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Supporting Material

Characterization of Antibiotic Peptide Pores using Cryo-EM and Comparison to Neutron Scattering

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Supplementary Materials

Examination of Antibiotic Peptide Pores using Cryo-EM and Comparison to Neutron Scattering

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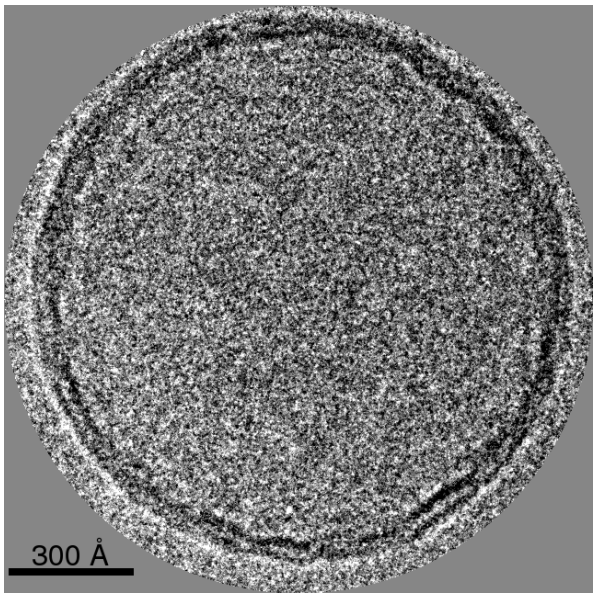

Figure S1A

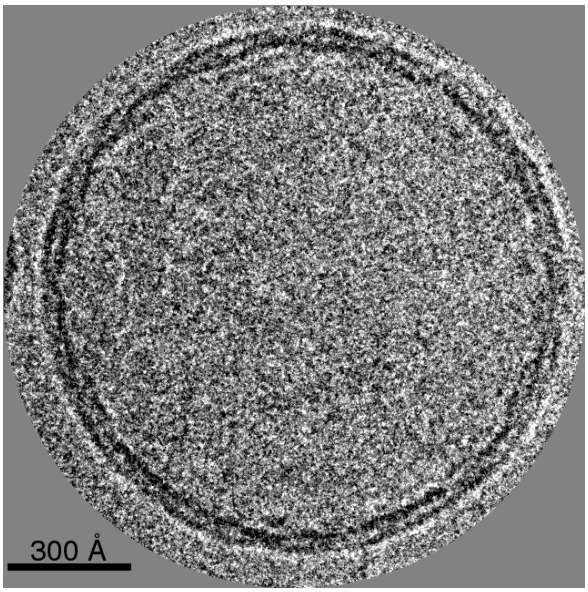

Figure S1B

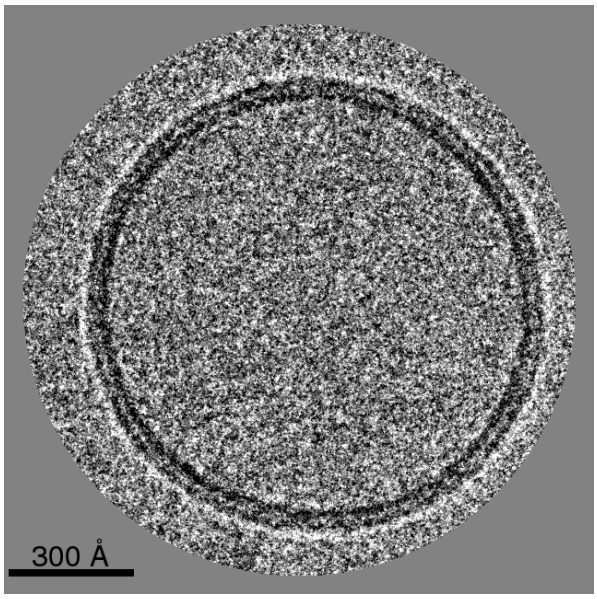

Figure S1C

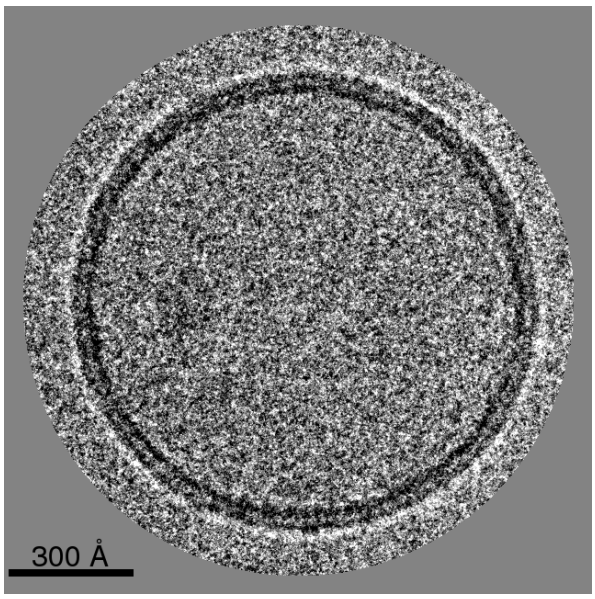

Figure S1D

Figure S1: Comparison of vesicle images with different lipid system. (A, B) images of DMPC/DMPG vesicle without Magainin. (C, D) images of POPC/POPG vesicle without Magainin. In the DMPC/DMPG without Magainin images, vesicles appear relatively smooth; however, interestingly, apparent bilayer thickness fluctuations were substantially stronger than a similar experiment performed with POPC/POPG. While this relative difference is not entirely unexpected due to the shorter chain-length in the DM membranes, the degree to which the bilayer seems to fluctuate in DMPC/DMPG membranes is somewhat surprising.

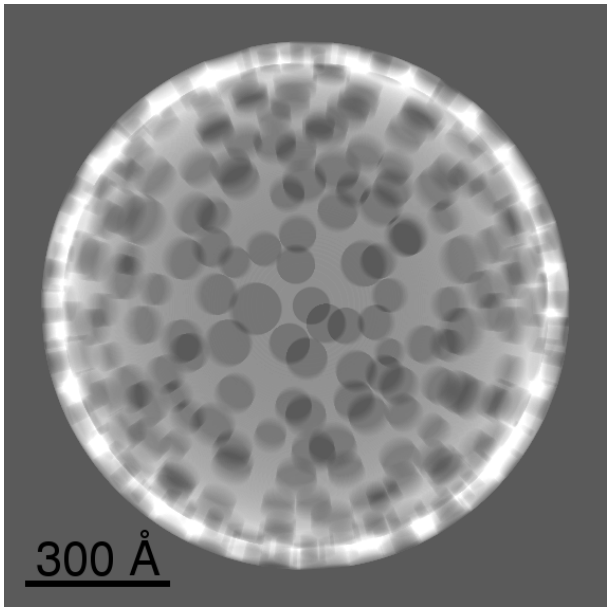

Figure S2A

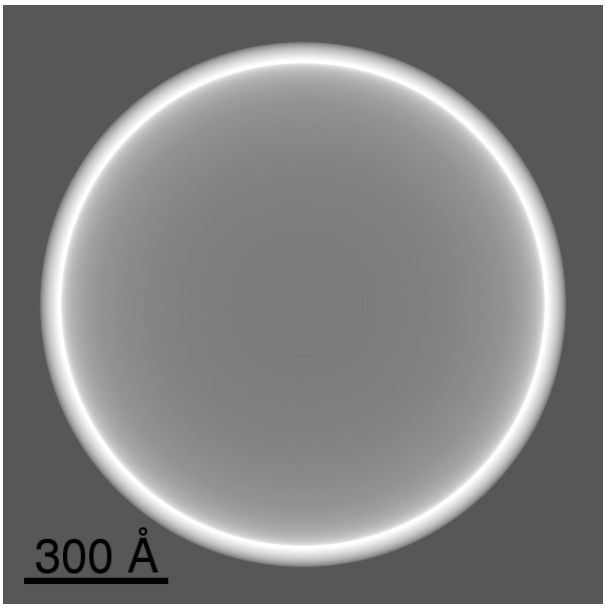

Figure S2B

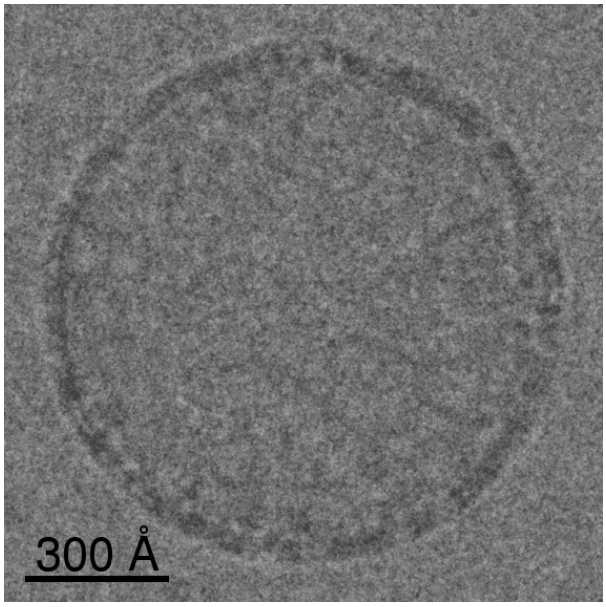

Figure S2C

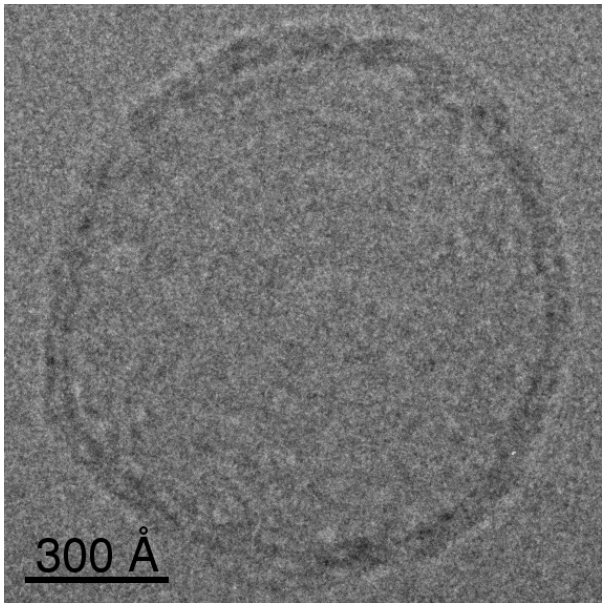

Figure S2D

Figure S2: Simulated vesicle with (A) and without (B) pores. The projection of spherical shells with a certain number of holes was generated to closely mimic the images of 'porous' vesicles. The projection of spherical shell without hole is used as a control. The bilayer was given no internal structure; because we are limiting ourselves to nearly planar regions of the bilayer, simulating the internal structure of the membrane was unnecessary. Non-overlapping pores of a given mean pore size and Gaussian pore size variation are placed on the surface, and then projections of the simulated vesicles were produced. Diameter and spherical shell thickness are 1056 Å and 46 Å, respectively. Mean pore size shown here is 80 Å and the pore size variation is 15%, 12 Å. (C) shows the simulated image (A) with CTF applied and noise added. (D) is a real image of DMPC/PG vesicle with magainin showing strongly perturbed appearance.

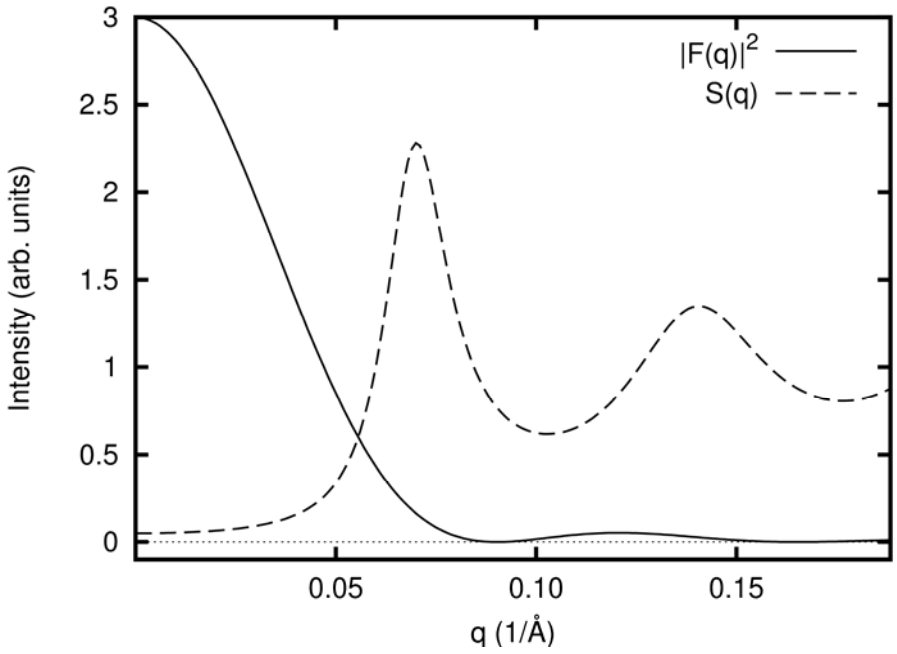

Figure S3: Decomposition of theoretical power spectrum into the structure factor, $S(q)$, of pore distribution and the form factor, $F(q)$, of a single pore, respectively. This figure shows $F(q)$ and $S(q)$ corresponding to pore size 83 Å and mean distance between pores (center to center) 108 Å.

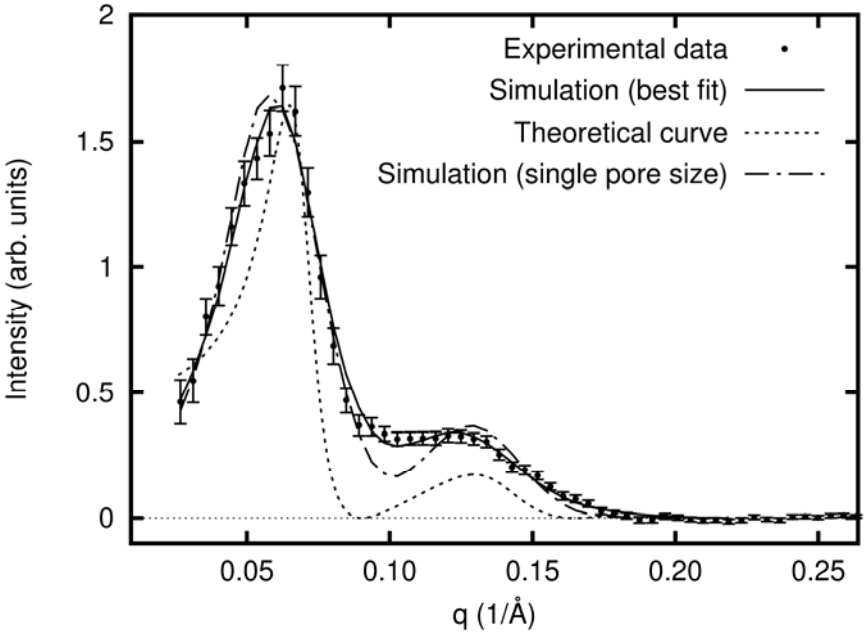

Figure S4: Comparison of theory, single pore size simulation and variable pore size simulation. The theoretical curve has the valley between the two peaks touching zero. The simulation with single pore size, which is close to the theoretical setup but with conic pore and slight curvature of membrane, is also shown. The simulation with variable pore size fits best with the experimental data.