Shiny new ELN

June 19, 2013

At the moment, most of my electronic notebook keeping has been on Sparklix. Happily, there is only one project there. It's the mucin project with David Live. It's taken me forever to do the work. I hate that... Anyhow, I've recorded everything there except for the data analysis part of the project.

Sparklix doesn't allow you to export an entire project, but you can export parts of it. Here are the parts up until now:

This is the meta-data I wrote about the project:

> MD simulations of mucin fragments with varying glycosylation.
>
> Protein sequence: ACE PRO PRO THR THR THR THR LYS LYS PRO NH2 (ACE and NH2 are neutral termination caps)
>
> The four threonines are treated in the following ways:
> * All four unglycosylated (called "protein" herein)
> * All four O-glycosylated with alpha-D-N-acetyl galactosamine (called "d4g")
> * All four O-glycosylated with alpha-D-mannopyranose (called "d4m")
>
> See the protocols for simulation treatments and analyses.

I set myself and David Live as members.

MD Simulations

Mucin- 0. Set up run environment

Mucin- 1. PDB file preparation

Mucin- 2. Generation of Topology and Input-Coordinate Files

Mucin- 3. MD simulation

Mucin- 4. Data curation