a)

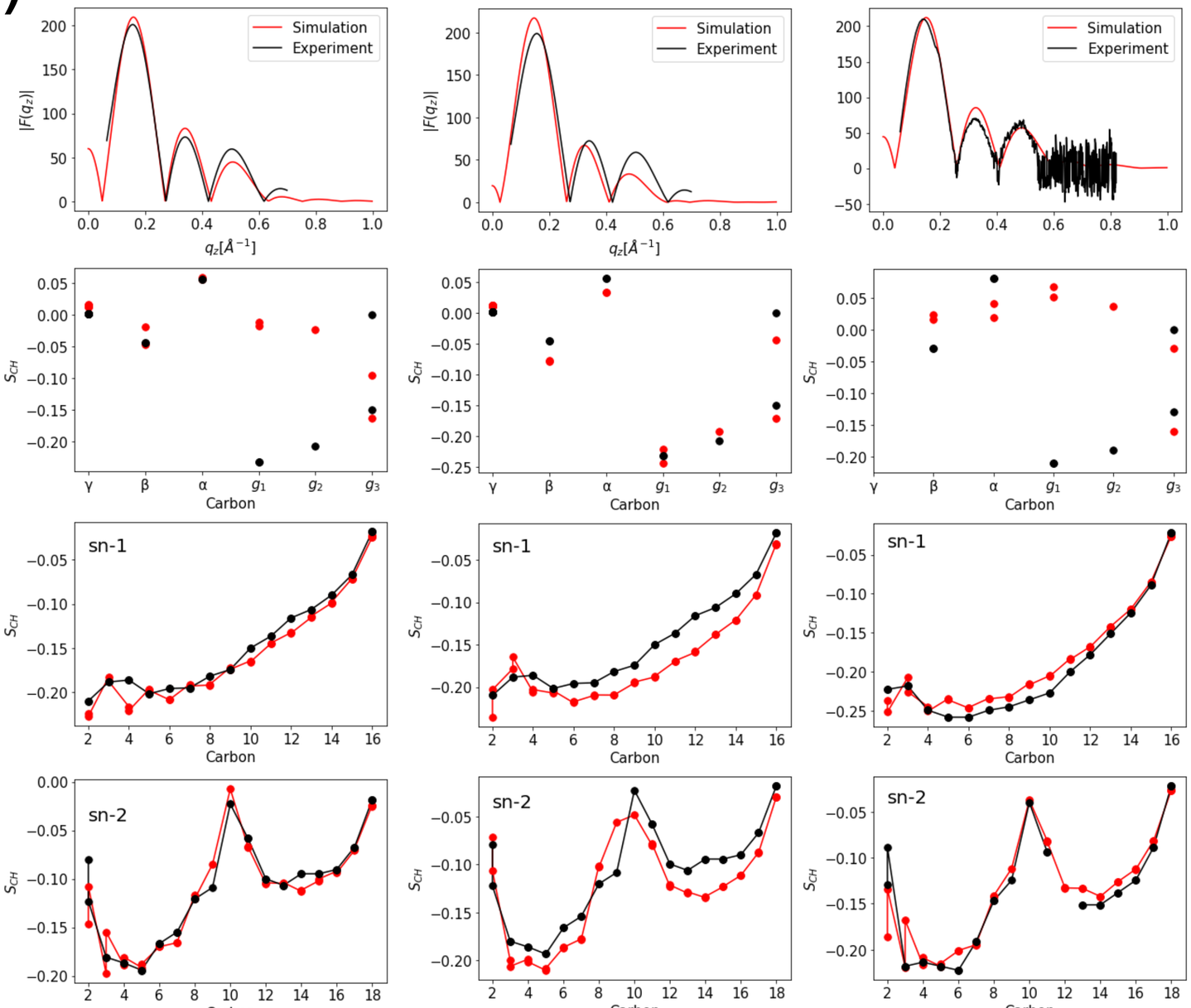
	headgroup	sn-1	sn-2	total	FFQuality	Forcefield	Molecules	Number of molecules	Temperature	DOI
0	0.61	0.84	0.82	0.76	514.766945	Slipids	POPC:SOL	(512:23943)	298.00	10.5281/zenodo.166034
1	0.63	0.70	0.76	0.69	713.024817	MacRog	POPC:SOL	(128:5120)	300.00	10.5281/zenodo.3741793
2	0.64	0.48	0.72	0.61	674.021485	MacRog	POPC:SOL	(288:14400)	298.00	10.5281/zenodo.13498
3	0.65	0.74	0.42	0.60	576.169287	ECC-lipids	POPC:SOL	(128:6400)	300.00	10.5281/zenodo.3335503
4	0.01	0.88	0.84	0.58		Berger	POPC:SOL	(256:10342)	300.00	10.5281/zenodo.1402417
5	0.02	0.83	0.78	0.55		Berger	POPC:SOL	(128:7290)	298.00	10.5281/zenodo.4643875
6	0.65	0.54	0.43	0.54	613.125521	ECC-lipids	POPC:SOL	(128:6400)	300.00	10.5281/zenodo.1118980
7	0.01	0.79	0.77	0.52	122.168365	Slipids	POPE:SOL	(500:25000)	310.00	10.5281/zenodo.3231342
8	0.10	0.87	0.57	0.51	140.087165	Slipids	POPE:SOL	(336:13460)	310.00	10.5281/zenodo.1293813
9	0.10	0.86	0.57	0.51	136.680061	Slipids	POPE:SOL	(336:13460)	310.00	10.5281/zenodo.1293813
10	0.16	0.64	0.69	0.50	297.214229	ECC-lipids, SPC water model, ECC-ions	POPS:SOL:SOD	(72:3600:72)	298.00	10.5281/zenodo.1488094
11	0.67	0.36	0.40	0.48	689.623863	CHARMM36	POPC:SOL	(256:9767)	300.00	10.5281/zenodo.1306800
12	0.67	0.37	0.38	0.47	902.726741	CHARMM36	POPC:SOL	(1024:51200)	298.15	10.5281/zenodo.5767451

b)

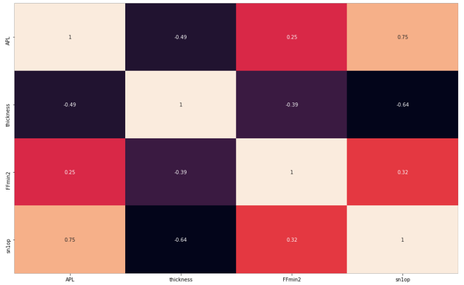
Overall best order parameters
Slipids POPC

Best order parameters for headgroup
CHARMM36 POPC

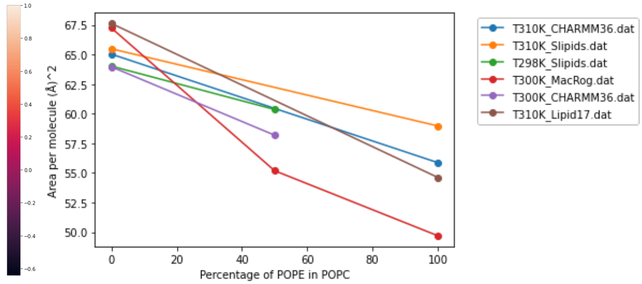
Best x-ray form factor
Slipids POPE



c)



d)



e)

	headgroup	sn-1	sn-2	total	FFQuality	Forcefield	Molecules	Number of molecules	Temperature	DOI
0	0.01	0.79	0.77	0.52	122.168365	Slipids	POPE:SOL	(500:25000)	310.0	10.5281/zenodo.3231342
1	0.10	0.86	0.57	0.51	136.680061	Slipids	POPE:SOL	(336:13460)	310.0	10.5281/zenodo.1293813
2	0.10	0.87	0.57	0.51	140.087165	Slipids	POPE:SOL	(336:13460)	310.0	10.5281/zenodo.1293813
3	0.54	0.52	0.27	0.44	197.034217	CHARMM36	SOL:POPE	(5760:144)	310.0	10.5281/zenodo.2641987
4	0.53	0.14	0.07	0.25	234.339081	CHARMM36	SOL:POPE	(25000:500)	310.0	10.5281/zenodo.3237461
5	0.09	0.12	0.35	0.19	264.439235	Lipid17	POPE:SOL	(500:25000)	310.0	10.5281/zenodo.4424292