**Sugars taskforce**

**1)** New bead definition for glucose, frutose, sucrose, maltose, cellobiose, kojibiose, sophorose, nigerose, laminarabiose, trehalose, etc. Two options:

1A) keep the mapping of [Lopes 2008](http://pubs.acs.org/doi/abs/10.1021/ct900313w), but change the beads based in MARTINI 3.0 approach.

1B) change the mapping.

- How to deal with Pentoses like ribose?

- How should we handle the different mappings for singe and joint sugar units?

**2)** check if the bonded parameters (specially if angles and dihedral in dissaccharides

are still good).

2A) same mapping: basically re-tune force constants, if necessary.

2B) new mapping: restart from zero.

**3)** Check water-octanol partition of the models

**4**) Check B22 of sugars (based in [Sikora 2017](http://pubs.acs.org/doi/abs/10.1021/acs.jctc.7b00374?journalCode=jctcce))

**5)** check some carbohydrate systems from the original paper ([Lopes 2008](http://pubs.acs.org/doi/abs/10.1021/ct900313w))

- water solutions of glucose and other sugars (density and effects in diffusion coefficients?)

- maltoheptaose oligomer (gyration radius and structure)

- amilose in water and in nonane. (structure in nonane – helix, in water – coil).

- curdlan in nonane

- effects of sugars in bilayers (like DPPC, POPC, etc).

**6)** other applications or mixed systems:

- cyclodextrin  [Lopes 2011](http://journals.plos.org/ploscompbiol/article?id=10.1371/journal.pcbi.1002020)

- cellulose [Lopes 2015](http://pubs.acs.org/doi/abs/10.1021/jp5105938)

- glycolipids (some bilayer properties) - [Lopes 2013](http://pubs.acs.org/doi/abs/10.1021/ct3009655), [Eerden 2015](http://www.sciencedirect.com/science/article/pii/S0005273615000656).

- lipopolyssacarides. ([Hsu 2017](http://onlinelibrary.wiley.com/doi/10.1002/jcc.24895/abstract), [Oosten 2016](http://www.sciencedirect.com/science/article/pii/S1093326315300899?via%3Dihub), [Hsu 2016](http://pubs.acs.org/doi/abs/10.1021/acs.jpcb.6b06615), [Ma 2015](http://pubs.acs.org/doi/abs/10.1021/acs.jpcb.5b07122))

- glycoproteins (solubility ?)

**7)** Survey of trisaccharides:

-automated mapping and parameterization of all possible trisaccharides, generated based on GLYCAM builder.

- based on that automated building and parameterization of any simple (i.e. non-branched) polysaccharide for MARTINI.

- comparison of dynamics of all trisaccharides to the ones present in nature.