Best order parameters for headgroup Best x-ray form factor Overall best order parameters **Slipids POPC Slipids POPE CHARMM36 POPC** 200 Simulation 200 — Simulation — Simulation 200 Number of FFQuality Forcefield Molecules Temperature DOI Experiment — Experiment — Experiment molecules 150 150 0.61 0.84 0.82 0.76 514.766945 POPC:SOL (512:23943) 298.00 10.5281/zenodo.166034 150 Slipids $|E(q_z)|$ 100 100 POPC:SOL (128:5120) 300.00 10.5281/zenodo.3741793 0.63 0.70 0.76 0.69 713.024817 MacRog 0.64 0.48 0.72 0.61 674.021485 MacRog POPC:SOL (288:14400)10.5281/zenodo.13498 50 POPC:SOL (128:6400) 0.65 0.74 0.42 0.60 576.169287 ECC-lipids 300.00 10.5281/zenodo.3335503 50 50 0.01 0.88 0.84 0.58 POPC:SOL (256:10342) 300.00 10.5281/zenodo.1402417 Berger 0.02 0.83 0.78 0.55 Berger POPC:SOL (128:7290)298.00 10.5281/zenodo.4643875 -50300.00 10.5281/zenodo.1118980 0.65 0.54 0.43 0.54 613.125521 ECC-lipids POPC:SOL (128:6400)0.6 0.0 0.2 0.4 0.8 1.0 0.0 0.2 0.4 0.6 0.8 1.0 0.0 0.2 0.6 8.0 1.0 $q_z[\mathring{A}^{-1}]$ $q_z[\mathring{A}^{-1}]$ 0.01 0.79 0.77 0.52 122.168365 Slipids POPE:SOL (500:25000) 310.00 10.5281/zenodo.3231342 0.10 0.87 0.57 0.51 140.087165 POPE:SOL (336:13460)310.00 10.5281/zenodo.1293813 Slipids 0.05 0.05 0.10 0.86 0.57 0.51 136.680061 POPE:SOL (336:13460) 310.00 10.5281/zenodo.1293813 Slipids 0.05 0.00 -0.00 -ECC-lipids, SPC water model, ECC-0.16 0.64 0.69 0.50 297.214229 POPS:SOL:SOD (72:3600:72) 298.00 10.5281/zenodo.1488094 0.00 ions -0.05-0.050.67 0.36 0.40 0.48 689.623863 CHARMM36 POPC:SOL (256:9767) 300.00 10.5281/zenodo.1306800 11 -0.05-0.10-0.10CHARMM36 (1024:51200) 298.15 10.5281/zenodo.5767451 0.67 0.37 0.38 0.47 902.726741 POPC:SOL -0.10-0.15-0.15-0.15-0.20-0.20-0.20-0.25 g_1 Carbon Carbon Carbon → T310K CHARMM36.dat T310K_Slipids.dat sn-1 T298K Slipids.dat sn-1 sn-1 -0.05→ T300K_MacRog.dat -0.05-0.05→ T300K CHARMM36.dat 60.0 T310K_Lipid17.dat -0.10-0.10-0.1057.5 [±]S −0.15 -0.15-0.15-0.20-0.20-0.20-0.25Percentage of POPE in POPC 12 14 10 10 12 14 10 12 14 16 Carbon Carbon Carbon 0.00 sn-2 sn-2 -0.05-0.05headgroup sn-1 sn-2 total FFQuality Forcefield Molecules Number of molecules Temperature -0.05310.0 10.5281/zenodo.3231342 0.01 0.79 0.77 0.52 122.168365 Slipids POPE:SOL (500:25000)-0.10-0.10S −0.10 0.10 0.86 0.57 0.51 136.680061 Slipids POPE:SOL (336:13460) 310.0 10.5281/zenodo.1293813 S_C 0.10 0.87 0.57 0.51 140.087165 Slipids POPE:SOL (336:13460) 310.0 10.5281/zenodo.1293813 -0.15-0.15-0.150.54 0.52 0.27 0.44 197.034217 CHARMM36 SOL:POPE (5760:144) 310.0 10.5281/zenodo.2641987 -0.200.53 0.14 0.07 0.25 234.339081 CHARMM36 SOL:POPE (25000:500)310.0 10.5281/zenodo.3237461 -0.20-0.20Lipid17 POPE:SOL 0.09 0.12 0.35 0.19 264.439235 (500:25000) 310.0 10.5281/zenodo.4424292 10 12 14 16 18 10 12 14 16 18 10 12 14 16 18 8 8 Carbon Carbon Carbon