

## Supplementary Information

### Label-free bacterial detection using polydiacetylene liposomes

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## **Synthesis of polydiacetylene liposomes**

10,12-pentacosadiynoic acid (PCDA,  $\geq 97.0\%$ , HPLC), 1,2-Bis(2-aminoethoxy)ethane (EDEA, 98%), ethylenediamine (EDA,  $\geq 99.5\%$ ), and surfactin (from *Bacillus subtilis*,  $\geq 98\%$ ) were purchased from Sigma Aldrich and used without further purification. According to previous report [S1], two types of diacetylenic monomers were synthesized. The amine-functionalized two diacetylene monomers were dissolved in chloroform at a molar concentration ratio of 1:1 for preparation of polydiacetylene liposome. After the solvent was removed using high-purity nitrogen gas, HEPES (5 mM, pH 8.0) buffer was added for making the concentration of lipid to 1 mM. After sonication of the suspension at 80 °C, the lipid aggregates were filtered. Before polymerization of diacetylenic monomers was performed, the resulting suspension was cooled at 4 °C for overnight. The monomers were then UV-irradiated (1 mW/cm<sup>2</sup>, 254 nm) for 30 s to make ene-yne alternating conjugation chains. Morphology and size of the conjugated polydiacetylene liposomes were analyzed with scanning electron microscopy (SEM, Supra55VP; Zeiss, 30 kV) and transmission electron microscopy (TEM, JEOL 2100 TEM, acceleration voltage; 200 kV).

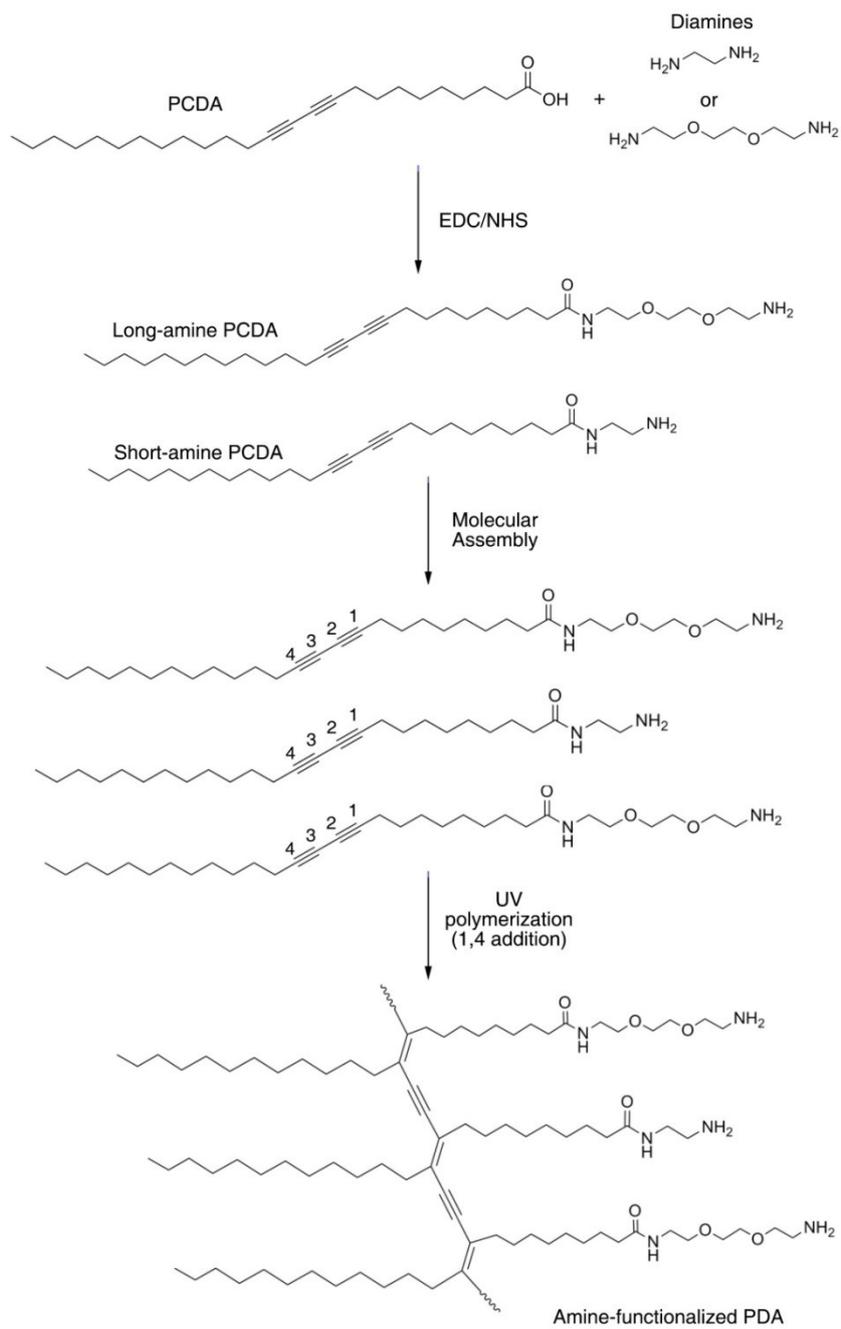
## **Chromatic changes in polydiacetylene liposomes induced by incorporating bacterial strains**

The chromatic changes in polydiacetylene liposomes were observed with optical and fluorescence microscope (Nikon Eclipse E800). The quantitative absorbance and fluorescence of the liposomes were measured using a spectrophotometer (UV/VIS Thermo Multiskan Spectrum, Vantaa) and a fluorescence microplate reader (Infinite 200pro, Tecan), respectively, at the specific time intervals after bacterial strains were incorporated. Each bacteria strains was grown on chloramphenicol (Duchefa Biochemie, C0113.0025) included LB broth agar (Merck-Millipore, #110285, #110283) plates and polydiacetylene liposomes in an incubator at 37°C.

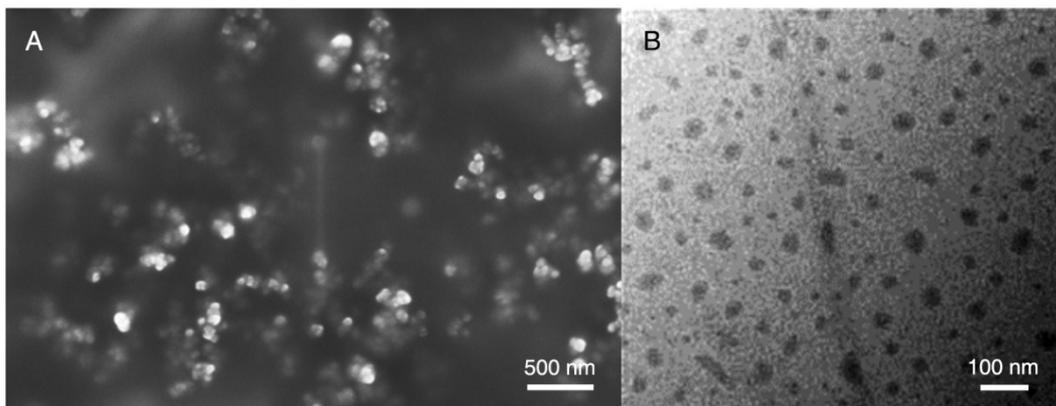
## **First-principle calculations**

All the free-energies in this work were calculated using the Perdew-Burke-Ernzerhof (PBE) functional and generalized gradient approximation (GGA) for the exchange-correlation to the density functional theory (DFT) [S2]. The projected augmented wave (PAW) method was used, as implemented in the Vienna ab initio simulation package (VASP code) [S3, S4]. Assembled structures comprised of short amine-functionalized diacetylenic

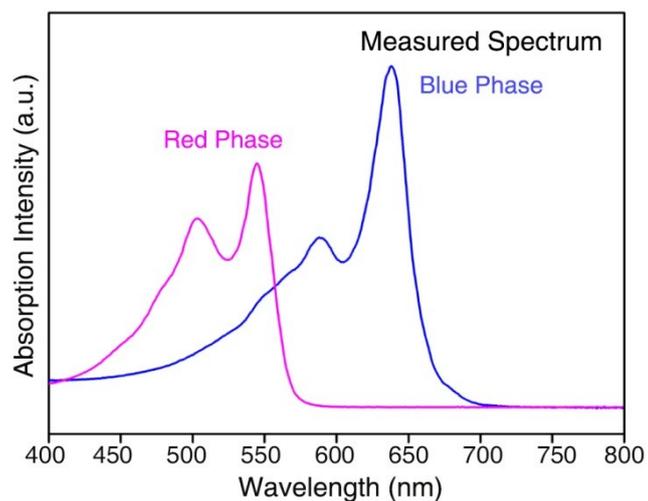
monomer (PCDA-EDA) were investigated, as simplified models of our liposomes. A 3D slab model with periodic boundary conditions was used with an energy cutoff of 500 eV, and an appropriate  $1 \times 4 \times 1$  k-points mesh with a high k-point density in the direction of the conjugated polymer chain was selected to ensure that the total energies converged within 5 meV per formula unit of PCDA-EDA. For all structures with different torsion angles between two neighboring monomers ( $0^\circ$ ,  $90^\circ$ , and  $180^\circ$ ), the residual forces on the atoms were relaxed below the force threshold of  $0.05 \text{ eV \AA}^{-1}$ . The absorption spectra of three structures were calculated from a dynamic dielectric constant obtained by the random phase approximation (RPA) [S5].



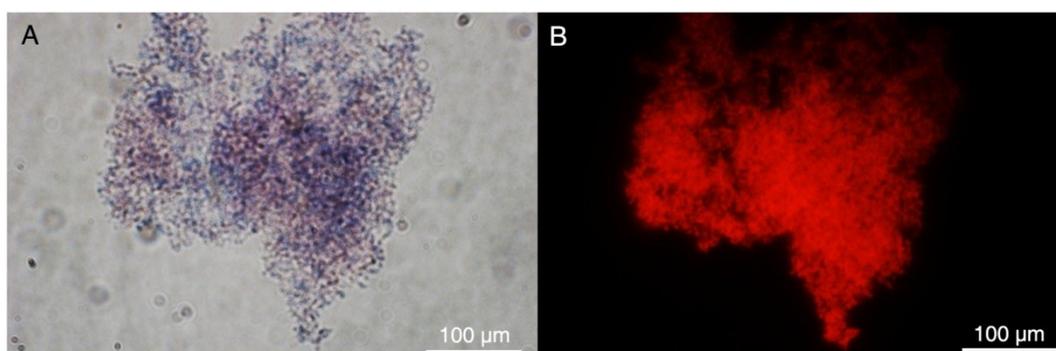
**Figure S1** Schematics for synthesis procedure of amine-functionalized PDA liposomes using two diacetylenic monomers



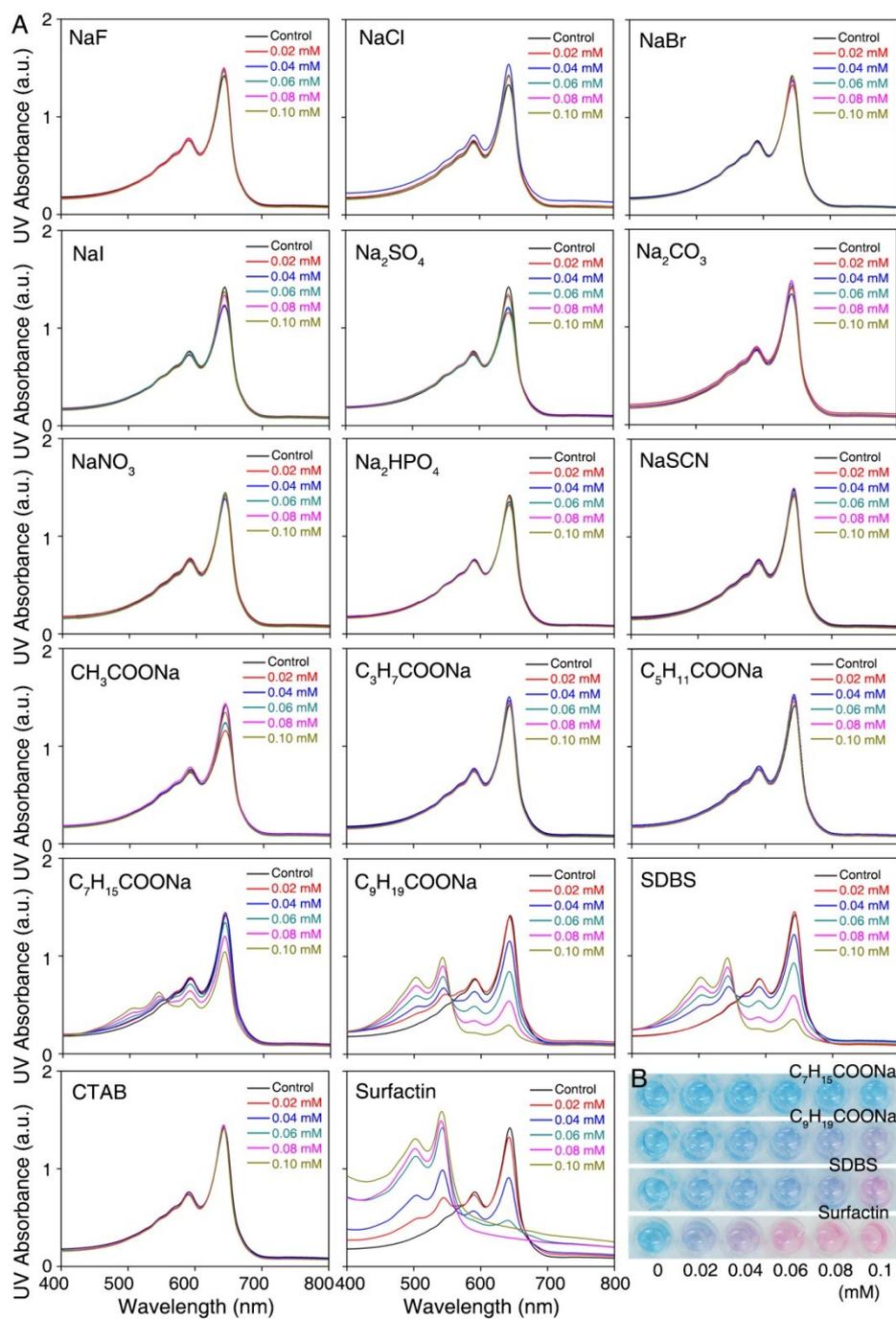
**Figure S2** SEM (a) and TEM (b) images of PDA liposomes suspended in phosphate-buffer-saline.



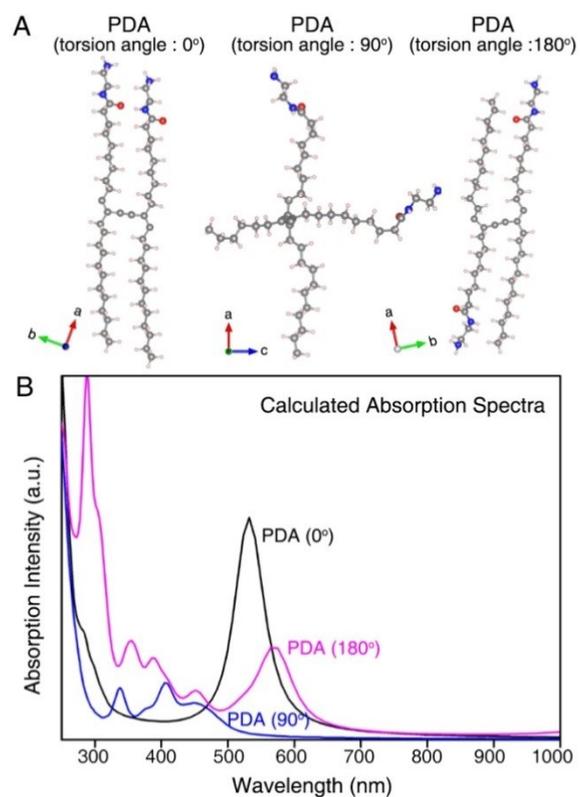
**Figure S3** Absorption spectra of PDA polymers before (blue phase) and after (red phase) incorporation of surfactin molecules.



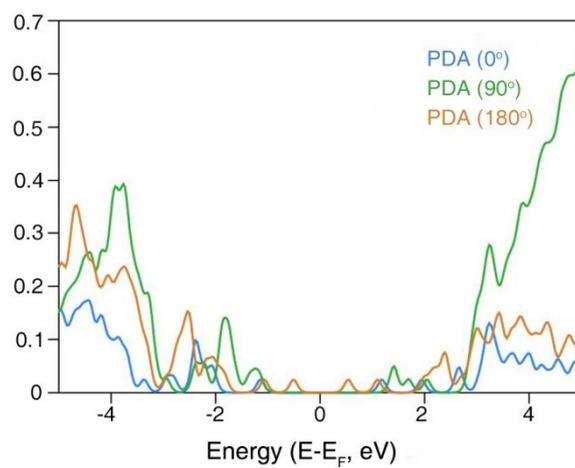
**Figure S4** Optical (a) and fluorescent (b) microscope images of PDA liposomes after incorporation of surfactin.



**Figure S5** (a) UV/Vis spectrum of 0.2mM of PDA solutions with different concentrations of the targets from 0.02 mM to 0.1 mM. (b) Representative optical images of PDA solutions after adding different concentrations of C<sub>7</sub>H<sub>15</sub>COONa, C<sub>9</sub>H<sub>19</sub>COONa, SDBS, and surfactin. The distinct colorimetric change in PDA solution after incorporating surfactin can be clearly observed.



**Figure S6** (a) Calculated chemical structures and (b) Absorption spectra of PDA polymers with various torsion angles between two neighboring amine-functionalized diacetylenic monomers. The red-green-blue axis exhibits the reference frame of each polymer, where the B-axis indicates the conjugation direction. Here, gray, pink, red, and blue balls indicated carbon, hydrogen, oxygen, and nitrogen atoms, respectively.



**Figure S7** Density of states (DOSs) of PDA structures with different torsion angle ( $0^\circ$ ,  $90^\circ$ , and  $180^\circ$ ). Relatively larger band gap was found in the PDA with torsion angle of  $90^\circ$  compared to other two groups.

## **Supplementary Movie Legend**

### **Supplementary Movie 1.**

Time-lapse images showing the fluorescent change in PDA-LB-agars after incorporation of NCIB3610 solutions.

## References

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- [S2] J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865.
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