Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.


# Supplementary Materials

## Nano-assemblies of Phosphonium-functionalized Diblock Copolymers with Fabulous Antibacterial and Relationships of Structure-Activity

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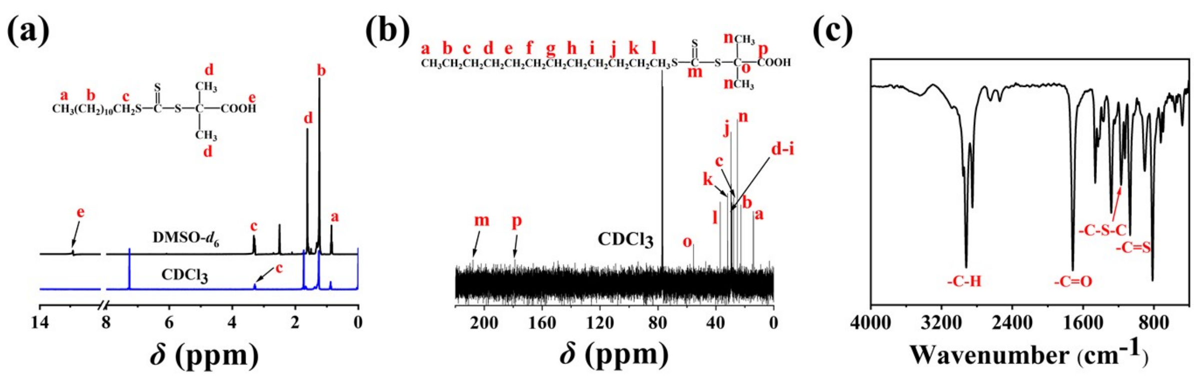


**Figure S1.** $^{1}$H (a) and $^{13}$C (b) NMR and FTIR (c) spectra of DCMAT.

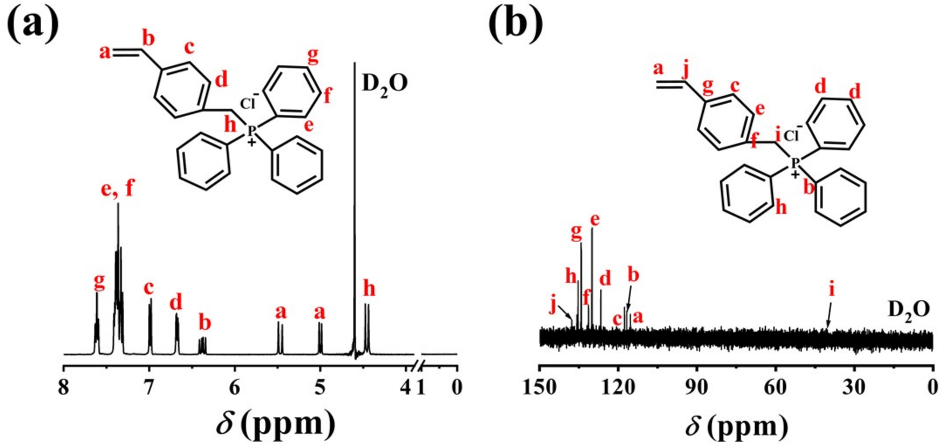


**Figure S2.** $^{1}$H (a) and $^{13}$C (b) NMR spectrum of $QPSPh_3IL$**.**

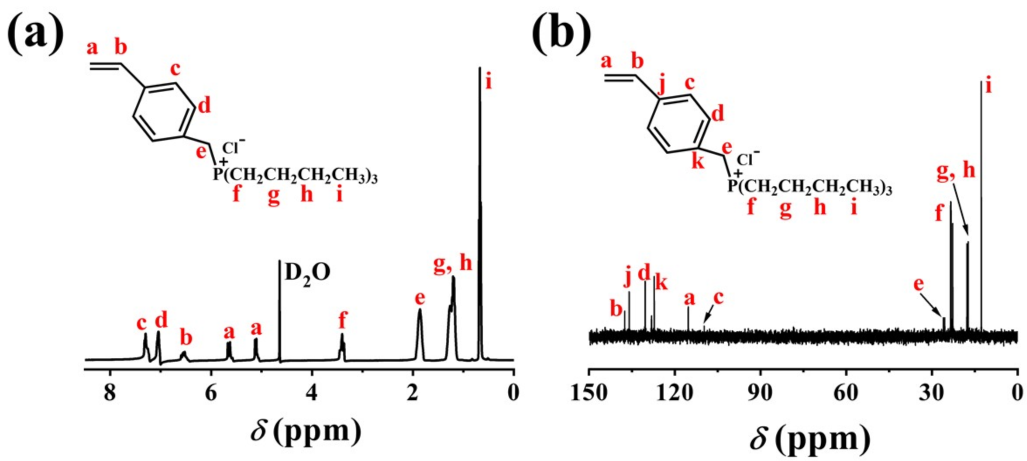


**Figure S3.** $^{1}$H (a) and $^{13}$C (b) NMR spectrum of $QPSBu_3IL$**.**

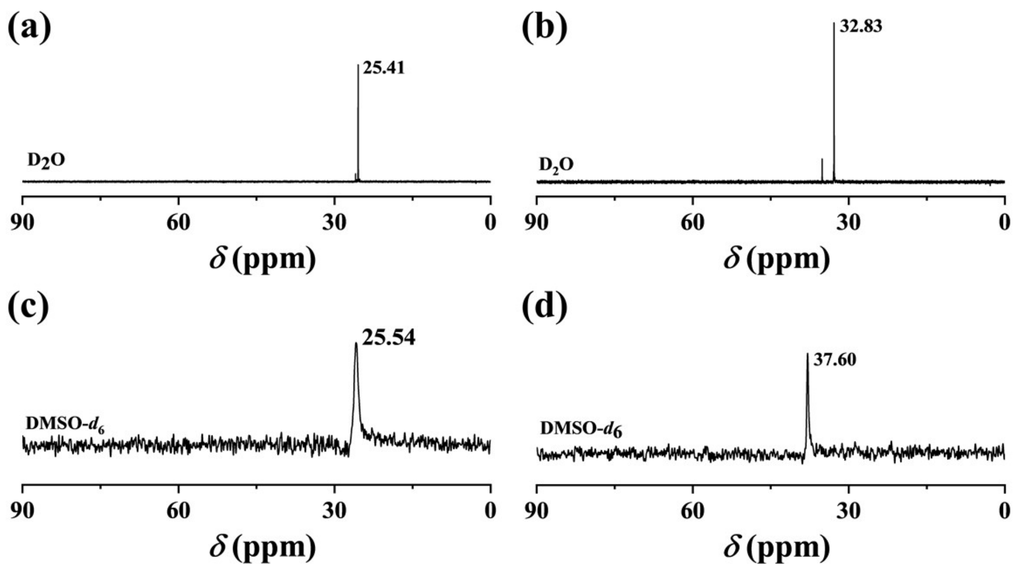


**Figure S4**. $^{31}P$ NMR spectra of $Bu_{60}$ (a), $Ph_{60}$ (b), $Bu_{60}St_{120}$-M (c) and $Ph_{60}St_{120}$-M (d).

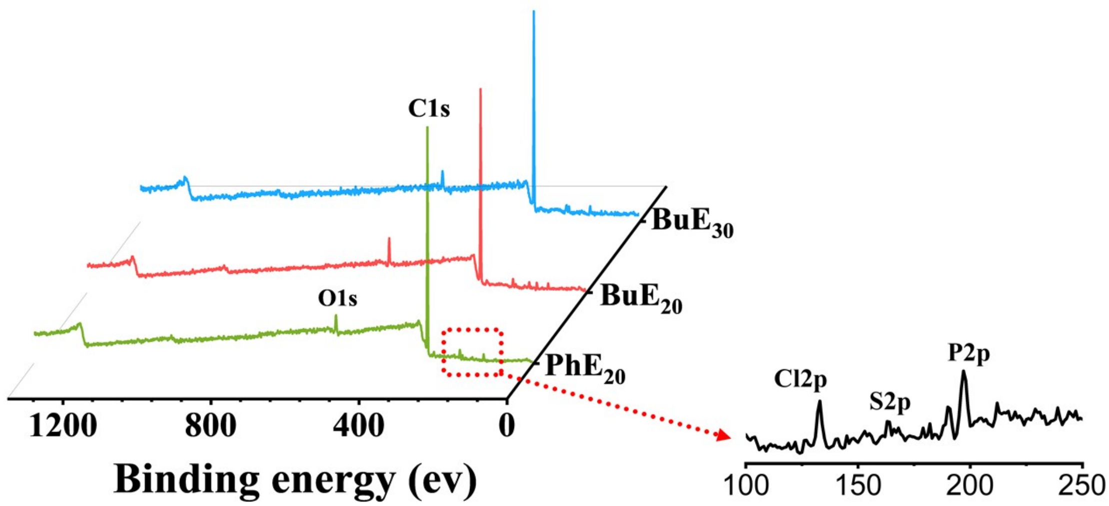


**Figure S5.** XPS analysis for $PhE_{20}$, $BuE_{20}$, and $BuE_{30}$ samples to identify the existence of carbon, oxygen, phosphorus, chlorine, and sulfur element.

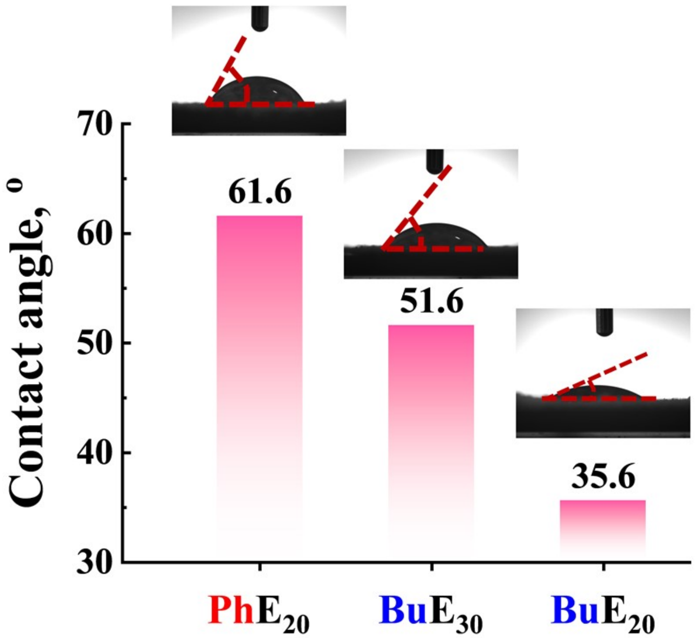


**Figure S6.** The contact angle of several PEGDMA crosslinked PFDCs.

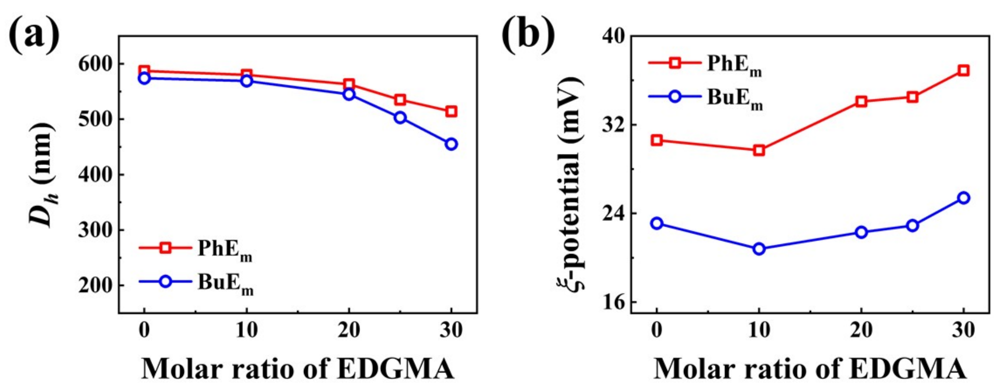


**Figure S7.** The molar ratio of EDGMA dependence of particle size ($D_h$, nm) (a) and $\xi$-potential (mV) (b).


**Figure S8.** Tyndall effect of $Bu_{60}St_y$ and $Ph_{60}St_y$ PFDCs in either methanol or 1,4-dioxane solvent.

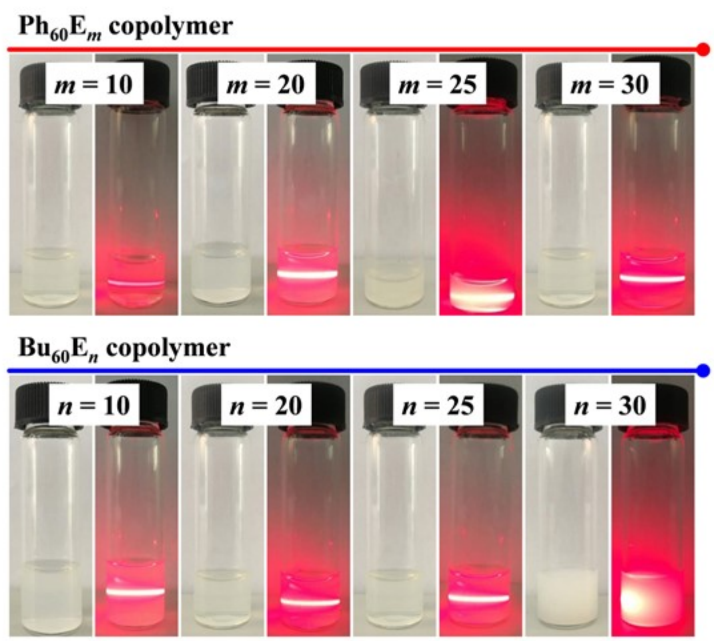


**Figure S9.** Tyndall effect of PEGDMA crosslinked PFDCs in methanol solution.

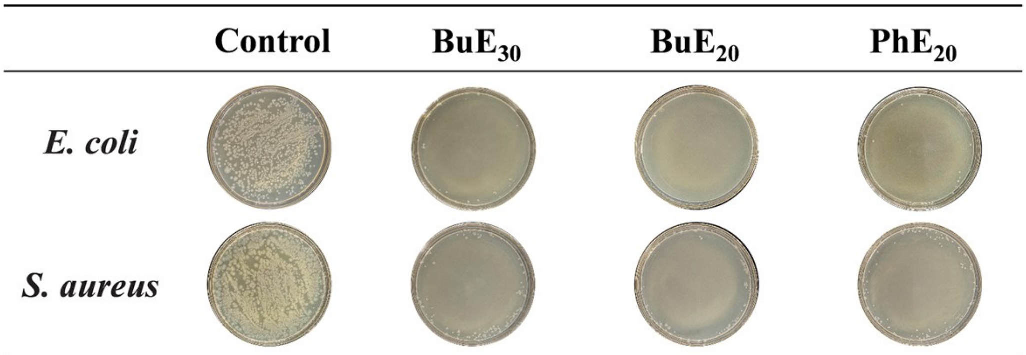


**Figure S10.** Photographs of the culture plates for *E. coli* and *S. aureus* after exposure to $PhE_{20}$, $BuE_{20}$, and $BuE_{30}$.

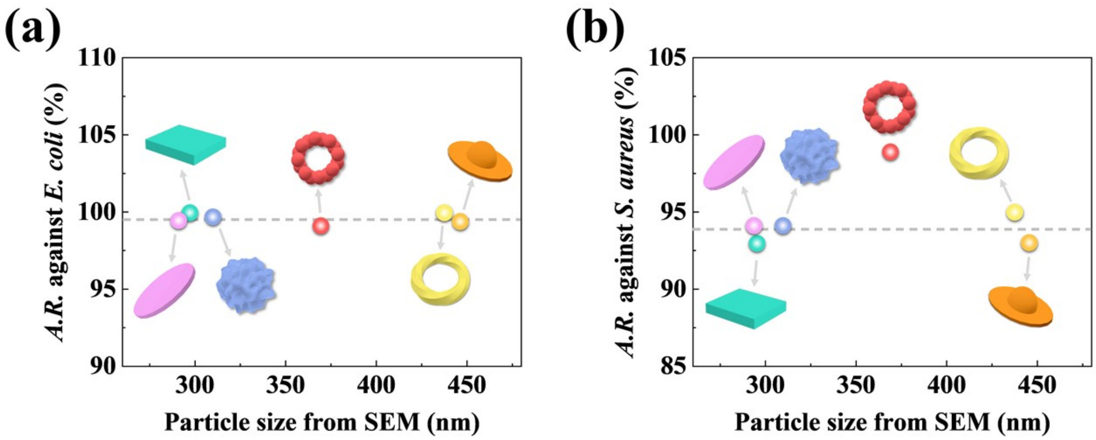


**Figure S11.** Antibacterial activity against *E. coli* (a) and *S. aureus* (b) of the PFDCs with special morphology. The diameter was obtained from the SEM result.

**Table S1.** Summary of molecular weight and conversion rate for all non-crosslinked PFDC diblock copolymers.

| Synthesis Media | Block Copolymer [a] | Targeted DP for St | Time (h) | *Conv.* (%) [b] | $M_{n,th}$ (g·mol$^{-1}$) [c] | $M_{n,APC}$ (g·mol$^{-1}$) | *Đ* |
|---|---|---|---|---|---|---|---|
| Methanol | $Bu_{60}St_{700}$-M | 700 | 16 | 97.6% | 94567 | 85644 | 1.25 |
| | $Bu_{60}St_{200}$-M | 200 | 16 | 97.5% | 42492 | 40818 | 1.17 |
| | $Bu_{60}St_{120}$-M | 120 | 16 | 97.8% | 34160 | 36452 | 1.16 |
| | $Bu_{60}St_{30}$-M | 30 | 16 | 96.9% | 24786 | 24223 | 1.12 |
| | $Ph_{60}St_{700}$-M | 700 | 18 | 98.6% | 98163 | 84184 | 1.25 |
| | $Ph_{60}St_{200}$-M | 200 | 18 | 98.5% | 46089 | 45574 | 1.10 |
| | $Ph_{60}St_{120}$-M | 120 | 17 | 96.8% | 37757 | 35274 | 1.13 |
| | $Ph_{60}St_{30}$-M | 30 | 16 | 95.1% | 28384 | 27666 | 1.12 |
| 1,4-Dioxane | $Bu_{60}St_{700}$-D | 700 | 18 | 98.8% | 94567 | 92742 | 1.21 |
| | $Bu_{60}St_{200}$-D | 200 | 15 | 97.0% | 42492 | 41453 | 1.14 |
| | $Bu_{60}St_{120}$-D | 120 | 16 | 97.2% | 34160 | 39280 | 1.13 |
| | $Bu_{60}St_{30}$-D | 30 | 17 | 96.7% | 24786 | 23217 | 1.12 |
| | $Ph_{60}St_{700}$-D | 700 | 17 | 98.0% | 98163 | 43580 | 1.24 |
| | $Ph_{60}St_{200}$-D | 200 | 18 | 98.0% | 46089 | 43070 | 1.24 |
| | $Ph_{60}St_{120}$-D | 120 | 17 | 97.2% | 37757 | 35685 | 1.16 |
| | $Ph_{60}St_{30}$-D | 30 | 18 | 98.8% | 28384 | 26090 | 1.15 |

[a] D: 1,4-dioxane; M: methanol.

[b] Determined by $^{1}$H NMR analysis.

[c] Theoretical number-average molecular weight was calculated by: $M_{n,th} = Conv. \times ([N_{\mathrm{monomer}}/N_{\mathrm{CTA}}]) \times M_{\mathrm{monomer}} + M_{\mathrm{n,macro\text{-}}CTA}$.

[d] *Đ* value was calculated by: $Đ = M_w/M_{n,APC}$.

**Table S2.** Particle properties of PEGDMA crosslinked PFDCs with different substrate ratios measured by DLS.

| **Sample** [a] | ***n*(Bu$_{60}$/Ph$_{60}$): *n*(EGDMA)** | **$D_h$ (nm)** [b] | **PDI** [c] | **ξ-potential (mV)** |
|---|---|---|---|---|
| Bu$_{60}$ | 1 : 0 | 574 | 0.108 | 23.1 |
| Ph$_{60}$ | 1 : 0 | 587 | 0.262 | 30.6 |
| BuE$_{10}$ | 1 : 10 | 569 | 0.124 | 20.8 |
| BuE$_{20}$ | 1 : 20 | 545 | 0.136 | 22.3 |
| BuE$_{25}$ | 1 : 25 | 503 | 0.202 | 22.9 |
| BuE$_{30}$ | 1 : 30 | 455 | 0.230 | 25.4 |
| PhE$_{10}$ | 1 : 10 | 580 | 0.256 | 29.7 |
| PhE$_{20}$ | 1 : 20 | 563 | 0.251 | 34.1 |
| PhE$_{25}$ | 1 : 25 | 535 | 0.247 | 34.5 |
| PhE$_{30}$ | 1 : 30 | 514 | 0.205 | 36.9 |

[a] Measured in methanol.

[b] Average hydrodynamic diameter of the resultant nanoparticles.

[c] Polydispersity index obtained from the accessory software.