Supporting Information

Multiple types of hydroxyl-rich cationic derivatives of PGMA for broad-spectrum antibacterial and antifouling coatings

Huimin Yuan,[a,b,c,#] Bingran Yu,[a,b,c,#] Li-Hai Fan,[d] Meng Wang,[d] Yiwen Zhu,[a,b,c] Xiaokang Ding,[a,b,c,*] and Fu-Jian Xu[a,b,c*]

[a]State Key Laboratory of Chemical Resource Engineering, Beijing University of Chemical Technology, Beijing 100029 China
[b]Key Laboratory of Carbon Fiber and Functional Polymers (Beijing University of Chemical Technology), Ministry of Education, Beijing 100029 China
[c]Beijing Laboratory of Biomedical Materials, Beijing Advanced Innovation Center for Soft Matter Science and Engineering, Beijing University of Chemical Technology, Beijing 100029 China
[d]College of Life Science and Technology, Beijing University of Chemical technology, Beijing 100029 China

[#]Both authors contributed equally to this work.
*Corresponding authors
E-mail address: xufj@mail.buct.edu.cn (F.J.X); dingxk@mail.buct.edu.cn (X.D.)

1. Molar ratio of DED and ED components in PGED-DED

The molar ratio of DED and ED components in PGED-DED is determined by using the areas of peaks (d, e) and (f, e', f' and f'') as shown in Fig. 1. For example, the peak area ratio of peaks (d, e) and (f, e', f' and f'') is 3.00/8.82. Let the molar fractions of DED and ED components in PGED-DED are x and y, respectively, the x and y can be calculated from Eq. S1 and Eq. S2:

$$x + y = 1 \quad \text{(Eq. S1)}$$

$$(2x + 2y + x + y)/(4x + 4y + 2x + 2y + 6x) = 3.00/8.82 \quad \text{(Eq. S2)}$$

As the solutions of the equations are x=0.47 and y=0.53, the molar ratio of the DED and ED components can be round up to 1:1.

2. Molar ratio of quaternary ammoniums (QAs) and tertiary amine groups in the quaternized polymers

Similarly, the molar ratio of QAs and tertiary amine groups in polymers can be calculated form their ^{1}H NMR spectra as shown in Fig. S1. For QPGDED-C_6H_{13}, the peak area ratio of peaks (3, 4) and (1, 2, 10-14) is 3.00/16.32. Let the molar fractions of QAs and tertiary amine components are x_1 and y_1, which can be calculated from Eq. S3 and Eq. S4:

$$x_1 + y_1 = 1 \quad \text{(Eq. S3)}$$

$$(3x_1 + 3y_1)/(2x_1 + 2y_1 + 3x_1 + 3y_1 + 11x_1) = 3.00/16.32 \quad \text{(Eq. S4)}$$

The solutions of the equations are x_1=1.03 and y_1=-0.03, indicating that all of tertiary amine groups of QPGDED-C_6H_{13} are quaternized.

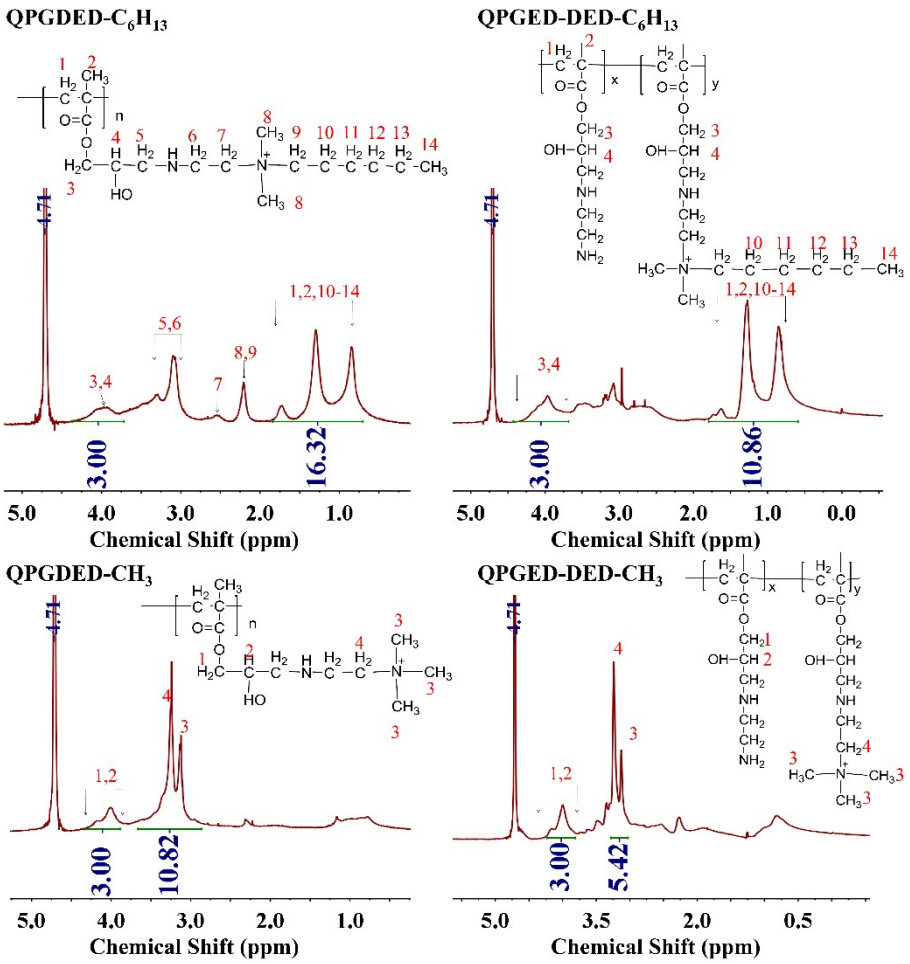

Fig. S1 ^{1}H NMR spectra of the QPGDED-C_6H_{13}, QPGDED-CH_3, QPGED-DED-C_6H_{13} and QPGED-DED-CH_3.

For QPGDED-CH_3, the area ratio of peaks (1, 2) and (3, 4) is 3.00/10.82. Let the molar fractions of QAs and tertiary amine components are x_2 and y_2, which can be calculated from Eq. S5 and Eq. S6:

$$x_2 + y_2 = 1 \quad \text{(Eq. S5)}$$

$$(3x_2 + 3y_2)/(2x_2 + 9x_2) = 3.00/10.82 \quad \text{(Eq. S6)}$$

The solutions of the equations are x_2=0.98 and y_2=0.02, indicating that 98% of

tertiary amine groups in QPGDED-CH_3 are converted to QAs.

The fractions of QAs in QPGED-DED-C_6H_{13} and QPGED-DED-CH_3 are determined to be 52.4% and 49.3% in a similar method. Since the molar ratio of DED and ED components in PGED-DED is approximately 1:1, we conclude that nearly all tertiary amine groups are converted to QAs.

3. X-ray photoelectron spectroscopy (XPS) characterization

The surfaces of glass slides decorated with PDA (**0**), QPGED-DED-C_6H_{13} (**1**), QPGED-DED-CH_3 (**2**), PGED-Ag (**3**), QPGED-DED-C_6H_{13}-Ag (**4**) and QPGED-DED-CH_3-Ag (**5**) were characterized by using XPS (Kratos AXIS HSi) equipped with a monochromatized Al Ka X-ray source (1486.6 eV photons).

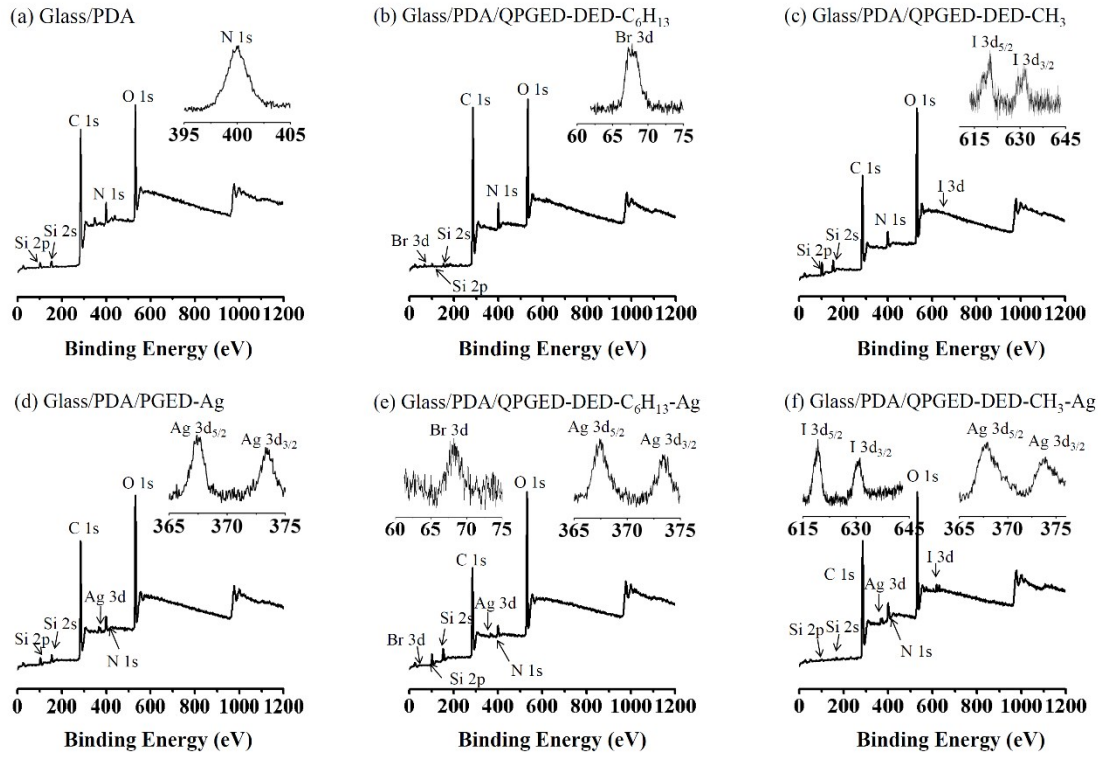

Fig. S2 Typical XPS wide-scan spectra of glasses coated with different materials.

In Fig. S2a, the binding energy peak of C 1s (284 eV) and N 1s (399 eV) indicates the formation of PDA film on glass slide surface due to the self-

polymerization of dopamine.[S1] Fig. S2b and S2c show the binding energy peak of Br 3d (69 eV) and I 3d5/2 (619 eV), I 3d3/2 (630 eV) respectively, due to the formation of quaternary ammonium salts. Fig. S2d-f show that the binding energy of Ag 3d5/2(368 eV) and Ag 3d3/2 (374 eV) appears after the cationic polymers are loaded with Ag. The XPS results qualitatively confirm that the antibacterial polymers are successfully grafted onto glass slides.

References

(S1) S. Hong, Y. S. Na, S. Choi, I. T. Song, W. Y. Kim, H. Lee, *Adv. Funct. Mater.* 2012, *22*, 4711-4717.