Supplementary Information

Bottlebrush-Like Highly Efficient Antibacterial Coating Constructed by α-helical Peptide Dendritic Polymers on Poly(styrene-*b*-(ethylene-*co*-butylene)-*b*-styrene) Surface

Yujia Zhang, [a] Ke Kang, [a] Nanhang Zhu, [a] Guohao Li, [a] Xiaoxi Zhou, [a]

Aimin Zhang, [b] Qiangying Yi *[a] and Yao Wu *[a]

[a] National Engineering Research Center for Biomaterials, Sichuan University, Chengdu 610064, P. R. China

[b] State Key Laboratory of Polymer Materials Engineering of China, Polymer Research Institute of Sichuan University, Chengdu 610065, P. R. China

* Corresponding authors

E-mail addresses: wuyao@scu.edu.cn (Y. W.), qyi@scu.edu.cn (Q. Y.)

Details in Molecular Dynamic Simulations.

The simulations were carried out by the GROMACS package,[1] version 2019.3, with the GROMOS 53A7 force filed.[2] The topology of α-helical peptide dendritic polymer was constructed by Automated Topology Builder (ATB) service,[3] and the PDB of the bacterial membrane model are available online at http://www.softsimu.org/downloads.shtml. The water model used was single point charge (SPC) model.[4] The equilibration process started with a 100 ps simulation under NVT conditions at 310 K. The electrostatic interactions were handled by the particle mesh Ewald (PME) method.[5] Van der Waals interactions were also given a shortrange cutoff of 1.2 nm, and all bonds were constrained with LINCS[6] to enable a 2 fs time step to be applied; the temperature was coupled to the v-rescale.[7] After NVT, a 1000 ps of NPT simulation were carried out with Nosé–Hoover thermostat[8] (310 K) and Berendsen barostat[9] (1 atm). The pressure coupling employed a semi-isotropic scheme in which x, y, and z directions are coupled independently at 1 atm with coupling time of 0.5 ps and compressibility of 4.5×10^{-5}.

For full simulation, a simplified model molecule of α-helical peptide dendritic polymer was placed above the surface of POPG and POPE with distance about 4.5 nm from the membranes surface. The simulation was lasted 100 ns and the snapshot was saved every 100 ps for analysis. All the graphs were produced using VMD.[10]

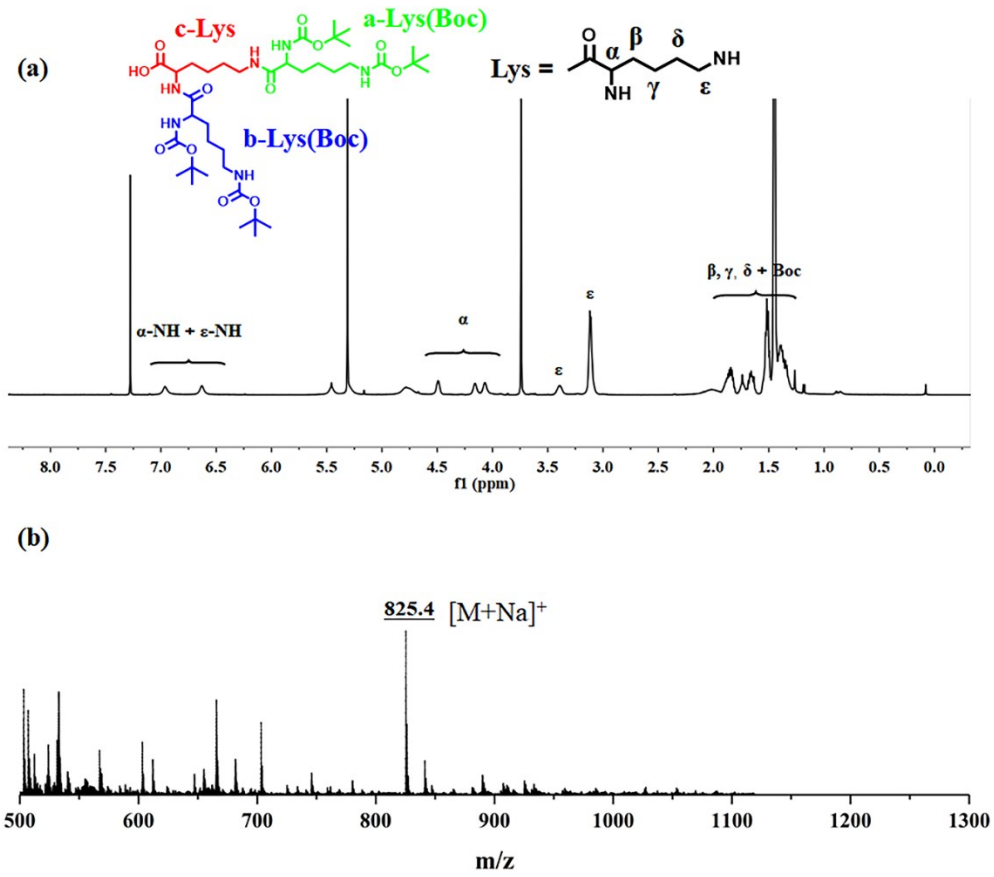

Figure S1. ^{1}H NMR spectra of compound **1** (a), MALDI-TOF-MS spectra of compound **1** (b).

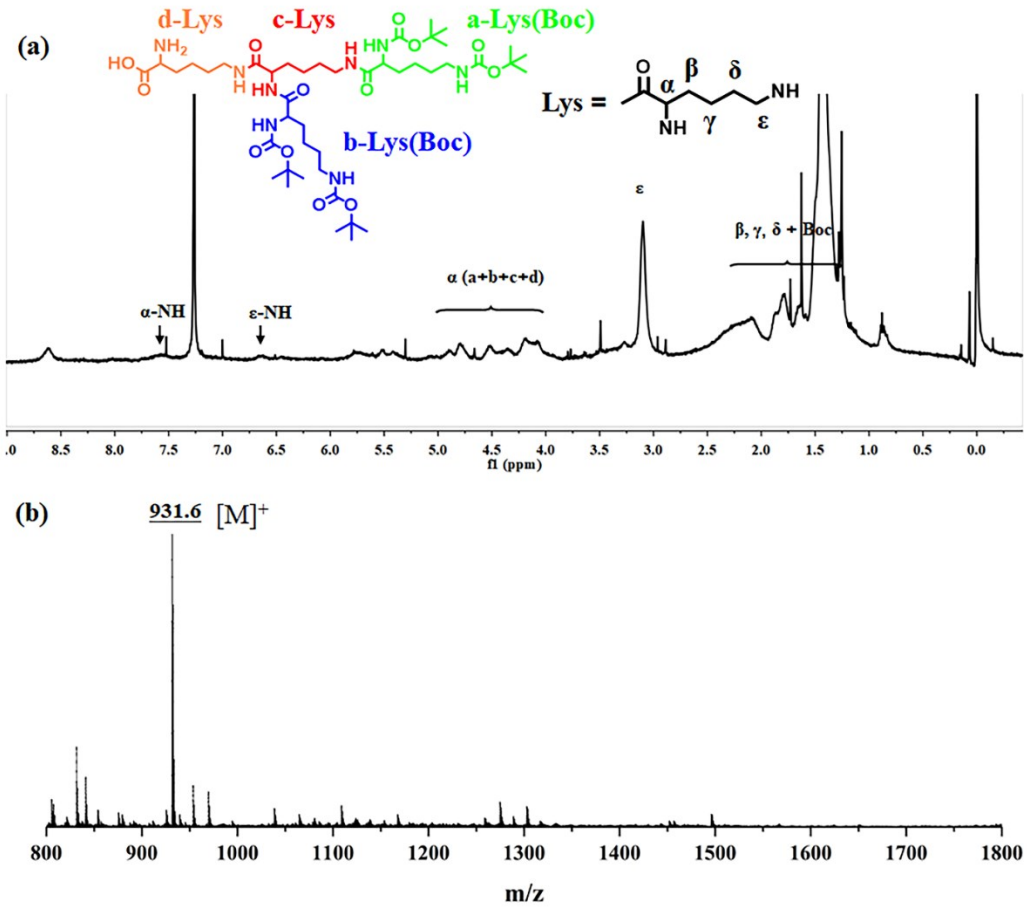

Figure S2. ^{1}H NMR spectra of compound **2** (a), MALDI-TOF-MS spectra of compound **2** (b).

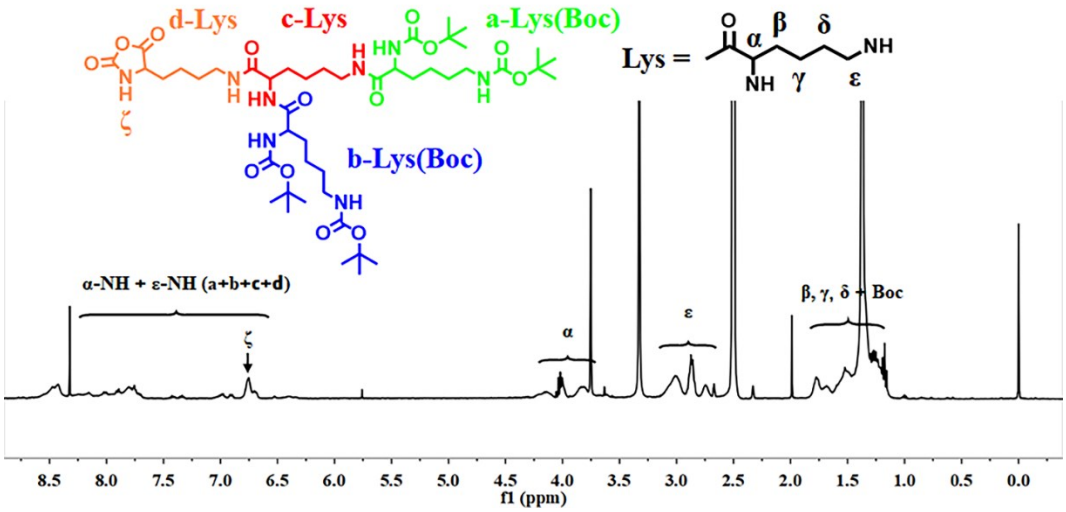

Figure S3. ^{1}H NMR spectra of compound **3**.

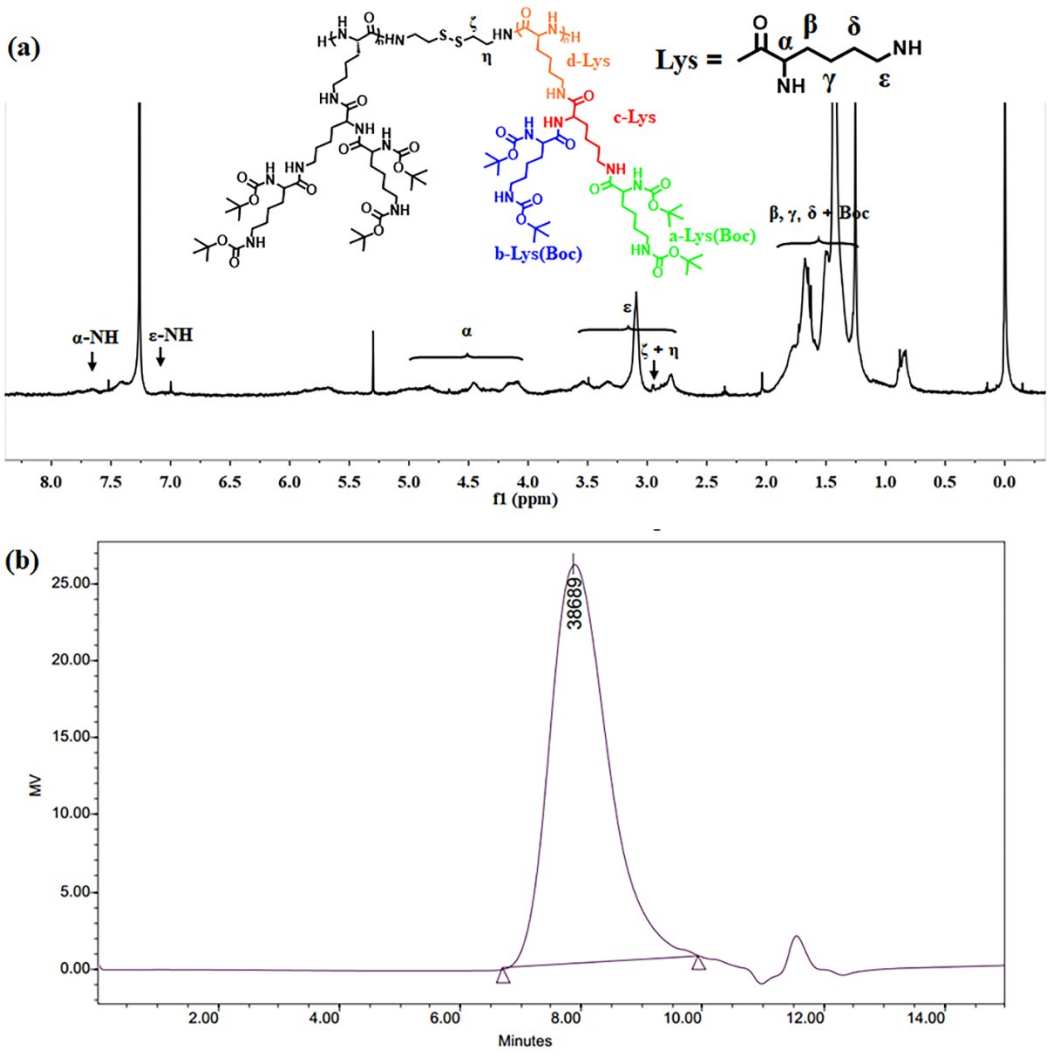

Figure S4. ^{1}H NMR spectra of compound **4** (a), GPC spectra of compound **4** (b).

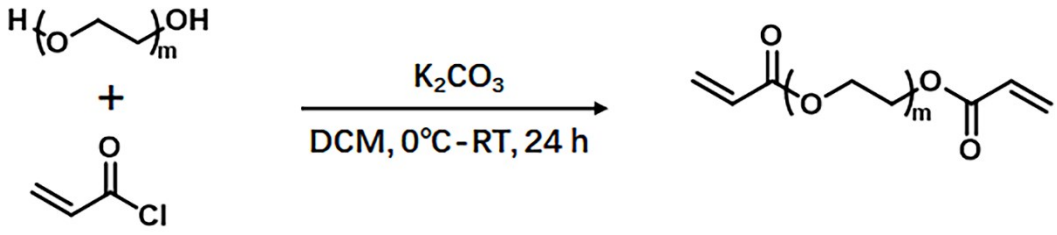

Figure S5. Synthesis of AC-PEG-AC.

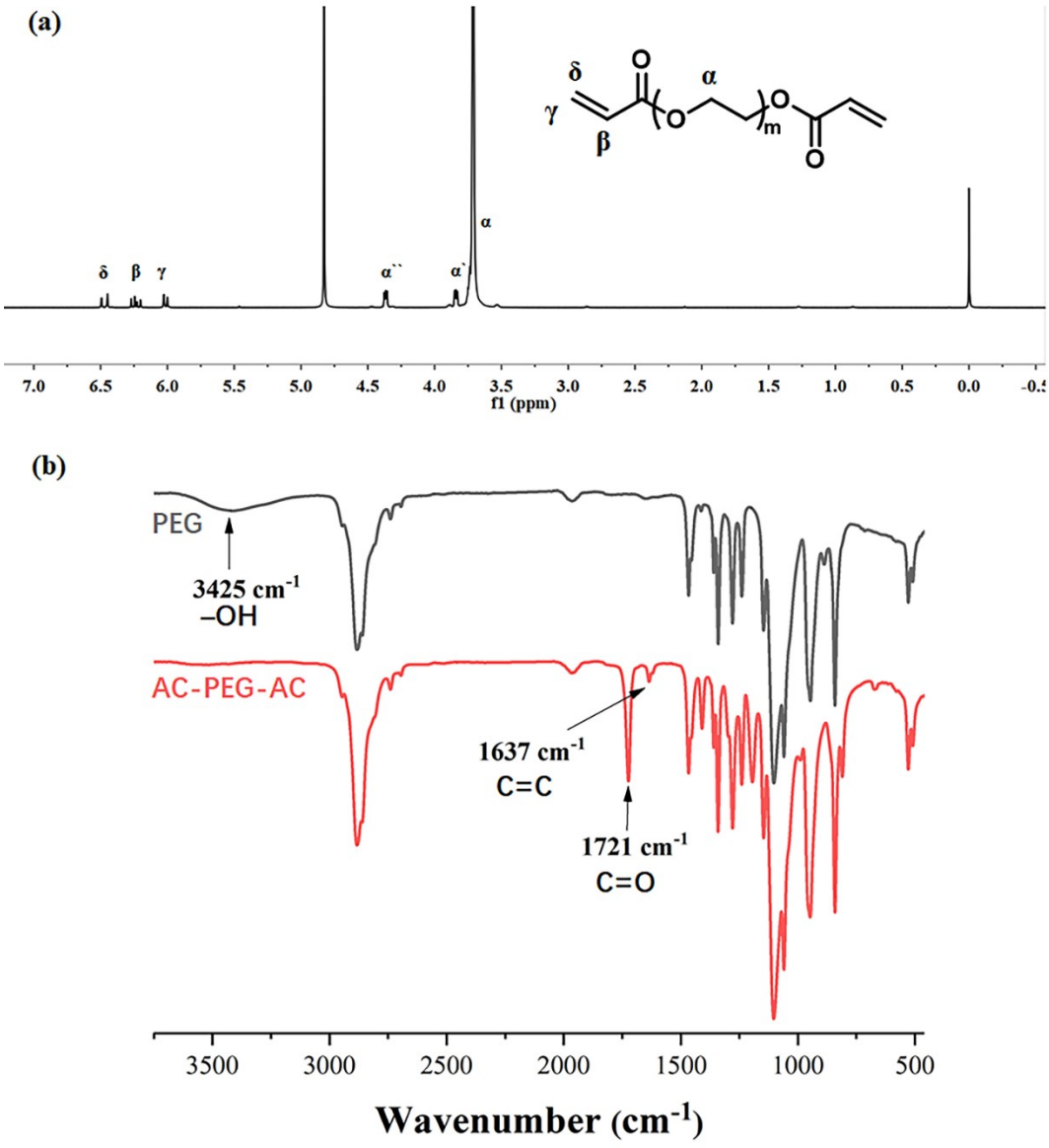

Figure S6. ^{1}H NMR spectra of AC-PEG-AC (a), FT-IR spectroscopy of PEG and AC-PEG-AC (b).

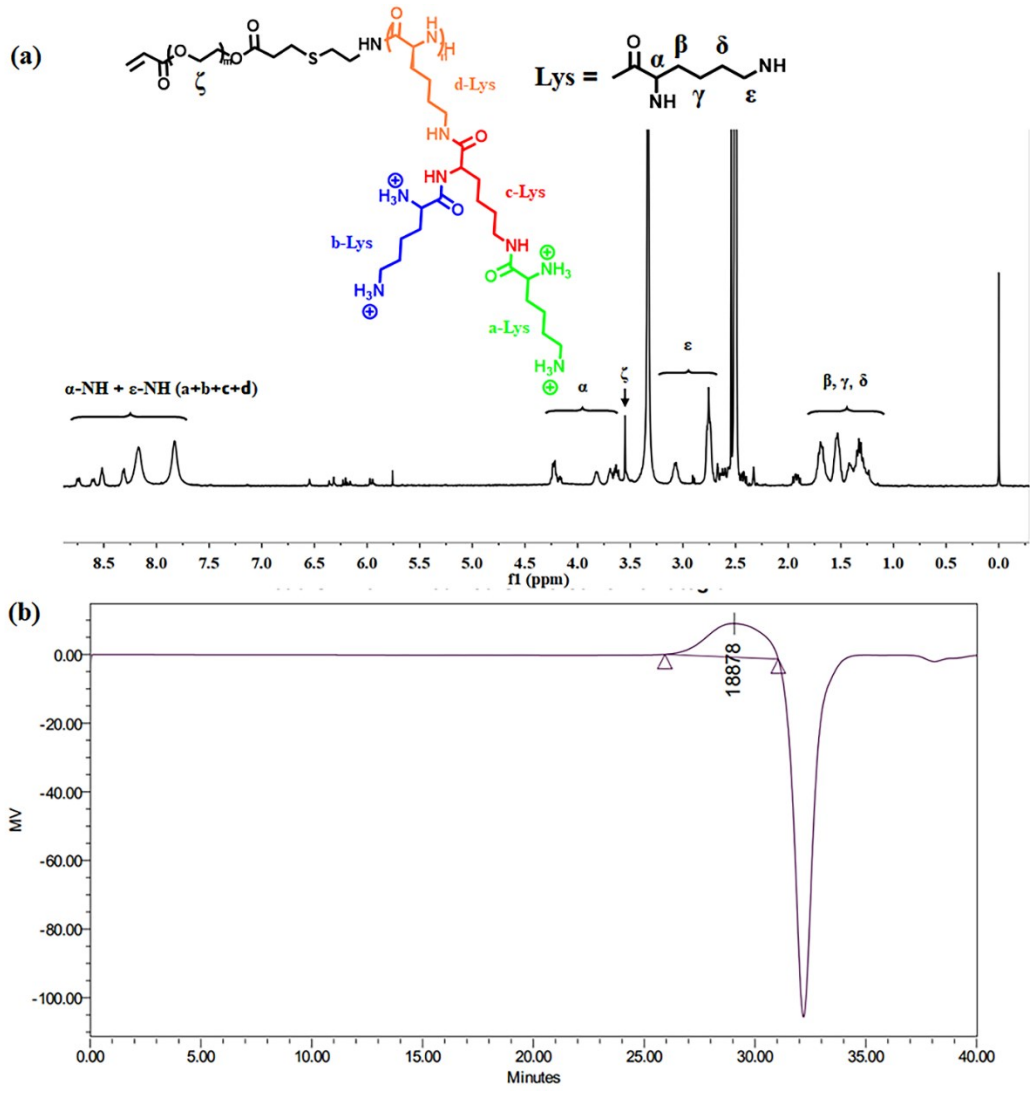

Figure S7. ^{1}H NMR spectra of compound **5** (a), GPC spectra of compound **5** (b).

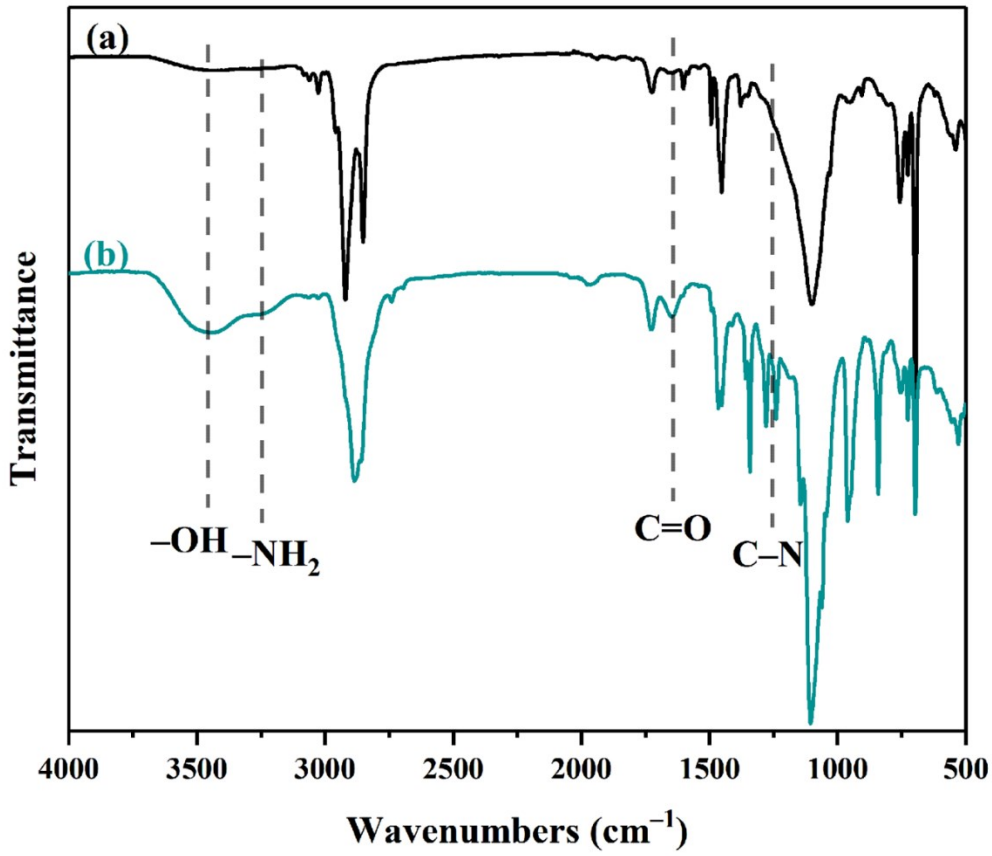

Figure S8. ATR FT-IR spectra of SEBS (a), SEBS-*g*-poly(Lys dendrimer) (b).

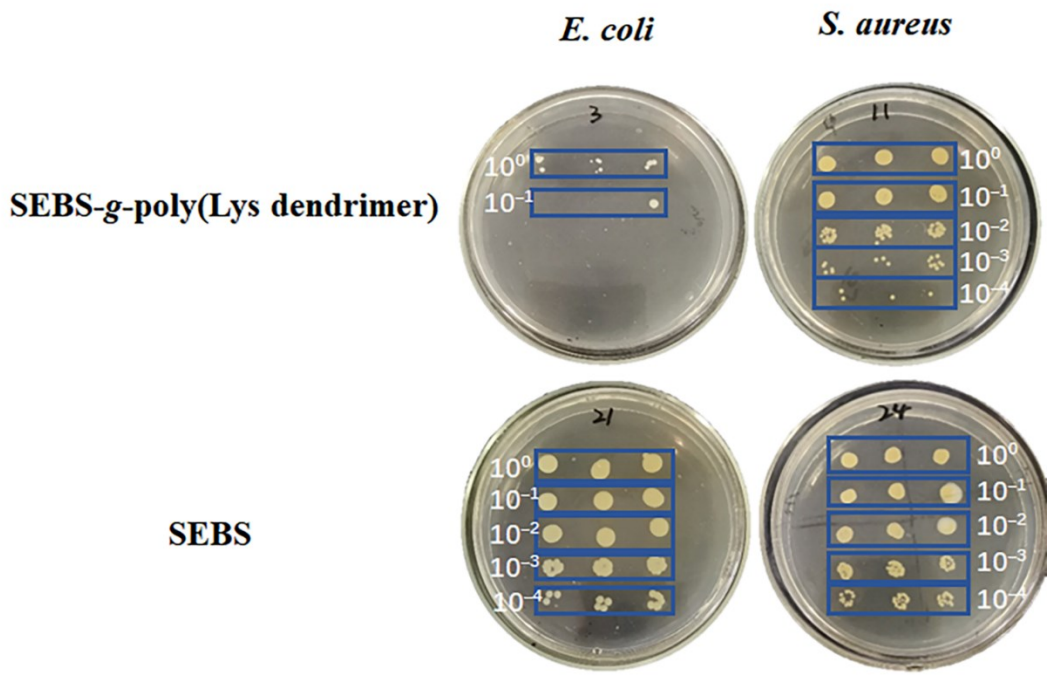

Figure S9. Photographs of agar plates for diluted bacteria suspension recovered from different samples.

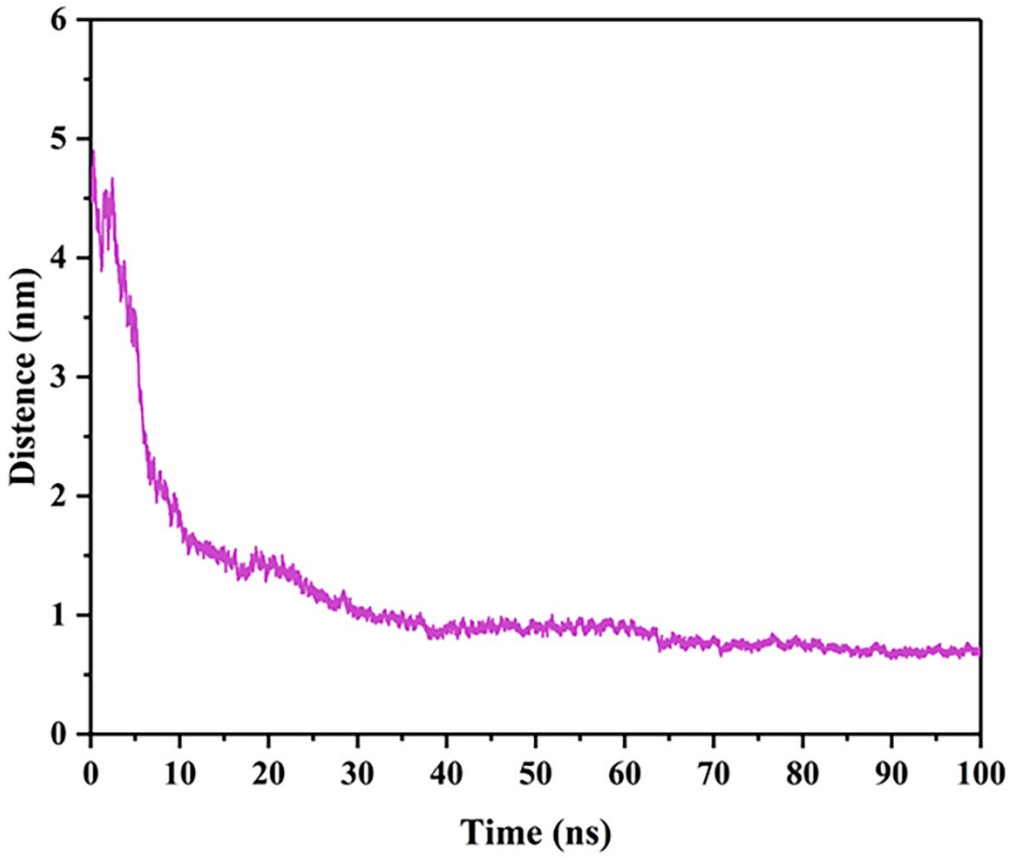

Figure S10. Distance between PEG-poly(Lys dendrimer) and the lipid bilayer.

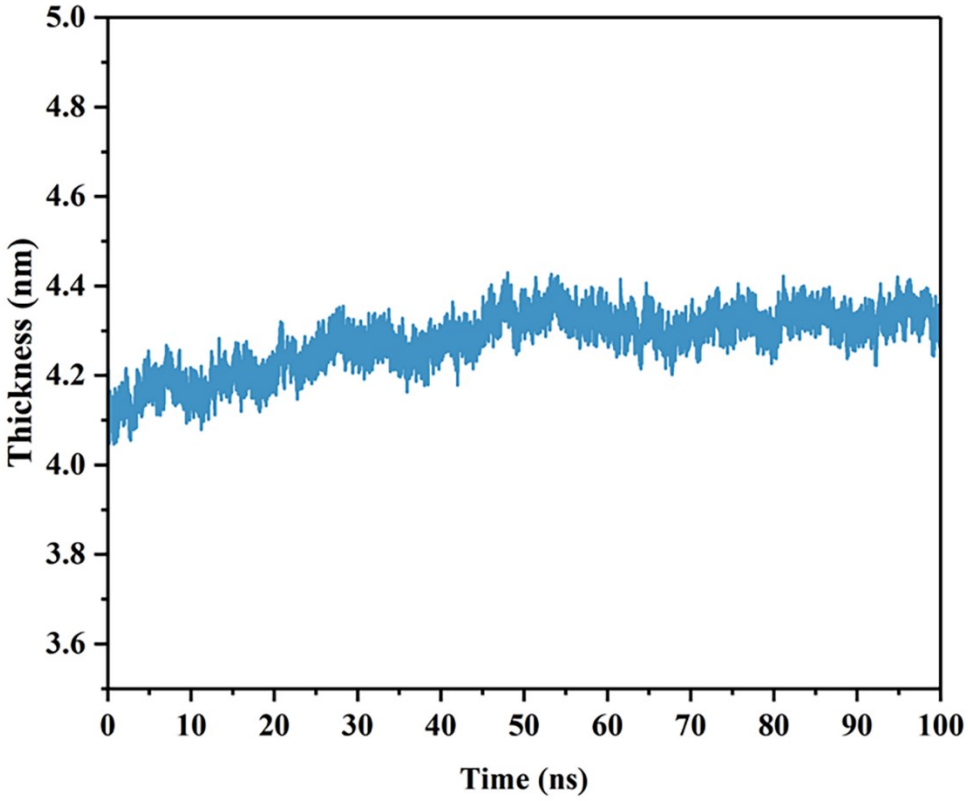

Figure S11. Thickness of the lipid bilayer.

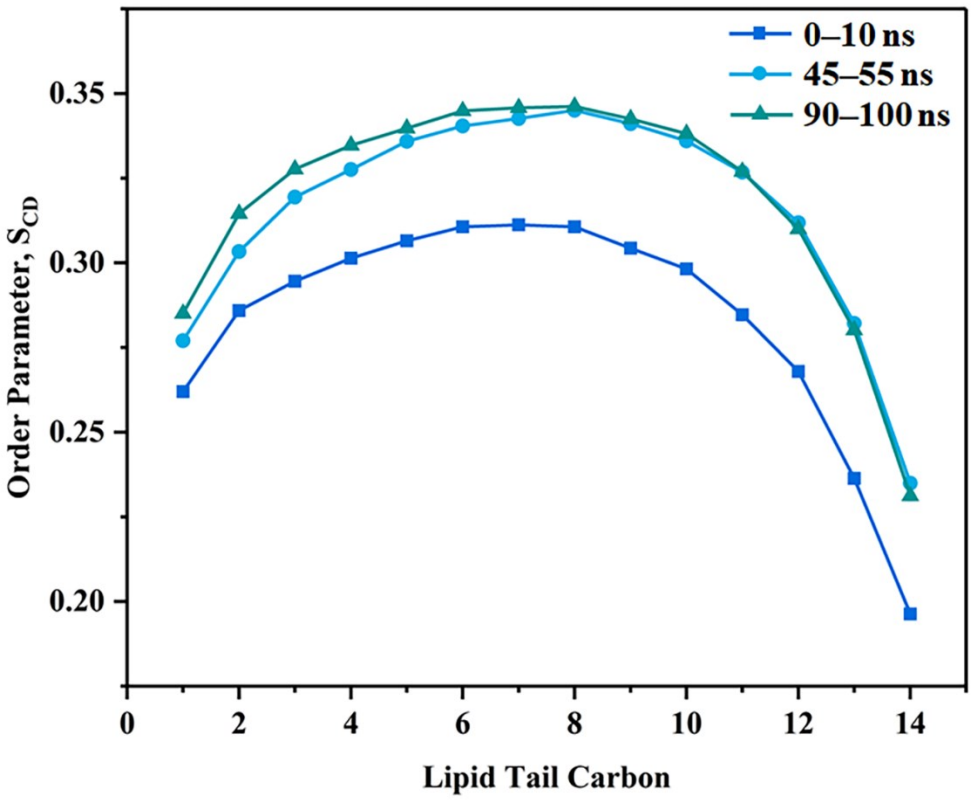

Figure S12. Deuterium order parameters S_{CD} of lipid tail groups (*sn*-1 chains).

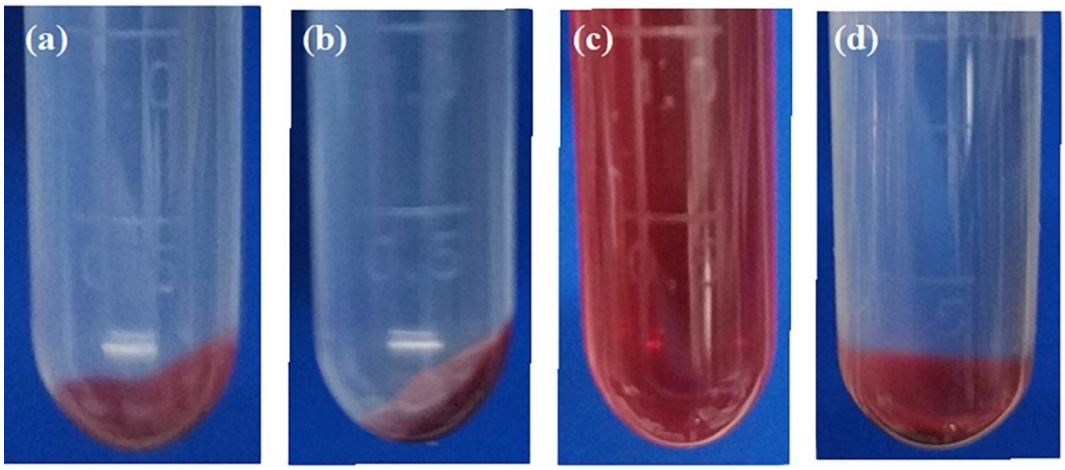

Figure S13. Photographs of centrifuged hemolysis assay samples, SEBS-*g*-ploly(Lys dendrimer) (a), SEBS (b), positive control (c), negative control (d).

Reference

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