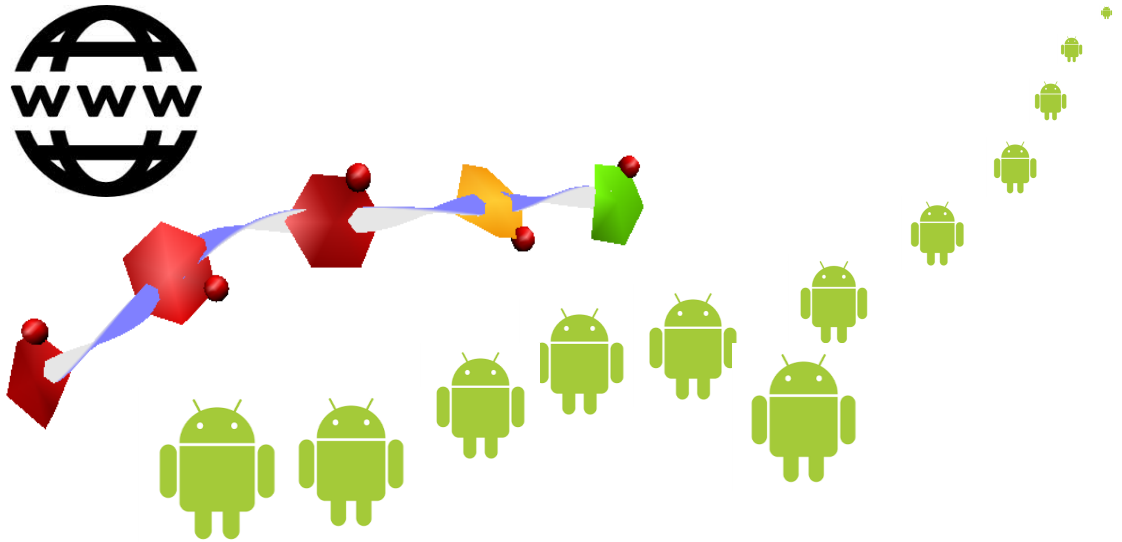
DESIGN AND DEVELOPMENT OF EFFECTIVE **WEB** AND **MOBILE** APPLICATIONS FOR VISUALIZING MOLECULAR STRUCTURE.



Michelle Kuttel

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University of Cape Town

http://www.cs.uct.ac.za/~mkuttel

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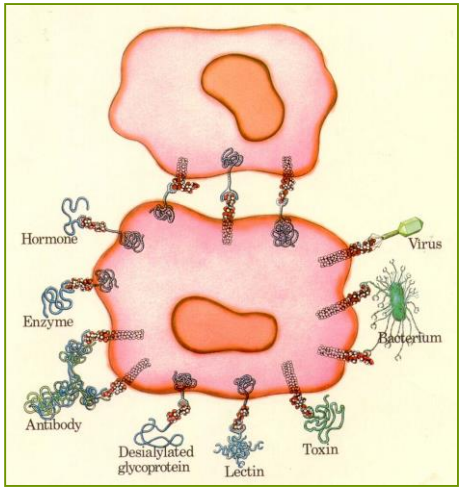
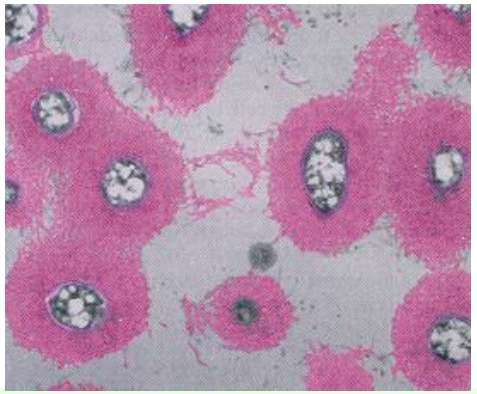
DEPARTMENT OF COMPUTER SCIENCE

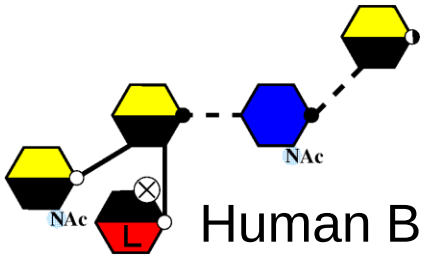
FOCUS: CARBOHYDRATES

- essential roles in cellular and molecular biology, in health and disease.
- e.g. modern bacterial vaccines target the carbohydrate capsule
- structure of great interest/importance for drug/vaccine/inhibitor design

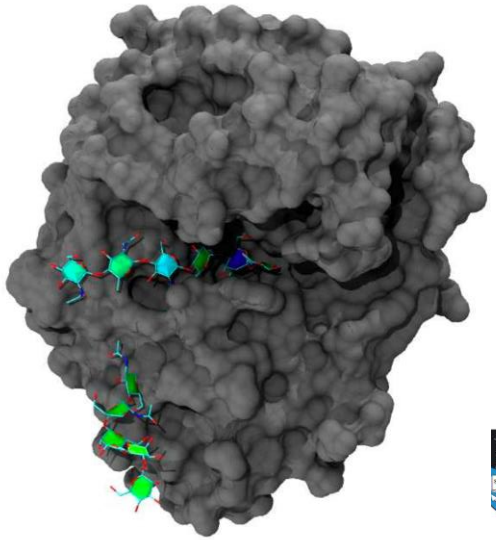




Haemophilus influenza bacteria expressing polysaccharide capsules.



Human Blood A antigen



CARBOHYDRATE MOLECULAR STRUCTURE REPRESENTATION

(E.G. SHIGELLA FLEXINERI SEROTYPE Y O-ANTIGEN REPEATING UNIT)

1D: ->2)aLRha(1->2)aLRha(1->3)aLRha(1->3)bDGlcNAc(1->

casper notation

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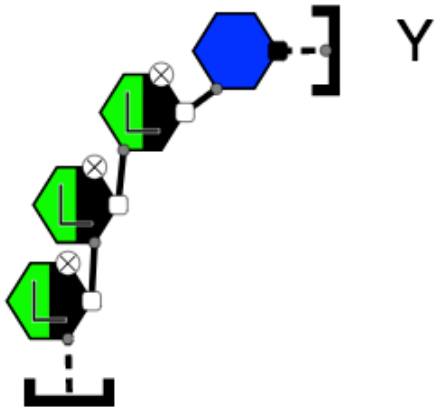
2D:



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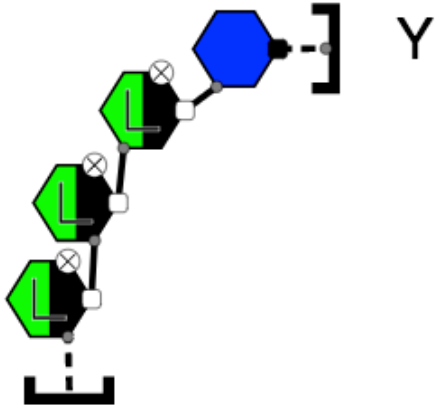
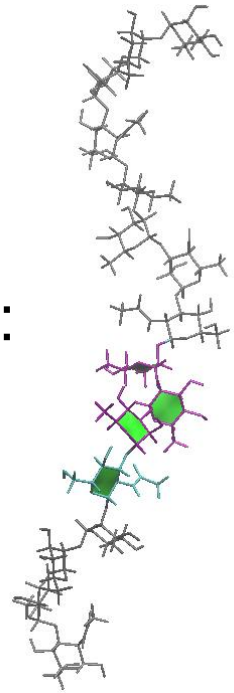


3D:



AIMS

- Design and develop (optimal) software tools to assist with:
  - researchers' investigation and exploration of carbohydrate structure
  - researcher discussions with collaborators or funders
  - chemistry education

SOFTWARE DEVELOPMENT APPROACH

- User-Centered design principles
- Iterative, explorative

- Design is important, but often neglected in development of **scientific software**.

There *is never a single optimal solution to a design problem, but rather a huge variety of alternative clear and effective designs*.

CARBOHYDRATE MOLECULAR STRUCTURE REPRESENTATION

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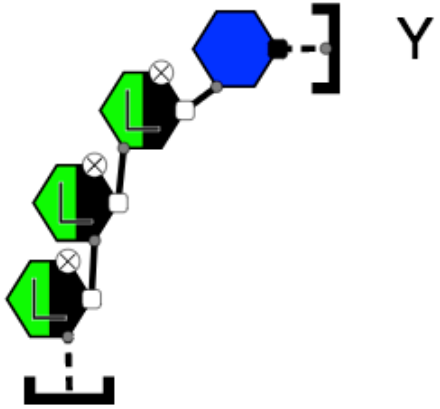

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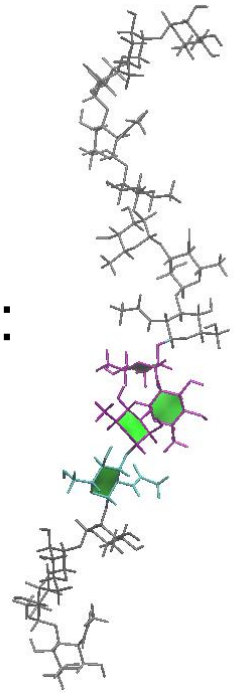

SOFTWARE FOR MOLECULAR STRUCTURE REPRESENTATION

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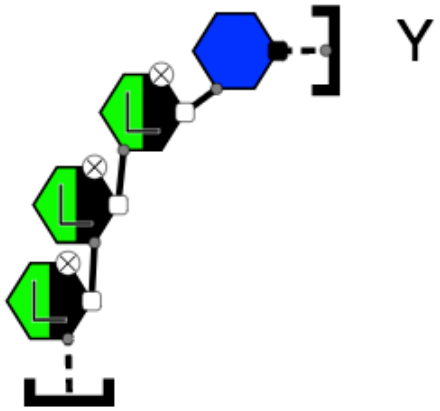
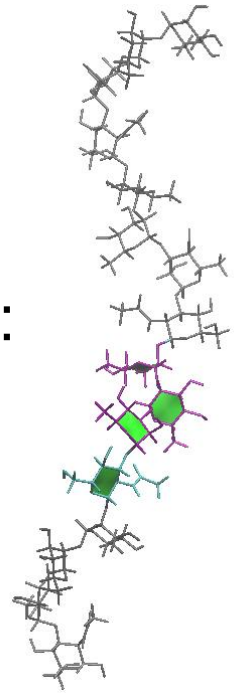
CarbBuilder

2D:



3D:



version 2
C#
improved building algorithm

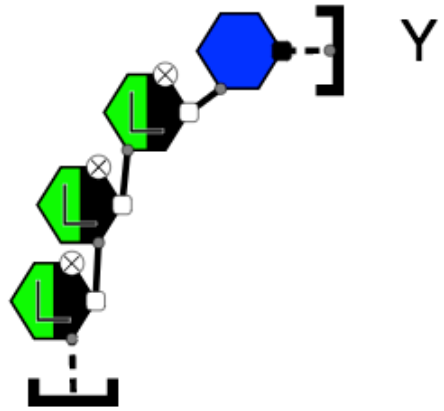
SOFTWARE FOR MOLECULAR STRUCTURE REPRESENTATION

1D: ->2)aLRha(1->2)aLRha(1->3)aLRha(1->3)bDGlcNAc(1->

Glycano

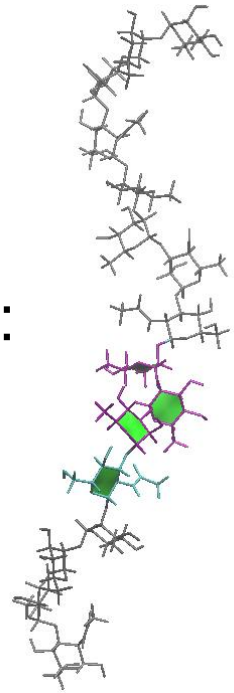
CarbBuilder

2D:



Y

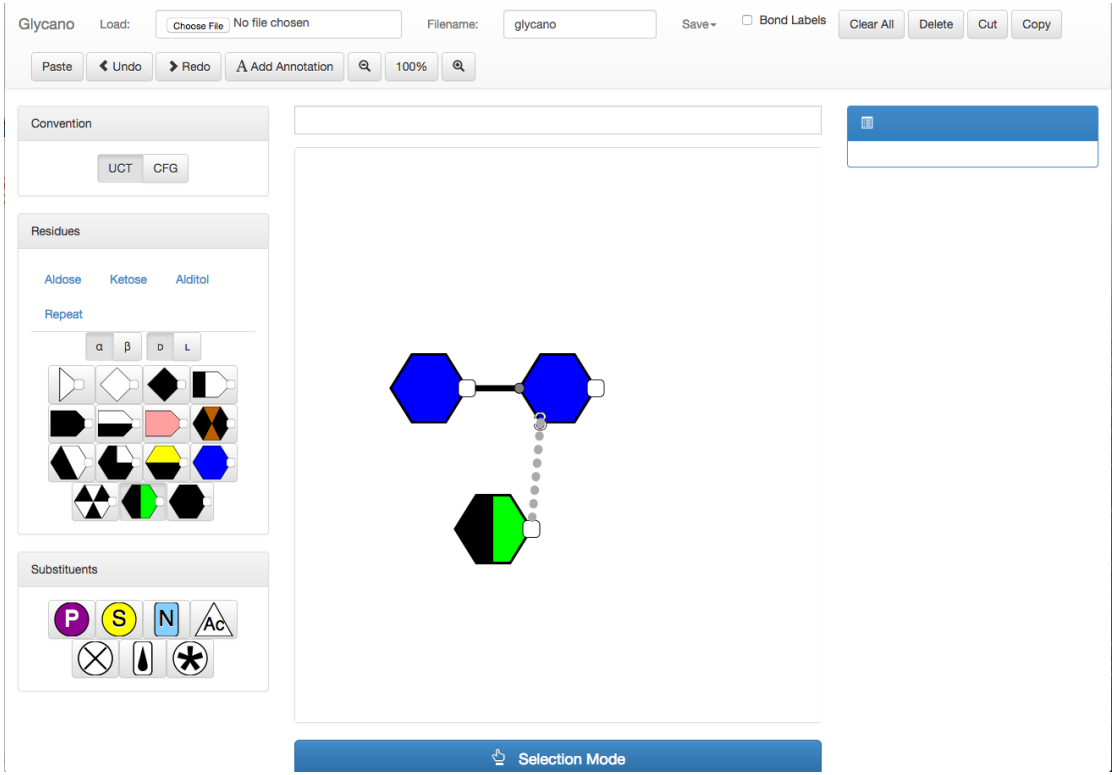
3D:



GLYCANO

- Original Java version now Javascript web application http://people.cs.uct.ac.za/~jwatson/

- Aims:
  - ease of access
    - no software to install
  - ease of use
    - minimize mouse clicks
  - testing new symbols for monosaccharides



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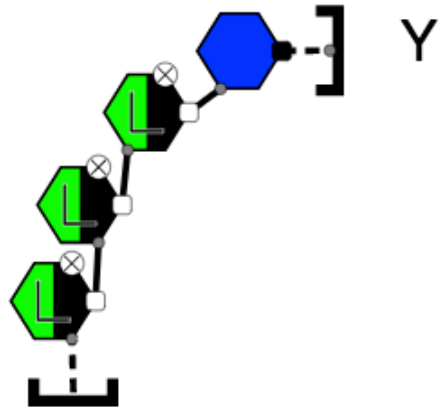

Y

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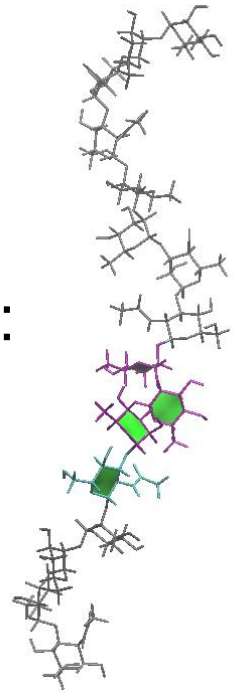

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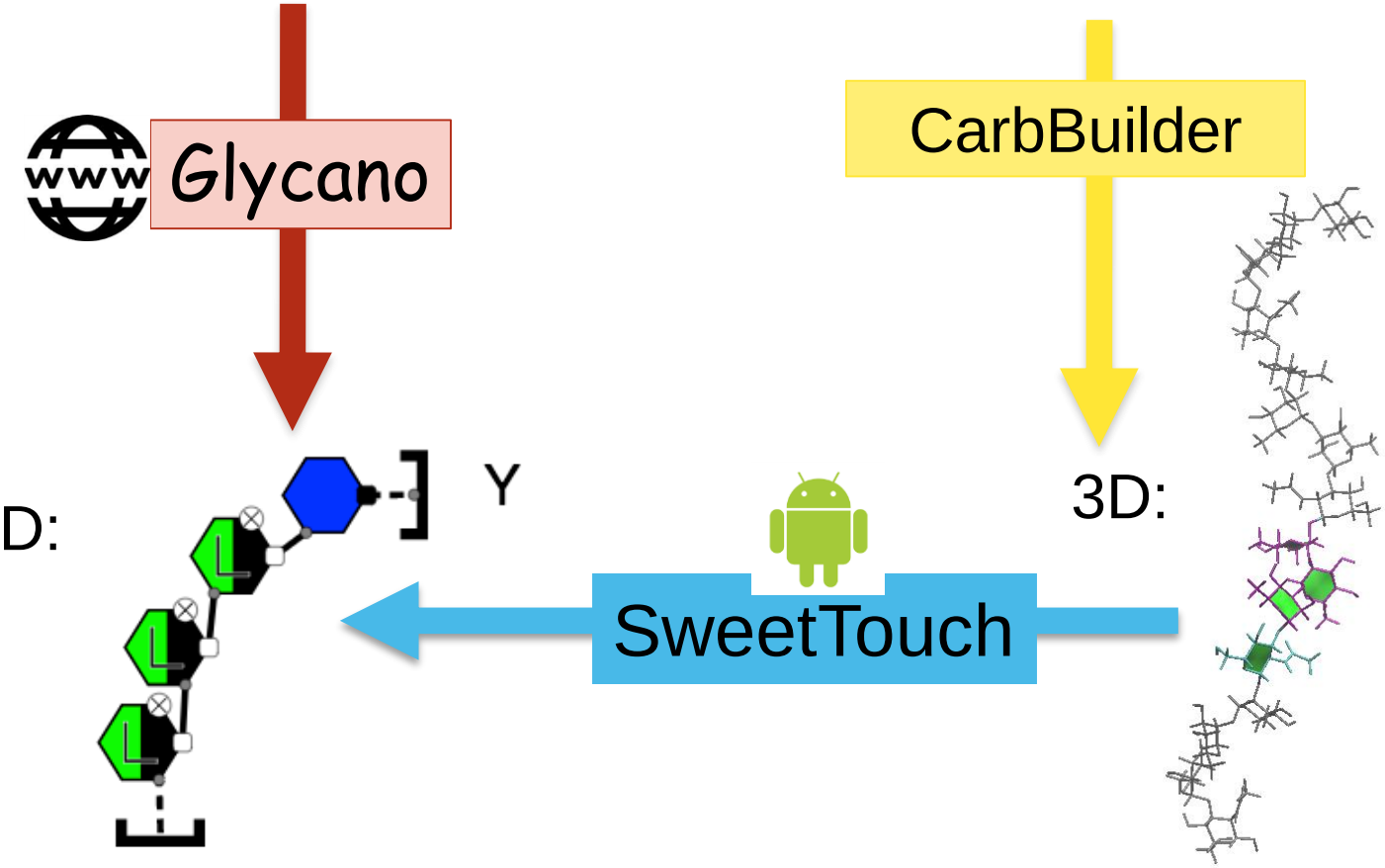
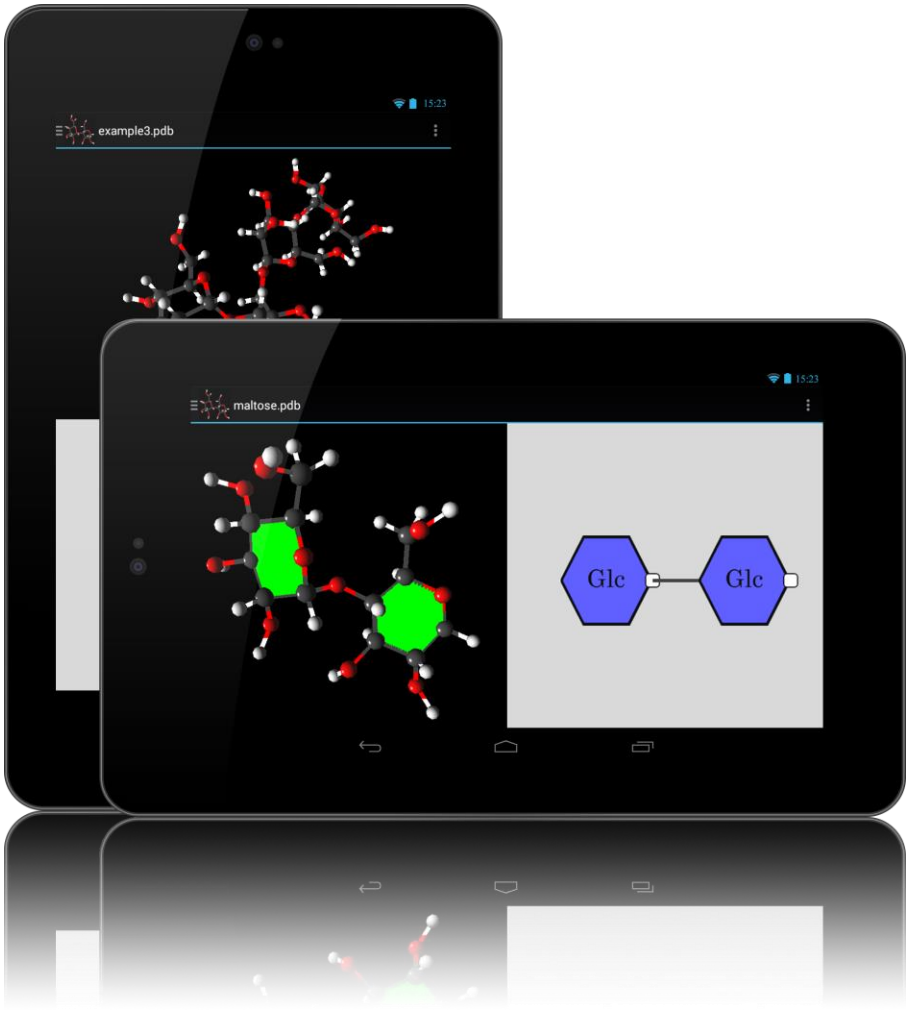
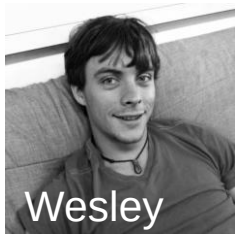


SweetTouch



An Open Source Android application for the 3D visualisation of molecules and the **identification** of carbohydrate rings.

4th year (Honours) project by:


Wesley Robinson

Mordechai Serraf

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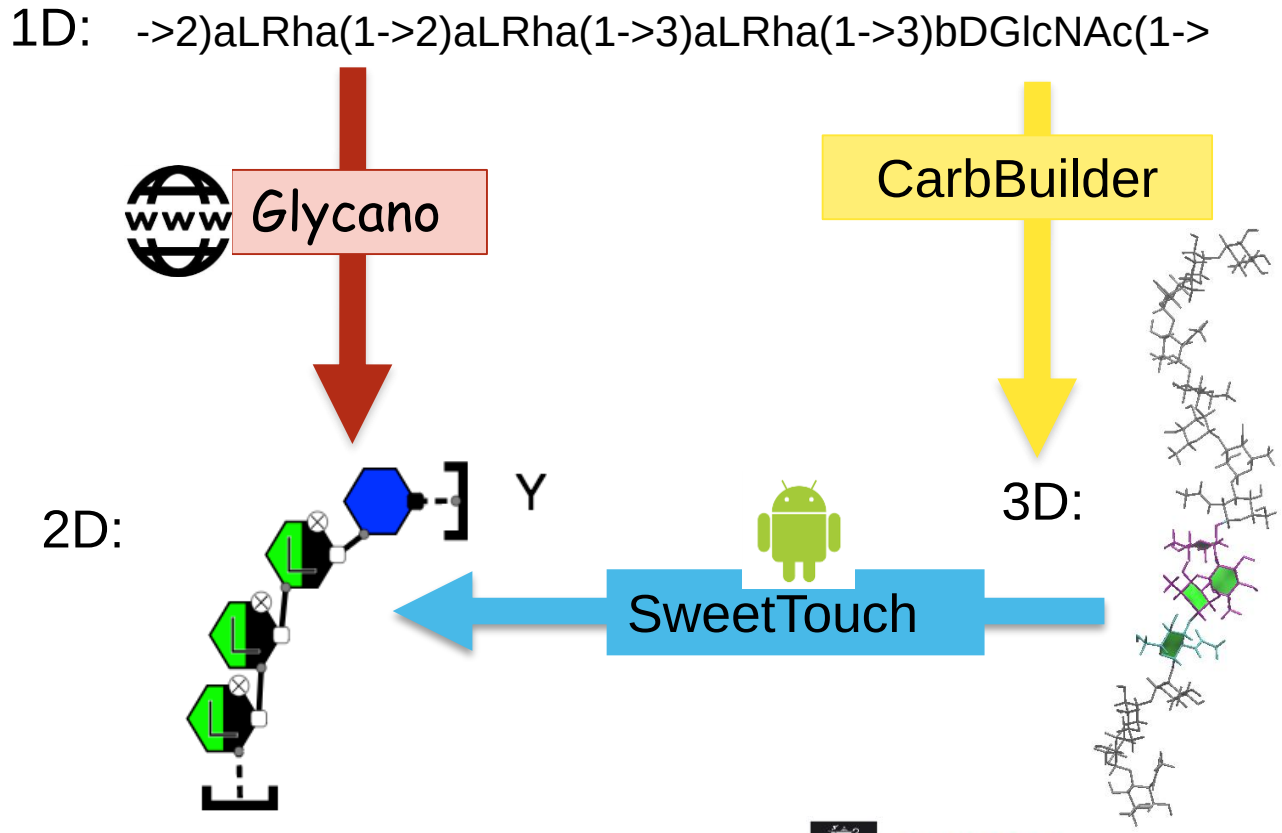
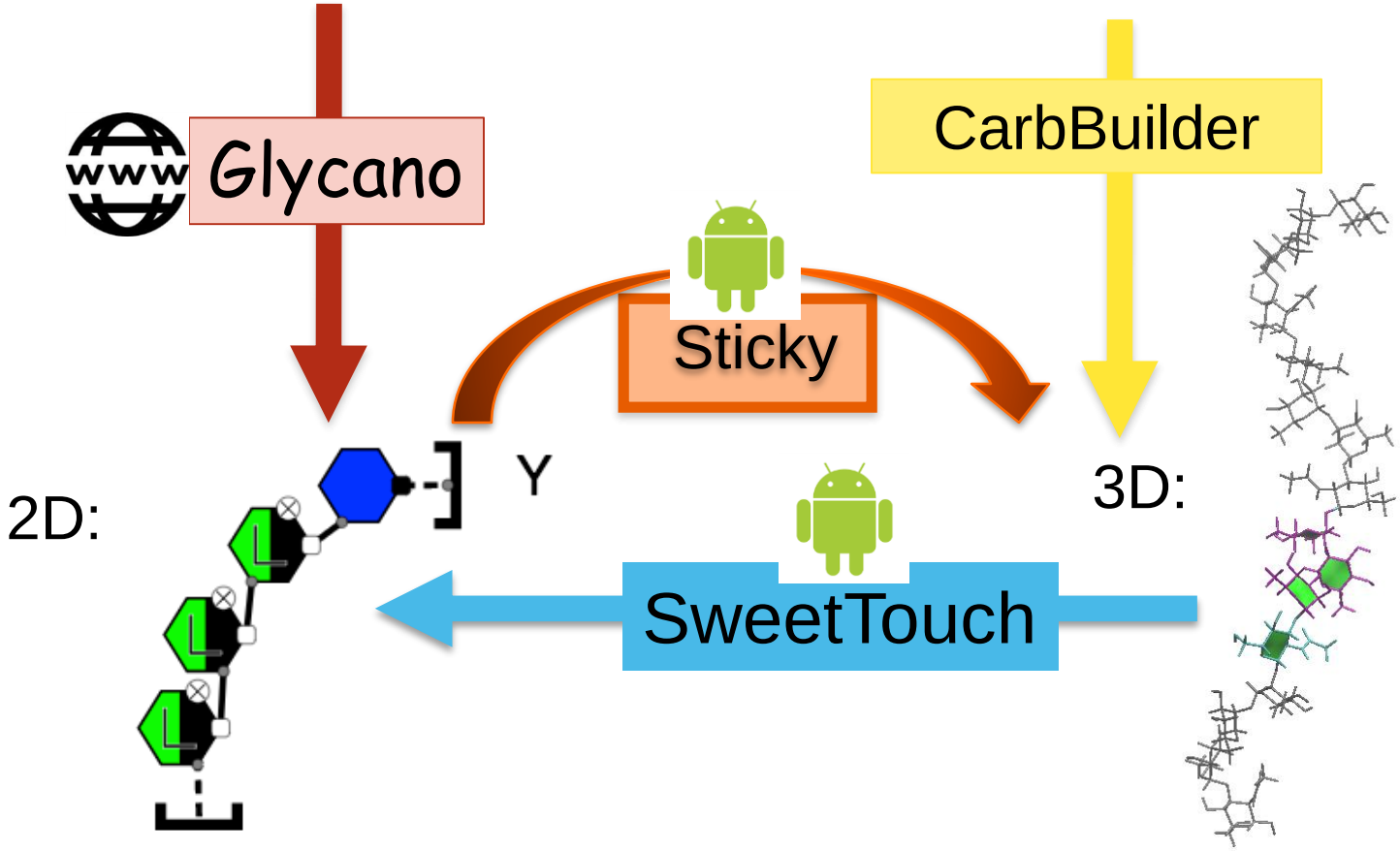
CONCLUSIONS

- Developing and refining a suite of software tools to help researchers investigate and explore carbohydrate structure



FUTURE WORK

1D: ->2)aLRha(1->2)aLRha(1->3)aLRha(1->3)bDGlcNAc(1->



ACKNOWLEDGEMENTS

University of Cape Town

James Watson

Mordechai Serraf

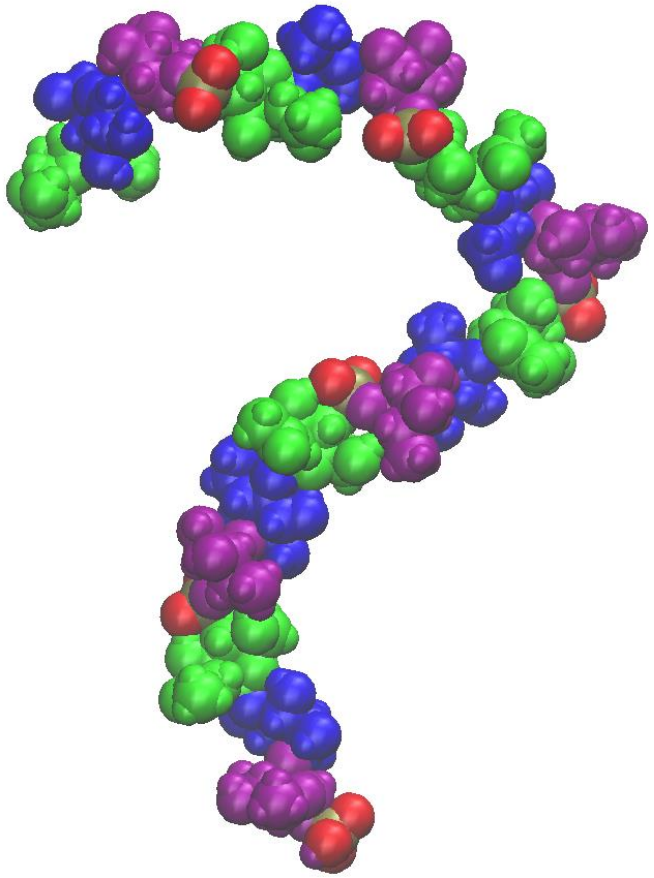
Wesley Robinson

Neil Ravenscroft

Stockholm University

Göran Widmalm

Financial Support

South African Medical Research Council

QUESTIONS?