



Interact on the web

- Feedback:
 - <https://forms.gle/SvkziuKfZSBhbQD46>
- Downloads:
 - <http://glycam.org/webinars>
- Current site:
 - <http://glycam.org>
- New site preview:
 - <https://dev.glycam.org>
 - Deployment expected by year end



Carbohydrate Modeling @ GLYCAM-Web

NIH Webinar 2020-08-14

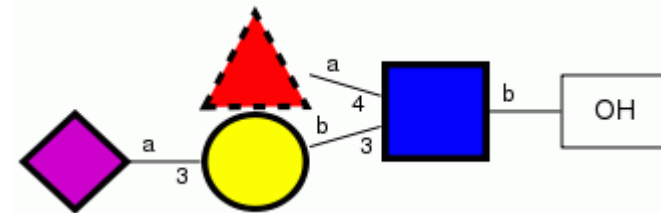
B. Lachele Foley



AUDIENCE PARTICIPATION!

Point & Click Interface

- First, a simple glycan (current site):



DNeu5Aca2-3DGalpb1-3[LFucpa1-4]DGlcpcNAcb1-OH

Build direction from non-reducing to reducing

1. **DNeu5Aca2-3DGalpb1-3**[LFucpa1-4]**DGlcpcNAcb1-OH**
2. DNeu5Aca2-3DGalpb1-3[**LFucpa1-4**]DGlcpcNAcb1-OH

- Go to glycam.org/cb

Websites referenced with the next slide

- Glycan Processing Figure:

- <https://www.ncbi.nlm.nih.gov/books/NBK1917/figure/ch8.f4/?report=objectonly>

- **From:** <https://www.ncbi.nlm.nih.gov/books/NBK1917/>

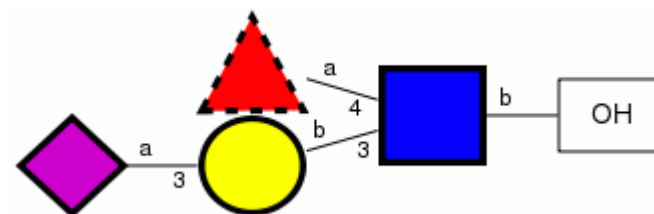
- Tree Image:

- <https://en.wikipedia.org/wiki/File:Person-tree.jpg>

- **From:** <https://en.wikipedia.org/wiki/Tree>

Point & Click Interface

- First, a simple glycan
([new site preview!](#)):



DNeu5Aca2-3DGalpb1-3[LFucpa1-4]DGlcpcNAcb1-OH



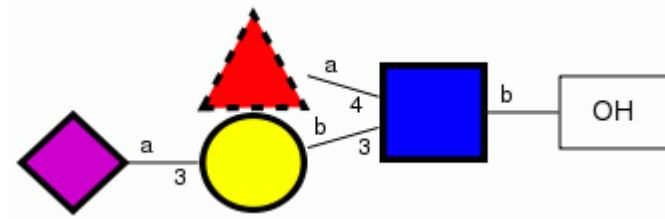
Build direction from reducing to non-reducing

Otherwise the same!

1. **DNeu5Aca2-3DGalpb1-3[LFucpa1-4]DGlcpcNAcb1-OH**
 2. DNeu5Aca2-3DGalpb1-3[**LFucpa1-4**]DGlcpcNAcb1-OH
- Go to dev.glycam.org/cb

Faster: Use the Libraries

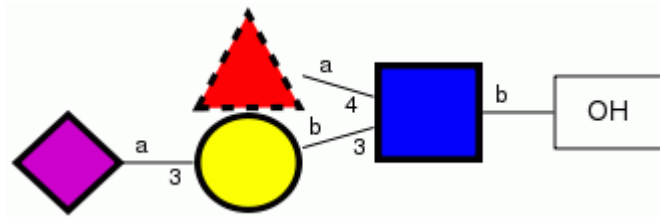
- Same glycan



- DNeu5Aca2-3DGalpb1-3[LFucpa1-4]DGlcNacp1-OH
- Current Site: glycam.org/oslibs
- **New site preview: dev.glycam.org/lib**

Even Faster/DIY: Enter Text

- Same glycan



- DNeu5Aca2-3DGalpb1-3[LFucpa1-4]DGlcNAcb1-OH
- Current Site: glycam.org/txt
- **New site preview: dev.glycam.org/txt**

Need a Glycosaminoglycan (GAG)?

- Quick background:
 - GAGs – polymers, some long, that alternate:
 - Hexosamine (e.g., GlcN, GalNAc)
 - Uronic acid (e.g., IdoA, GlcA)
 - Often sulfated, sometimes highly
- **Current Site: glycam.org/gag**
- New site preview: dev.glycam.org/gag



SHOULD GLYCAM MODELS MATCH PDB STRUCTURES?

Short answer: Should be close, usually

- Carbohydrates are flexible *and* inflexible
 - Sometimes in unexpected ways
 - Our site tries to present common shapes
- Crystallization can cause the unexpected
 - Do not assume either is wrong
 - If very different, consider carefully
 - Contact us if uncertain
 - If concerned: contact study authors



Acknowledgments

- All of you!
 - NIH
 - PDB
 - CCRC
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