NMRLIPIDS PROJECT 1

## Report for lipid bilayer model structural quality

## MATCH - NMRlipids project

## I. FORM FACTOR

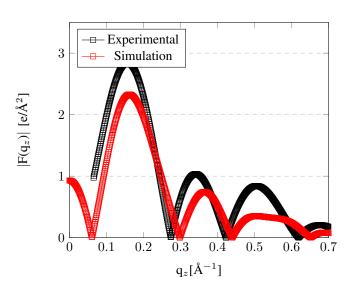


Fig. 1. Form factors. The results in this demonstration show that the lipid bilayer is too thin compared to experiments.

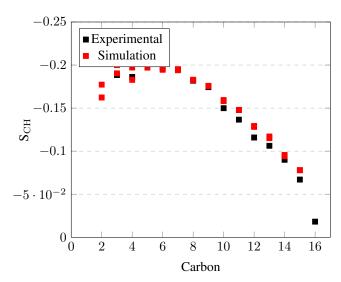


Fig. 3. *Sn*-1 acyl chain order parameters. The results in this demonstration show that the bilayer *sn*-1 acyl chain structure is well described by this model.

## II. ORDER PARAMETER

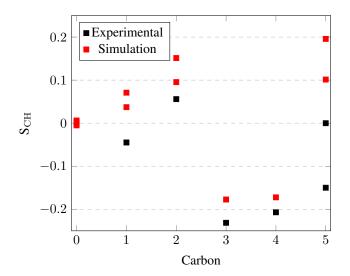


Fig. 2. Headgroup and glycerol backbone order parameters. The results in this demonstration show that the glycerol backbone and choline headgroup structures are not well described by this model.

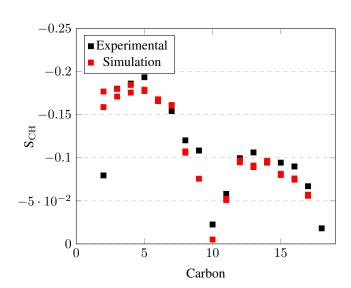


Fig. 4. *Sn*-2 chain order parameters. The results in this demonstration show that the bilayer *sn*-2 acyl chain structure is well described by this model, except for carbons C2 and C9.