March 11, 2014

1 SIMtoEXP software

The details of the program can be found in [1]. Here, a brief introduction to the software will be given.

SIMtoEXP is a program to analyze the bilayer structure along the bilayer normal. It reads in the number density of each atom in lipids and peptides and calculate the form factor from the bilayer electron density profile,

$$F(q_z) = \int_{-z_0}^{z_0} \rho(z) dz. \tag{1}$$

An assumption made here is that x-ray form factor is properly represented by the Fourier transform of an average electron density profile, while, strictly, x-ray form factor is equal to. Within Born approximation, the X-ray intensity is a statistical (time) average over absolute form factor squared,

$$I(q_z) = \left\langle |F(q_z)|^2 \right\rangle \tag{2}$$

An electron density profile of a DOPC bilayer simulated by S-lipid force field is shown in Fig. reffig:DOPC. The exact parsing of atoms into each component group is shown in Fig. . Parsing with more components can be achieved, but one shown is the same parsing employed in SDP modelling for x-ray data, which will be discussed in a later chapter.

Calculated form factor is shown in . In order to obtain reliable structure from simulations, simulations with various area per lipid were done. A simulation that best matches the experimental form factor was chosen and analyzed to obtain the bilayer thickness. For systems with Tat, Tat was fixed at various z coordinates at various area per lipid. Table reftb:Tat shows chi squared values for all the simulations performed for this study. As seen in Table reftb:Tat, smaller chi squared was obtained for larger z values. While the smallest χ^2 was obtained at $z = 20\mathring{A}$, this simulation was considered artifactual because it is difficult for the bilayer thickness to be modified so much for a rather small insertion of Tat. Since the experimental data already suggest that bilayer thickenss was decreased as increasing concentration of Tat, Tat must be embbed by an appreciable amount in the bilayer.

While physical reasoning can be employed to eliminate some of small χ^2 simulations, simulations with $A_L =$ and $z_{Tat} = 18, 16, 14$ seem to be all good.

As Fig. shows, simulated form factors look very similar albeit small differece in χ^2. Instead of taking the smallest χ^2 as the best structure for this system, we averaged three simulations weighted by their χ^2 as ...

References

[1] Norbert Kuerka, John Katsaras, and JohnF. Nagle. Comparing membrane simulations to scattering experiments: Introducing the simtoexp software. *Journal of Membrane Biology*, 235(1):43–50, 2010.