In this report, we ran pure DOPC lipid simulations at 310 k , at constant area per lipid equal to 68 A^2, 70 A^2, 72 A^2, 74 A^2. The system has 64 DOPC lipids and 3921 spc waters. We ran the systems with both Berger force field and Poger 53a6 gromos force field.

For Berger force field, each simulation was ran for 80 ns, while for Poger force field, each simulation was ran for 160 ns. The xray form factors were calculated from the first and second half of the simulation to compare for convergence.

1 Convergence

In Fig 1, we showed that the form factor converged well within the simulation timescale. Though with Poger force field, they diverge a little, the positions of the peaks and also the positions where the form factor equals to 0 do not change.

2 Compare with experiment

We compare the xray form factor calculated from different area per lipid to the experiment. Since we already showed the convergence of our simulation, the data we used below are only from the second half of the simulation.

Since the absolute value in form factors can be scaled, so it is better to compare the position where the form factors intersecting 0. We have three observations:

- It is clear that when the area per lipid increases, the form factor shifted the high q region.
- Form factor of simulation at constant area per lipid of 68 A^2 agrees better with experiment. This is true for both force fields.
- Berger a68 agrees better than Poger a68 with the experiment (from the position of the second intersection to 0).

3 Propose work to do

The comparsions we made between simulations and experiment are only qualitative. We notice your group have used more quantitatively χ^2 comparison. Also your group have a SDP model which you may prefer to compare to simulation rather than raw experimental data.

We put our data in the dropbox shared with Kiyo. So you guys can do further comparison. Once we established which area per lipid simulation data agrees the best with experiment, we can back calculated the required surface tension to fix the system to that area per lipid. And further add peptides to the system with a prefixed surface tension to see the change of form factors and compare with experiments.

Another thing to note that in your experiment, the peptide should be on both side of the bilayer. However, the original PNAS paper has a concentration difference of peptide on different bilayer leaflets. Therefore it may not reflect the experimental conditions. It seems to me that it is very hard to control the peptide on one side of the bilayer in multistack bilayer systems, we may need to run simulations with peptides on both sides in order to compare with experiment. In that case, the most hypersized results would be the peptide thinner the bilayer, and we probably would see this trend from simulation. If you guys can extract the binding modules, we may also calculated that from simulation, which may add an extra point to the work.

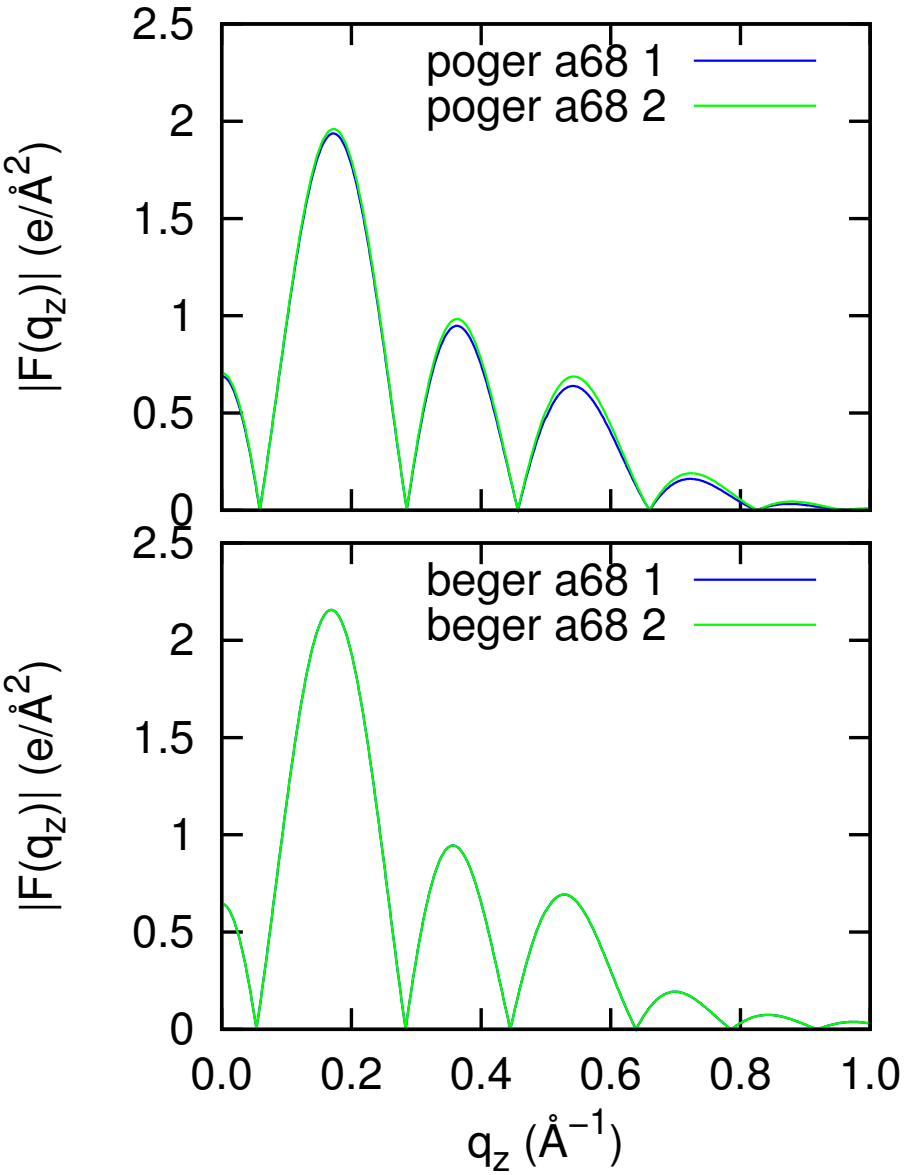

Figure 1: Xray form factor calculated from Berger force field and Poger force field. Blue line was calculated from the first half of the simulation while the green line was from the second half of the simulation. Simulations were ran with a constant area with area per lipid as 68 A^2

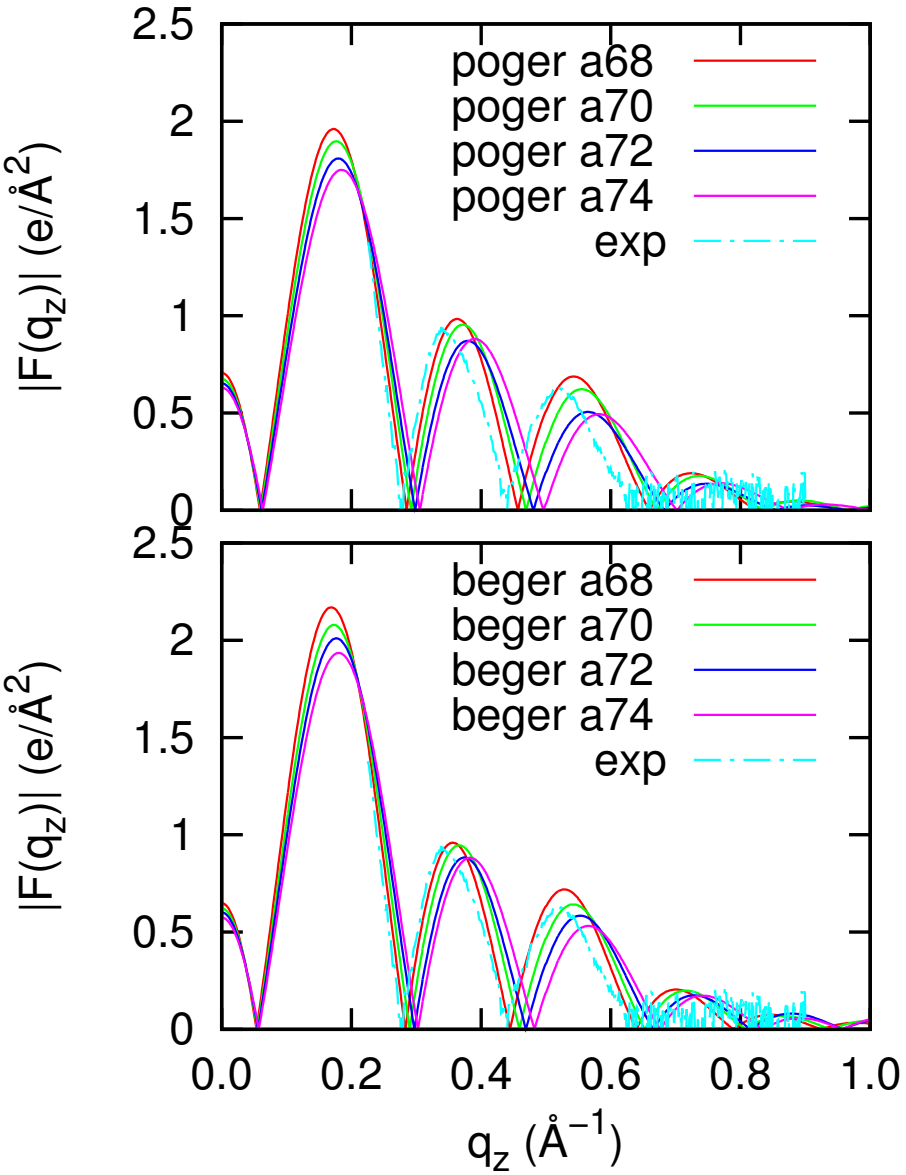

Figure 2: Xray form factor calculated from Berger force field and Poger force field. Blue line was calculated from the first half of the simulation while the green line was from the second half of the simulation. Simulations were ran with a constant area with area per lipid as 68 A^2