UV Absorption Enhanced Polydopamine Coating

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Materials and experiments.

Dopamine hydrochloride (98%), tetrabutylammonium hexafluorophosphate (Bu_4NPF_6) (99%), and ferrocene (99.5%) were all purchased from J&K Scientific Ltd. (Beijing, China). 1H-imidazo[4,5-b]pyridine-2(3H)-thione (HIPT, 99%) was purchased from Bide Pharmatech Co., Ltd. 2-Mercapto-5-methoxyimidazole[4,5-b]pyridine (MMDP, 99%), 5-Methoxy-2-mercaptobenzimidazole (MOBI, 99%) and Rhodamine B (RhB, 99%) were purchased from Energy Chemical (Shanghai, China). Ammonia aqueous solution (25-28 wt %), Sodium chloride (NaCl, 99%), ethanol (anhydrous, 99%) and acetonitrile (99%) were purchased from Kelong Chemical (Chengdu, China). All plastic substrates were purchased from shangjiu. Rubber & Plastic Company (Shanghai, China). All chemical reagents were used directly without further purification.

Fabrication of PDA-i (i=1 to 26) coatings.

Taking PDA-1 for example, dopamine monomer (5 mg, 0.026 mmol) and HIPT (10 mg, 0.066 mmol) were added to a mixed solvent of ethanol (2 mL) and Tris-HCl buffer (6 mL) with a concentration of 200 mM, pH=8.5. After shaking for 10 minutes in a shaker at a temperature of 25 °C, a polycarbonate (PC) substrate measuring 1 mm x 10 mm x 30 mm was placed to the above system. Then the system was shaken in the shaker at 25 ℃ for 24 h. After that, the above PC plate was rinsed three times with ethanol and water respectively, and then soaked in a solution of water and ethanol (3:1) for 24 h, and the solution was changed every 6 hours. Finally, the coating was gently dried with a hair dryer and named PDA-1 for later use. PDA-i (i=0 and 2-26) was prepared using a similar method, and the detailed reaction conditions were presented in **Table S1b**.

Theoretical calculations.

The energy levels of the molecular orbits were obtained using density functional theory (DFT) by Gaussian 09 software. The molecular orbits of probable intermediates were outputted at the B3LYP/6-31G* level with solvation model density (SMD). Moreover, the ESPs were calculated by Multiwfn (Multiwfn 3.7), and the images of ESP were obtained through VMD (1.9.3). The coordinates of the model structure after optimization were shown in **Table S2**.

Post-modification of PDA coatings.

Take PM-14 for example, MMDP (8 mg, 0.044 mmol) was added to a mixed solvent of ethanol (2 mL) and Tris-HCl buffer (6 mL) with a concentration of 200 mM, pH=8.5. After shaking for 10 minutes in a shaker at a temperature of 25 °C, the PC plate coated with PDA-14 was placed into the above system. Then the mixture was still shaken in the shaker at 25 ℃ for 24 h. After that, the above PC plate was rinsed three times with ethanol and water respectively, and then soaked in a solution of water and ethanol (3:1) for 24 h, and the solution was changed every 6 hours. Finally, the post-modified PDA coating was gently dried with a hair dryer and named PM-14 for later use. PM-i (15-26) were prepared using a similar method, and the detailed reaction conditions were presented in **Table S1c**.

The efficiency of protecting Rhodamine B from UV photocatalytic degradation

The UV degradation protection experiment of rhodamine B was completed according to the previously reported procedures[1]. Typically, 5 mg of titanium dioxide was first added to a vial containing 10 mL of 1×10^{-5} M RhB aqueous solution, and stirred for

half an hour in the dark. The mouth of the vial was covered with naked PC plate, PDA (PDA-0) coated PC plate and P(DA-MMDP) (PDA-1) coated PC plate before irradiating it with UV rays. Then a UV phototherapy instrument (312 nm) was applied to study their protection efficiency. Note that the height from the lamp tube to the bottle mouth was 5 cm. At regular intervals (t), 1 mL of the solution in the vial was taken out and centrifuged to remove the titanium dioxide. Then ultraviolet-visible (UV-Vis) spectrophotometer was used to measure the absorption of the RhB solution at 552 nm. The UV protection efficiency could be obtained through equation $I=A_t / A_0 \times 100\%$, where A_0 is the absorption of the RhB solution without exposed to UV light, A_t is the absorption of the RhB solution irradiated by UV light for t minutes.

UV protection efficiency

The naked PC plates, PDA (PDA-0) coated PC plates and P(DA-MMDP) (PDA-1) coated PC plates were exposed to UV light (UV phototherapy instrument, 312 nm) for four hours, and these samples were then tested for mechanical properties, UV absorption and thermal stability before and after exposure to UV light. Note that the height from the lamp tube to the plates was 5 cm.

Fabrication of PDA and P(DA-MMDP) coated fabrics

Dopamine hydrochloride (16 mg, 0.084 mmol) was dissolved in a mixed solvent of ethanol (2 mL) and Tris-HCl buffer (6 mL) with a concentration of 200 mM, pH=8.5. After shaking for 10 minutes in a shaker at a temperature of 25 °C, a piece of non-woven fabric with a diameter of 2.5 cm was added to the above solution. Then the mixture was still shaken in the shaker at 25 °C for 24 h. After that, the above fabric was

rinsed three times with ethanol and water respectively, and then soaked in a mixed solution of water and ethanol (3:1) for 24 h, and the solution was changed every 6 hours. Finally, the fabric was gently dried with a hair dryer and named Fabric-1 for later use. P(DA-MMDP) coated fabric (Fabric-2) was prepared by the same method, except that MMDP (16 mg, 0.088 mmol) was additionally added to the above reaction system.

Hydroxyl radicals generated from UV-light illuminated fabrics

Naked fabric (Fabric-0), PDA coated fabric (Fabric-1) and P(DA-MMDP) coated fabric (Fabric-2) were added into freshly prepared terephthalic acid, disodium salt solution (6 mL, 3 mM). Then these mixed systems were illuminated by a UV phototherapy instrument (312 nm) at a distance of 5 cm for 3 h. Took 1 mL of the solution from the above system every one hour to measure its fluorescence intensity. Fluorescence intensities (Em 425 nm) from the generated hydroxylterephthalate (HTA) were measured while excitation wavelength was set at 315 nm. The generation of hydroxyl free radical of terephthalic acid, disodium salt solution (water) under UV-light illumination was also measured. Moreover, the generation of hydroxyl free radical of Fabric-0, Fabric-1 and Fabric-2 in dark also examined as control.

Stability testing of hydroxyl radicals generated from UV-light illuminated Fabric-2

Fabric-2 were added into freshly prepared terephthalic acid, disodium salt solution (6 mL, 3 mM). Then these mixed systems were illuminated by a UV phototherapy instrument (312 nm) at a distance of 5 cm for 1 h. 1 mL of the solution from the above system was taken to measure its fluorescence intensity after illumination. The above procedure was repeated five times, and the fluorescence intensity after each irradiation

was measured. The efficiency of generating hydroxyl radicals during each UV irradiation of Fabric-2 could be obtained through equation $E=I_t / I_1 \times 100\%$, where I_1 was the value of the fluorescence intensity after the first irradiation, and I_t is the value of the fluorescence intensity after the t-th irradiation.

Antibacterial activity of fabrics

Escherichia coli (*E.coli*) was dispersed in a sterile liquid medium and incubated in an incubator at 37 °C for overnight (18-24 h). The bacteria were detected by spectrophotometer (Thermo Fisher) prior to use to ensure that bacteria were in logarithmic growth phase (approximately 1×10^8 CFU/mL). Then the cultures of the mid exponential-phase bacterium were diluted with phosphate buffered saline (PBS) to approximately 10^5 CFU/mL for later use.

Fabric-0, Fabric-1 and Fabric-2 were placed in 6-well plate and inoculated with 100 μL of diluted bacterial suspension, respectively. All samples were exposed to UV light (UV phototherapy instrument, 312 nm) for different time (10 min, 20 min and 30 min). It is worth noting that lamp tube to the fabrics was 15 cm. Meanwhile, another set of samples was covered and stored in dark environment for the same duration. Afterward, the fabrics were soaked in 10 mL of sterilized PBS solution, and then the mixture was shaken vigorously for 1 min. An aliquot of 0.1 mL of the mixture solution was taken out and diluted 10-fold and then placed on an agar plate and incubated at 37 °C for 18 h. Finally, 0.1 mL of solution was taken from the bacterial stock solution (10^5 CFU/mL) and diluted 1000-fold and then placed on an agar plate and incubated at 37 °C for 18 h as control sample. The reduction rate of bacteria was calculated based on the numbers

of colony forming units on agar plate according to equation 1:

Reduction of bacteria (%) = (B − A) / B × 100% (1)

where B is the number of colonies forming units of control, and A is the number of colonies forming units of light exposed samples and dark samples.

UV photocatalytic dye degradation by fabrics

Fabric-0, Fabric-1 and Fabric-2 were added into freshly prepared 1×10^{-5} M RhB aqueous solution. Let the above system stand in the dark for half an hour. Then a UV phototherapy instrument (312 nm) was applied to study their photocatalytic degradation efficiency. Note that the height from the lamp tube to the bottle mouth was 5 cm. t minutes after irradiation, 0.5 mL of the solution in the well plate was taken out. Then UV-Vis spectrophotometer was used to measure the absorption of the RhB solution at 552 nm. The UV photocatalytic degradation efficiency could be obtained through equation $I=(1-A_t / A_0) \times 100\%$，where A_0 is the absorption of the RhB solution without exposed to UV light, A_t is the absorption of the RhB solution irradiated by UV light for t minutes. In addition, the dye degradation of the above system in the dark was also examined as a control.

Cytocompatibility investigation

NIH-3T3 fibroblasts were cultured at 37 °C in a 5% CO_2 atmosphere in Dulbecco's Modified Eagle's Medium prepared with 10% fetal bovine serum and 1% penicillin-streptomycin. The cell viability of each group was detected by MTT assay. Briefly, cells were incubated in 12-well plates at a density of 20,000 cells per well for 12 h and treated with Fabric-2 for 30 min under UV311 irradiation (Fabric-2@UV). As a control,

Fabric-2 was exposed directly to the cells for 30 minutes (Fabric-2). Likewise, cells not contact to Fabric-2 were irradiated with UV311 for 30 min (UV). Note that viability of untreated cells was detected by MTT assay too. Additionally, NIH-3T3 cells were incubated in 12-well plates at a density of 20,000 cells per well for 12 hours. The same treatment as above was then performed and live/dead staining was recorded using an inverted fluorescence microscope to confirm NIH 3T3 cell viability and morphology.

In Vivo Antimicrobial Wound Healing

A mouse wound model was established and processed to evaluate the antibacterial and wound repair effects of Fabric-2 under ultraviolet irradiation. All studies with these animals followed the Animal Ethics Standards (no. 2020064A; WCHSIRB-D-2017-263) of the Animal Ethics Committee of West China Hospital of Sichuan University, Chengdu, China. All animals used in this study were from Dashuo Experimental Animal Co., Ltd. (Chengdu, China). Twenty male Kunming mice (6-8 weeks; 28-32 g, 5 per group) with circular wounds (~40 mm^2) were randomly divided into 4 groups. After the wounds of each group were infected with 100 μL *E. coli* suspension (~1×10^8 CFU mL^{-1}) for 24 hours, the wounds were treated with normal saline; UV light; Fabric-2 and Fabric-2@UV for 30 minutes. On the second day of treatment, bacteria were collected from the wounds of the mice to quantify the number of bacteria. At different times after treatment (0, 1, 2, 3, 4, 5, 7, 9, 11, 13 days), the wounds of the four groups of mice were observed and photographed, and the body weight of the mice was recorded. After 13 days of treatment, mice were sacrificed and wound tissues were collected. The collected wound tissues were fixed with 10% formalin and embedded in

paraffin for sectioning. Finally, these wound tissue sections were used for histological and immunological analysis.

Characterization

SEM images of PDA coatings were obtained on an FEI Nova NanoSEM 450. The test mode is backscattered electron mode, and the test voltage is 15kV. The surface roughness and thicknesses of the PDA coatings were acquired on AFM of AIST-NT Smart SPM. Specifically, the samples were manipulated using tweezers to leave steps that could be used to measure coating thickness. Electron energy-loss spectroscopy mapping (EELS mapping) was performed on HORIBA X-max detector within a SU-8010 scanning electron microscope. And X-ray photoelectron spectroscopy (XPS) was conducted with Escalab 250Xi (Thermo Scientific, USA) by using Al Kα radiation. The CaseXPS software (Version 2.3.16) was used to analyze the survey scan XPS spectra and deconvolute the narrow-scan XPS spectra of the S 2p and O 1s of the samples, using adventitious carbon to standardize the C 1s binding energy (284.5 eV). Moreover, UV-Vis absorption spectra and UV-Vis transmittance spectra were carried by using UV-Vis light spectrophotometer (PerkinElmer, Lambada 650). The measured spectral range is 290-800 nm with slit of 1 nm. Furthermore, water contact angles were tested by a Data-Physics OCA 25, with 8 μL of the water drop. the CV measurement was carried out on the CHI760E electrochemical workstation. This test was completed by using PDA coatings coated indium tin oxide as the working electrode, Pt wire as the counter electrode, and Ag/AgCl as the reference electrode in a 0.1 M Bu_4NPF_6 acetonitrile solution. And, the Fc/Fc^+ couple was used as an internal reference. Note

that the preparation method of the coating applied on the working electrode was the same as that applied on the PC. Also, the thermal stability of samples before and after UV irradiation were evaluated by using thermogravimetric analysis (TGA, 209F3 IR thermal gravimetric analyser, Netzsch, Germany) tests from room temperature (25 °C) to 800 °C with a ramp rate of 10 °C/min under nitrogen atmosphere. Moreover, the mechanical behavior of samples before and after UV irradiation were test by a universal testing machine (Model 5967, Instron, USA) at a strain rate of 2 mm/min. For each measurement, five samples were measured for an average value. Fluorescence spectra were recorded on the F98 fluorescence spectrophotometer (Shanghai Lengguang Technology Co., Ltd.) with the excitation and emission slit width at 10 nm. Image-J software was used to measure the wound area of each group for analysis.

Statistical analysis

The data were presented as mean ± standard deviation. Statistical significance was calculated using either Student's t-test or one-way ANOVA followed by Newman Keuls Multiple Comparison Test. A p-value less than 0.05 was considered significant.

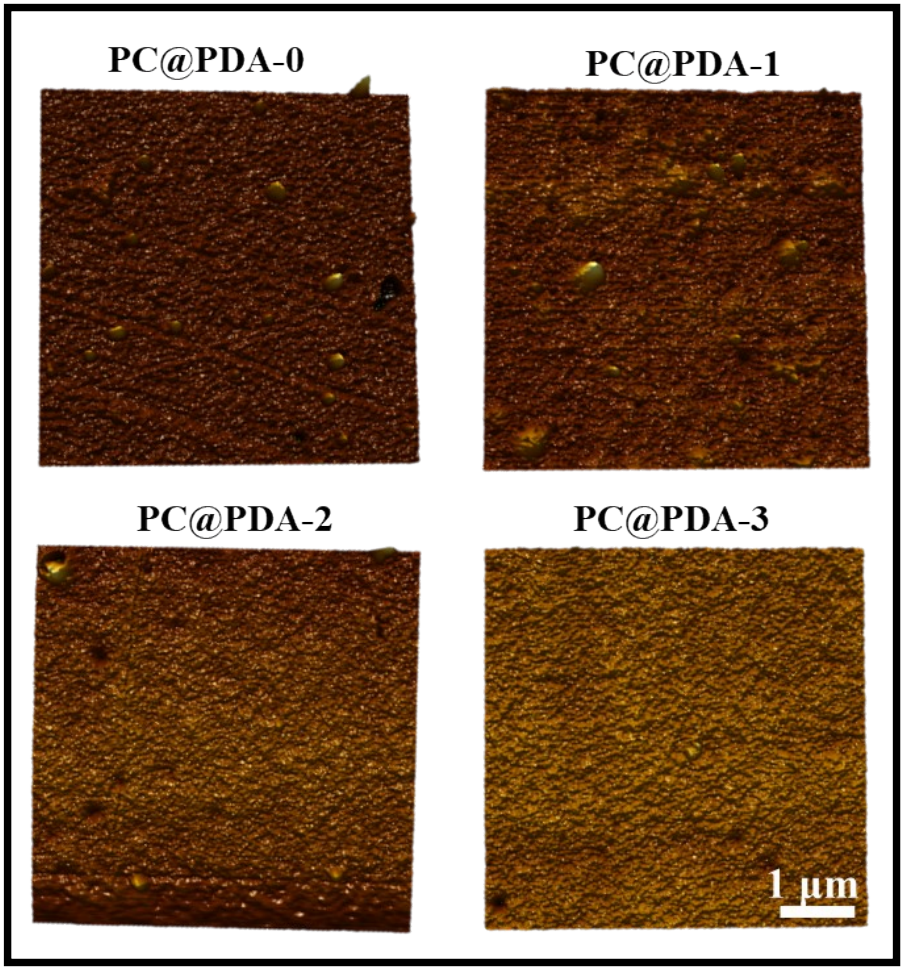

Figure S1. 3D AFM height images of PC@PDA-i coating, where i = 0-3.

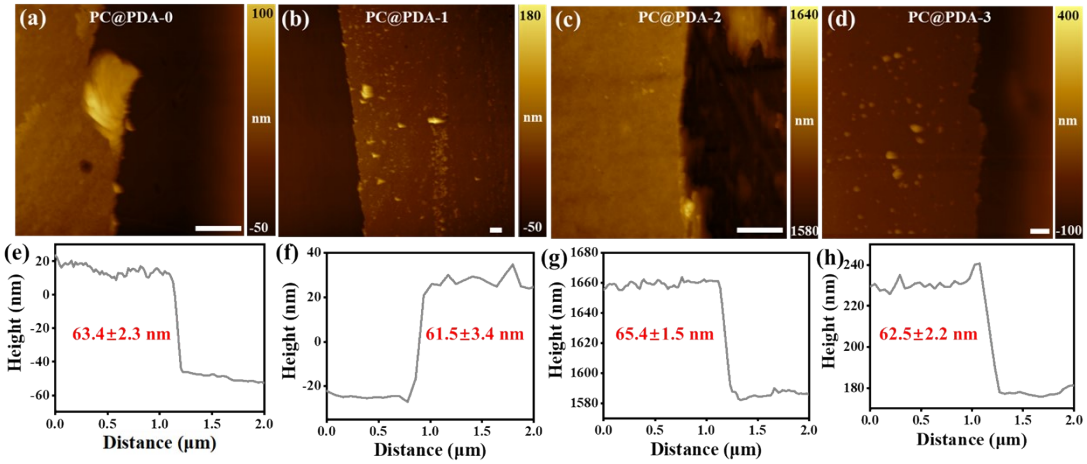

Figure S2. Thickness of PDA coatings. (a)-(d) AFM images of PDA coatings, respectively, (a) PC@PDA-0, (b) PC@PDA-1, (c) PC@ PDA-2, (d) PC@ PDA-3, scale

bars, 1 μm. (e)-(h) Corresponding height chart, respectively, (e) PC@PDA-0, (f) PC@PDA-1, (g) PC@ PDA-2, (h) PC@ PDA-3.

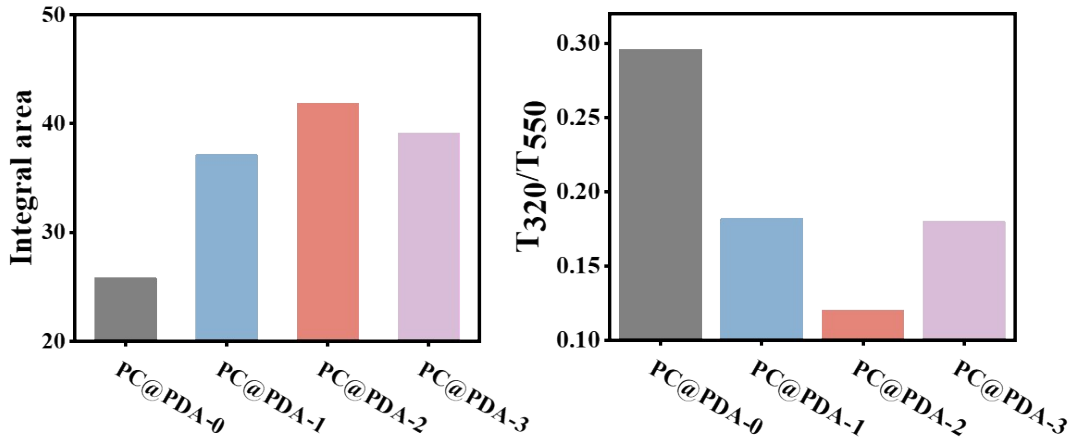

Figure S3. Quantitative analysis of the UV enhancement of PDA coatings. (a) Integral area values of UV absorption curve (shown in Figure 2a) from 290 to 400nm. (d) The ratio of transmittance at 320 nm and 550 nm in UV transmittance curve (shown in Figure 2b).

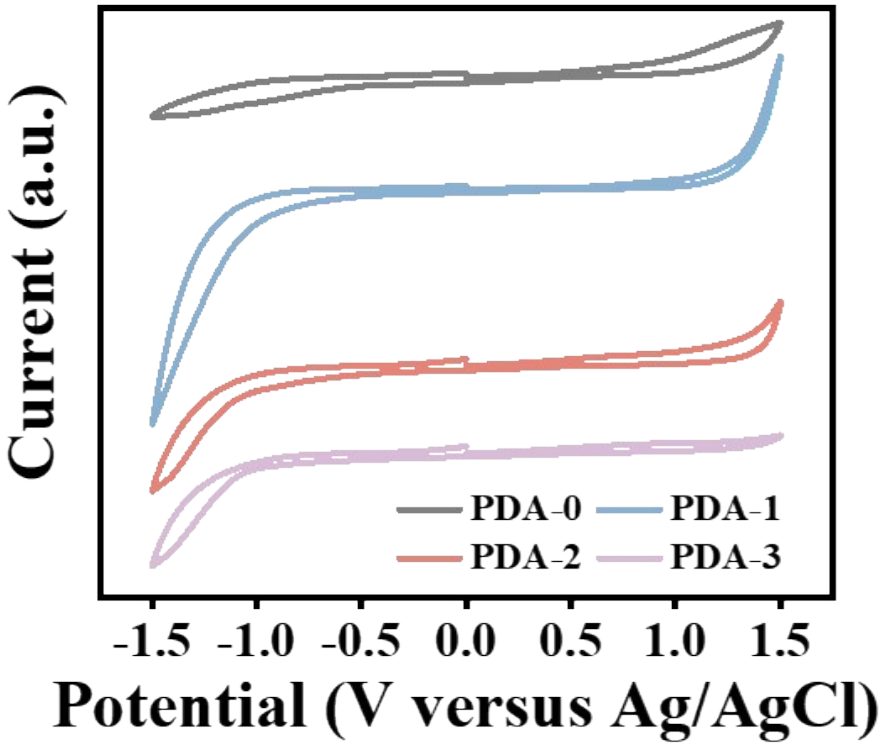

Figure S4. Cyclic voltammograms testing of the PDA coatings.

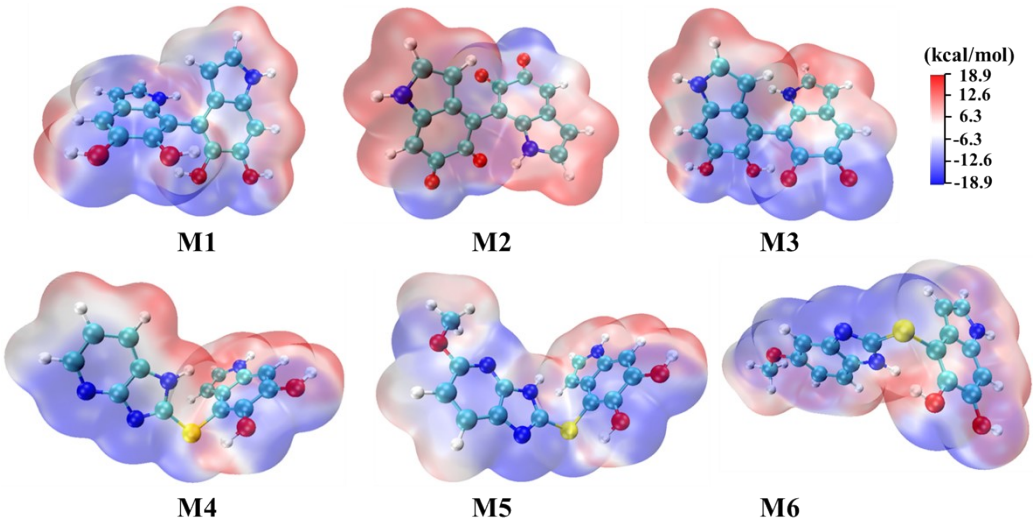

Figure S5. ESP photographs of M1-M6.

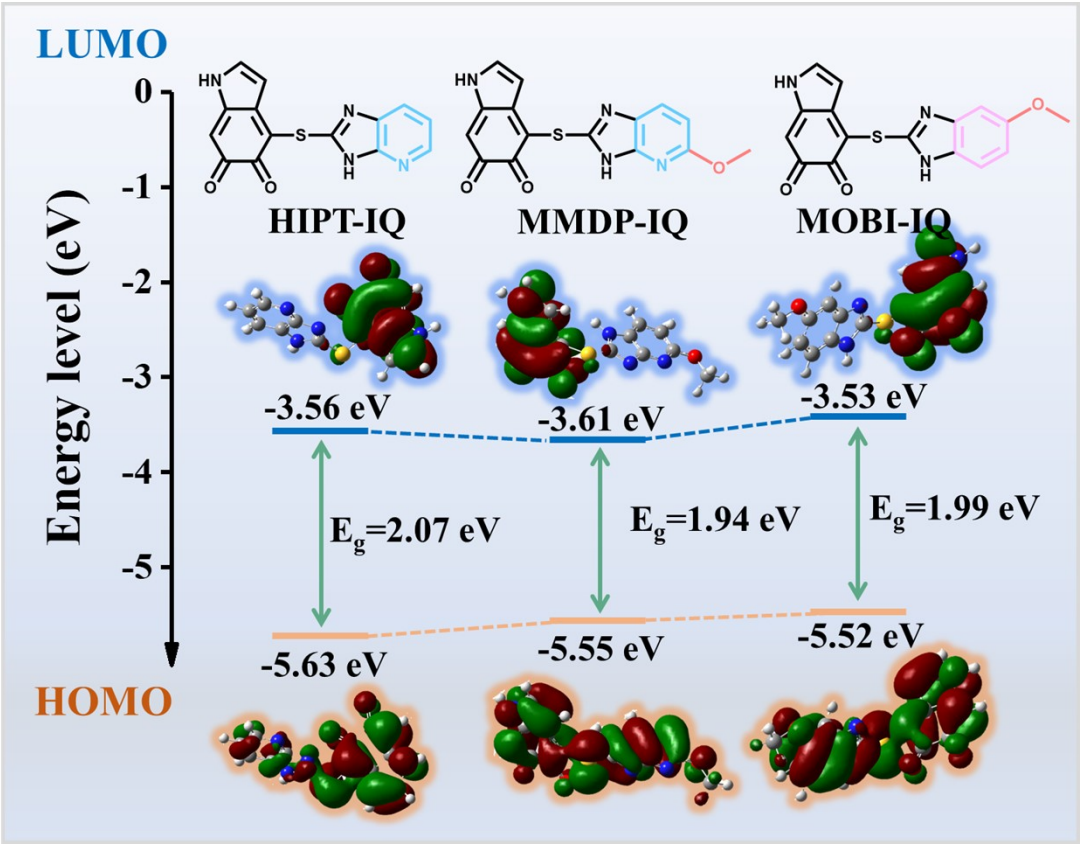

Figure S6. Chemical structures of TH-IQs and theoretical calculated frontier molecular orbital using DFT calculations at the B3LYP/6-31 G* level with solvation model density.

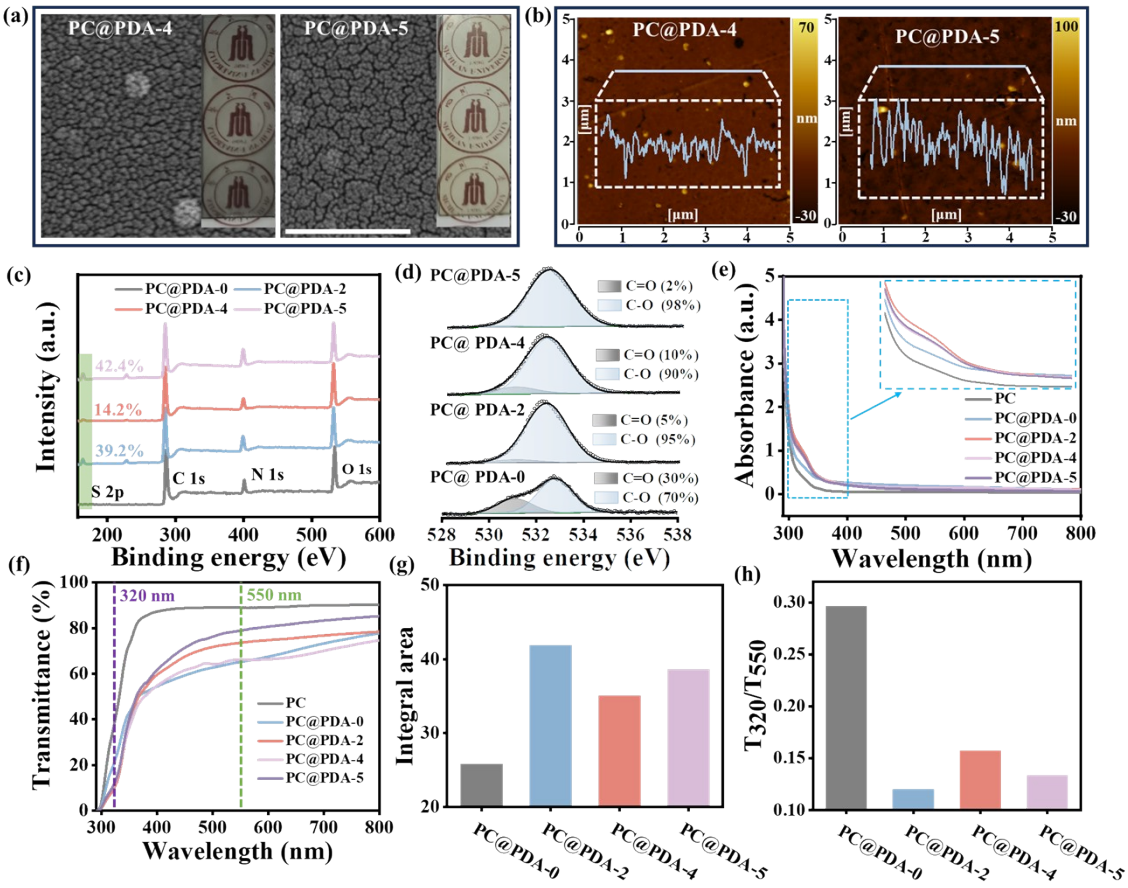

Figure S7. Characterization of PDA coatings with different MMDP doping amount. (a) SEM and optical images of PDA coatings, scale bar, 500 nm. (b) AFM height images of PDA coatings (Inset: corresponding height fluctuation along the blue line from Figure S7b). (c) XPS survey spectra of PDA coatings. (a.u.: arbitrary units). (d) O 1s peaks in XPS spectra of PDA coatings. (e) UV-Vis absorption spectra of naked PC and PDA coated PC ranging from 290 to 800 nm. (f) UV−Vis light transmittance spectra of naked PC and PDA coated PC ranging from 290 to 800 nm. (g) Integral area values of UV absorption curve (shown in Figure S7e) from 290 to 400nm. (h) The ratio of transmittance at 320 nm and 550 nm in UV transmittance curve (shown in Figure S7f).

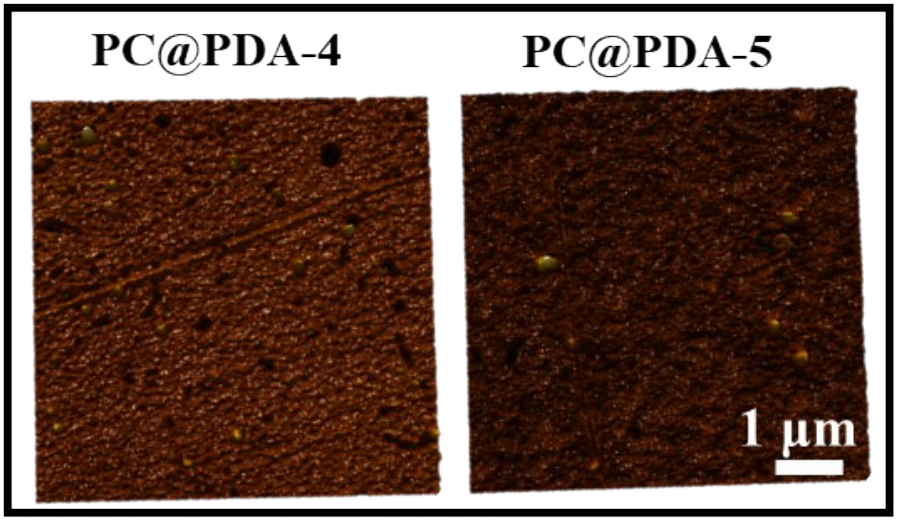

Figure S8. 3D AFM height images of PC@PDA-i coating, where i = 4-5.

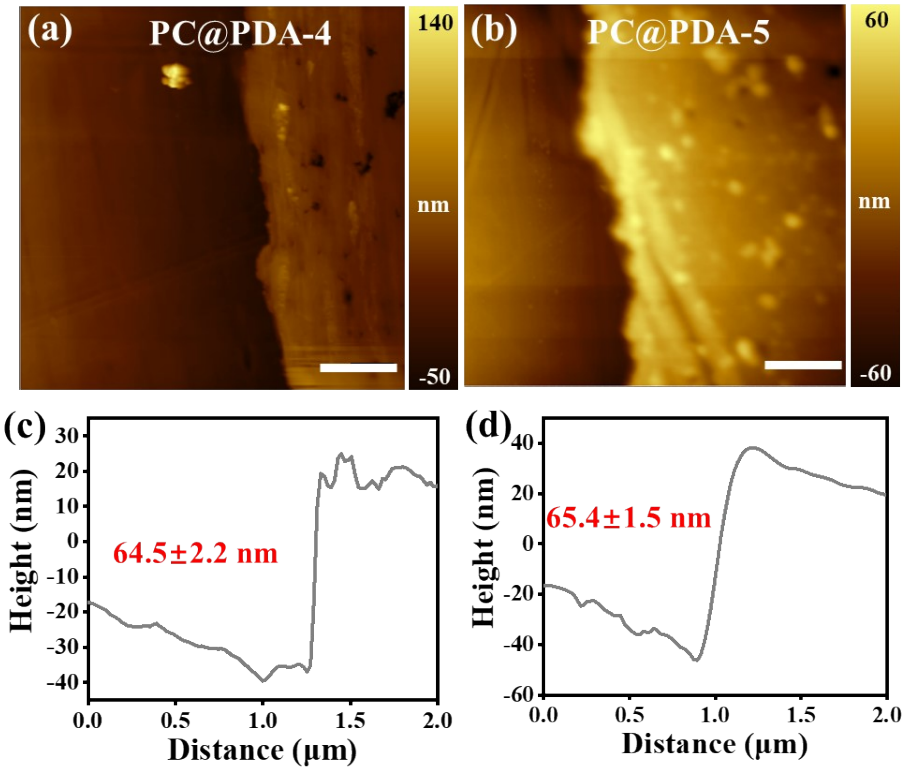

Figure S9. Thickness of PDA coatings. (a)-(b) AFM images of PDA coatings, respectively, (a) PC@PDA-4, (b) PC@PDA-5, scale bars, 1 μm. (c)-(d) Corresponding height chart, respectively, (c) PC@PDA-4, (d) PC@PDA-5.

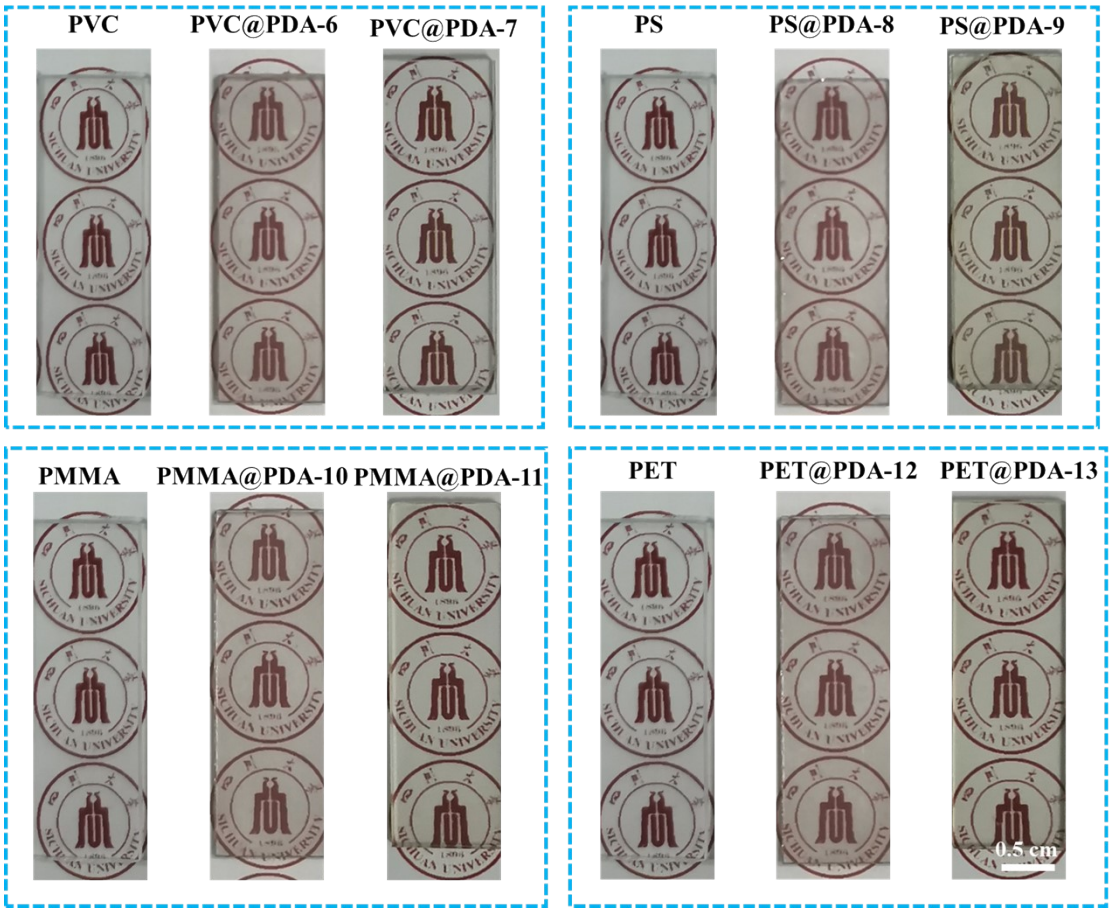

Figure S10. Optical images of different substrates uncoated and coated with PDA.

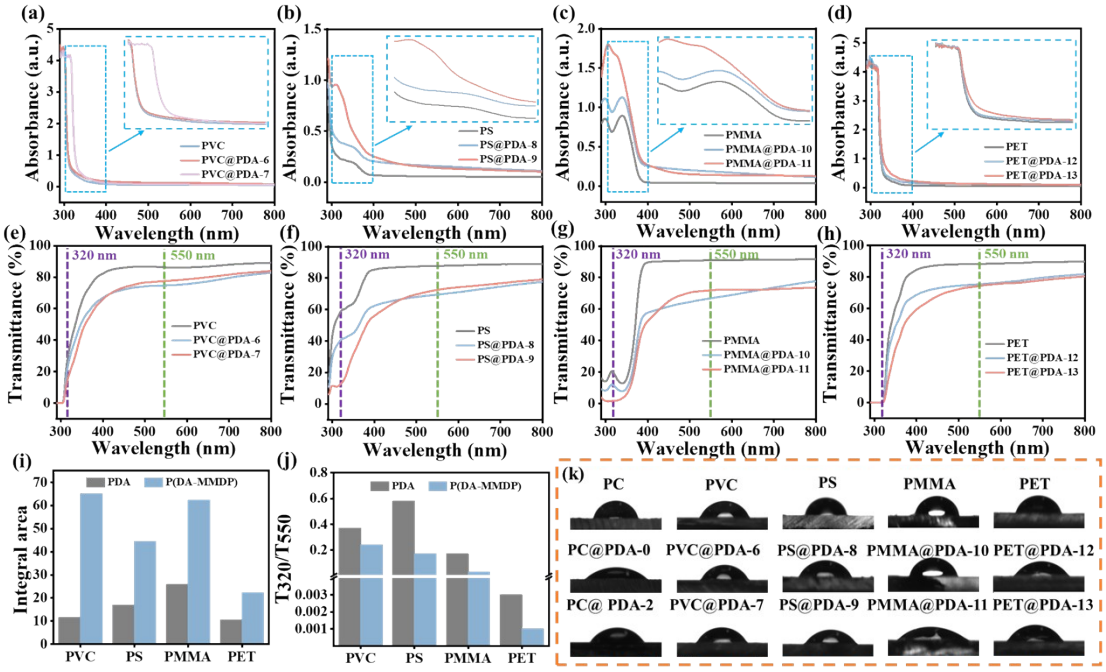

Figure S11. UV absorption enhancement of MMDP-doped PDA coatings. (a)-(d) UV-Vis absorption spectra of PDA and P(DA-MMDP) coating on different substrate ranging from 290 to 800 nm, respectively, (a) PVC, (b) PS, (c) PMMA, (d) PET. (e)-(h) UV−Vis light transmittance spectra PDA and P(DA-MMDP) coating on different substrate ranging from 290 to 800 nm, respectively, (e) PVC, (f) PS, (g) PMMA, (h) PET. (i) Integral area values of UV absorption curve (shown in Figure. S7(a)-(d)) from 290 to 400nm. (d) The ratio of transmittance at 320 nm and 550 nm in UV transmittance curve (shown in Figure. S7(e)-(h)). (k) Pictures of water droplets on different surface.

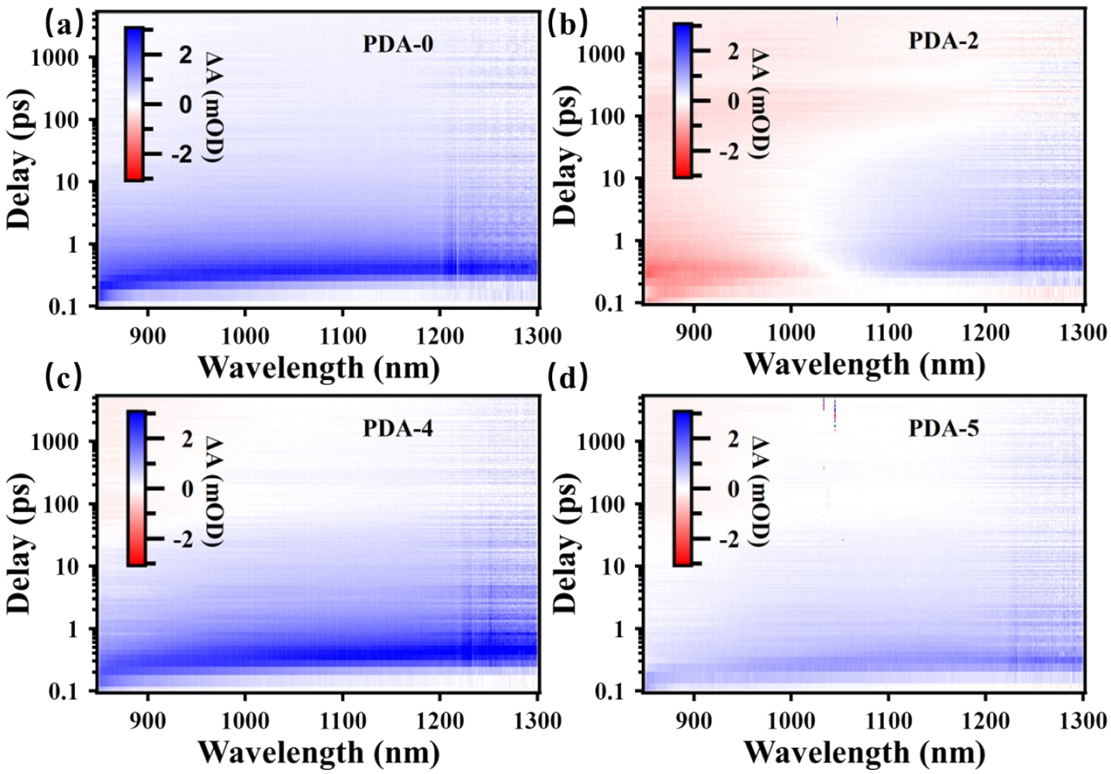

Figure S12. Pseudocolor images of the TA spectra at all decays. The horizontal and vertical axes corresponding to the probe wavelength and pump-probe delay, respectively. As indicated by the color scale bar, the color intensity represents the magnitude of the TA signal.

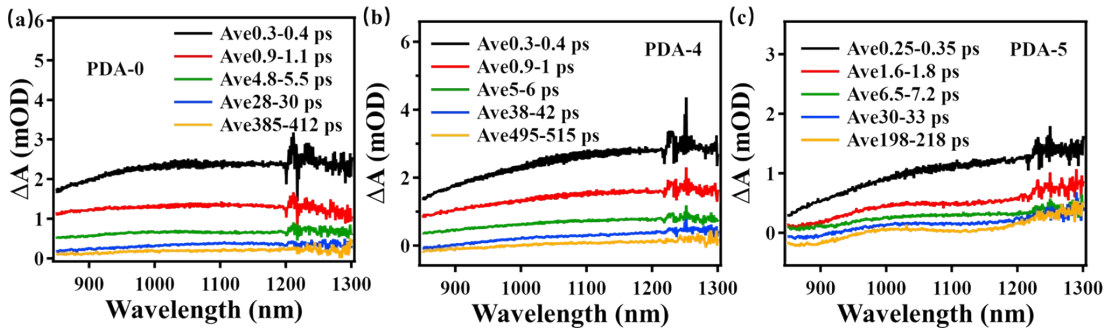

Figure S13. Transient absorption spectra of PDA-i (i=0, 4 and 5) at indicated delay times.

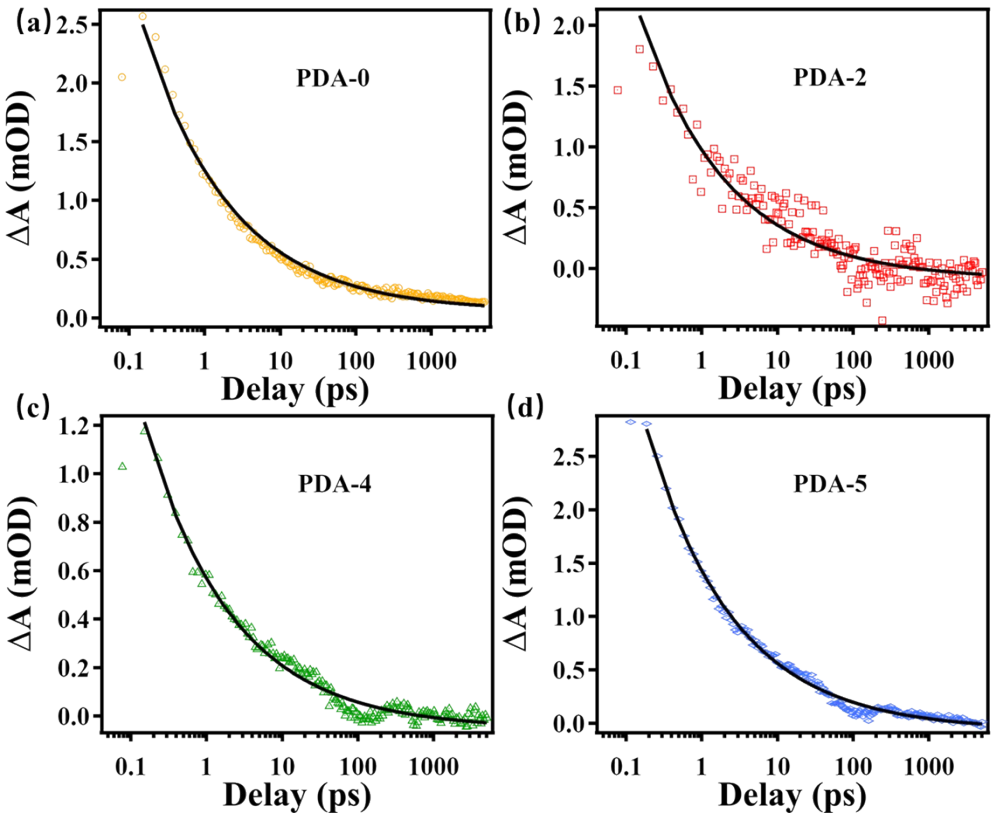

Figure S14. The EIA kinetics traces of PDA-i (i= 0, 2, 4 and 5). These traces can be described by a power law function with a power of -0.377±0.006.

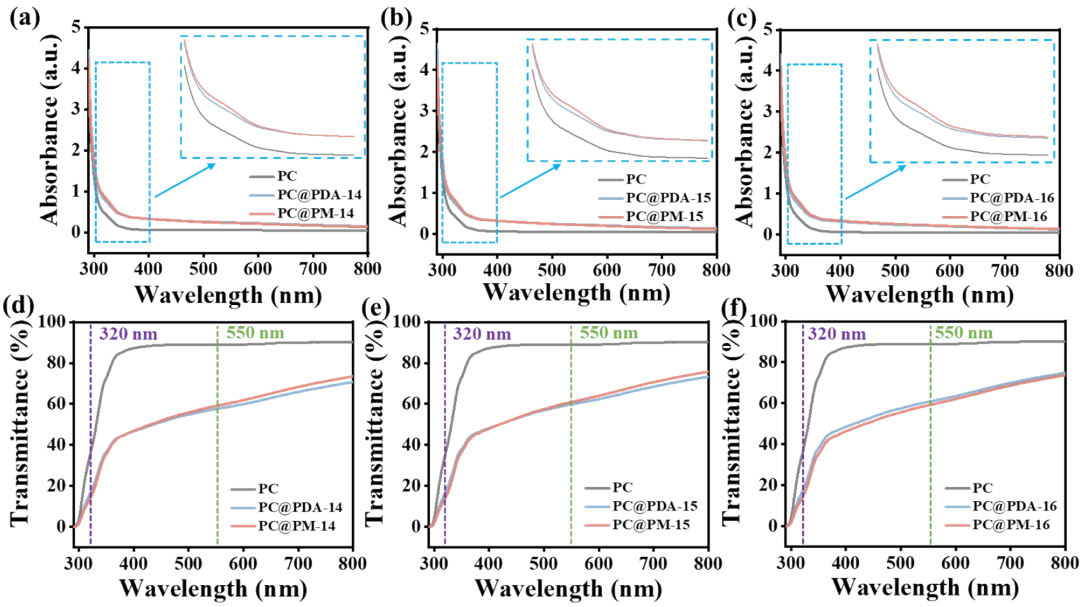

Figure S15. Effect of reaction pH on UV absorption of PDA coatings. (a)-(c) UV-

Vis absorption spectra of PDA coatings before and after modification at different reaction pH, respectively, (a) pH = 8.5, (b) pH = 9.5, (c) pH = 10.5. (d)-(f) UV−Vis light transmittance spectra of PDA coatings before and after modification at different reaction pH, respectively, (d) pH = 8.5, (e) pH = 9.5, (f) pH = 10.5. (PDA coating thickness = 60 nm, reaction time = 24 h, reaction temperature = 25 ℃)

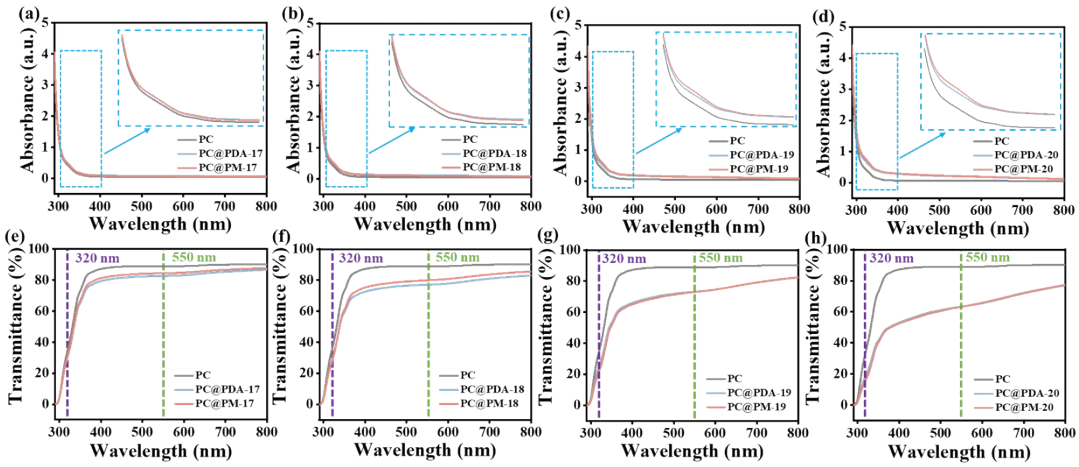

Figure S16. Effect of thickness on UV absorption of PDA coating. (a)-(d) UV-Vis absorption spectra of PDA coatings before and after modification with different PDA coating thickness, respectively, (a) PDA coating thickness = 20 nm, (b) PDA coating thickness = 30 nm, (c) PDA coating thickness = 45 nm, (d) PDA coating thickness = 60 nm. (e)-(h) UV−Vis light transmittance spectra of PDA coatings before and after modification with different PDA coating thickness, respectively, (e) PDA coating thickness = 20 nm, (f) PDA coating thickness = 30 nm, (g) PDA coating thickness = 45 nm, (h) PDA coating thickness = 60 nm. (reaction pH = 10.5, reaction time = 24 h, reaction temperature = 25 ℃)

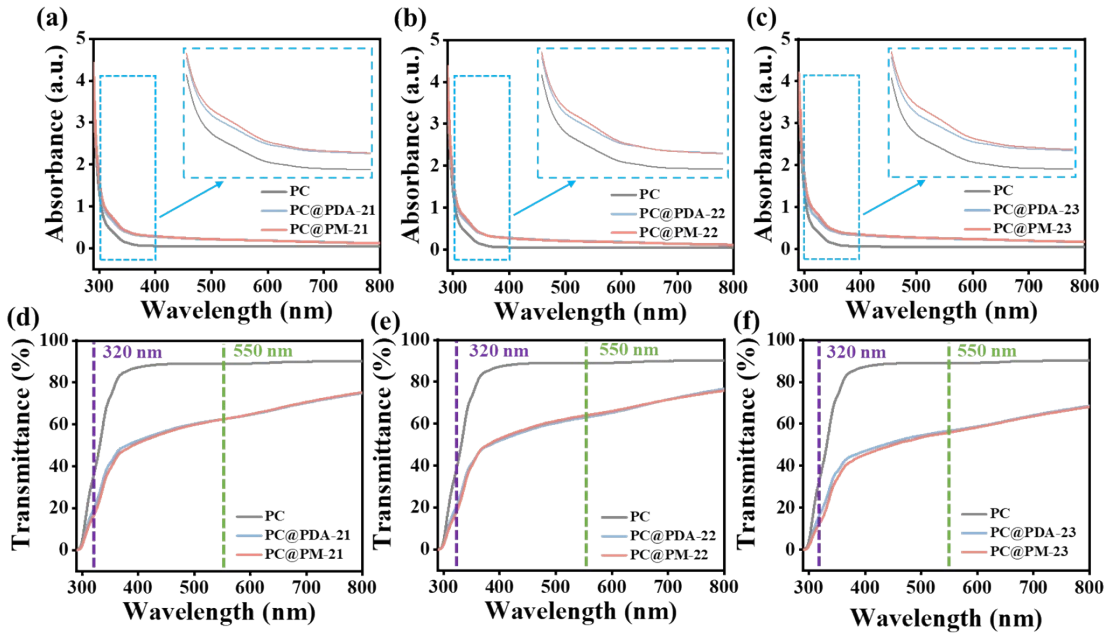

Figure S17. Effect of the reaction time and temperature on UV absorption of PDA coatings. (a)-(d) UV-Vis absorption spectra of PDA coatings before and after modification with different modification reaction time and temperature, respectively, (a) reaction time = 24 h, reaction temperature = 25 ℃, (b) reaction time = 48 h, reaction temperature = 25 ℃, (c) reaction time = 24 h, reaction temperature = 42 ℃. (d)-(f) UV−Vis light transmittance spectra of PDA coatings before and after modification with different modification reaction time and temperature, respectively, (d) reaction time = 24 h, reaction temperature = 25 ℃, (e) reaction time = 48 h, reaction temperature = 25 ℃, (f) reaction time = 24 h, reaction temperature = 42 ℃. (reaction pH = 10.5, PDA coating thickness = 60 nm).

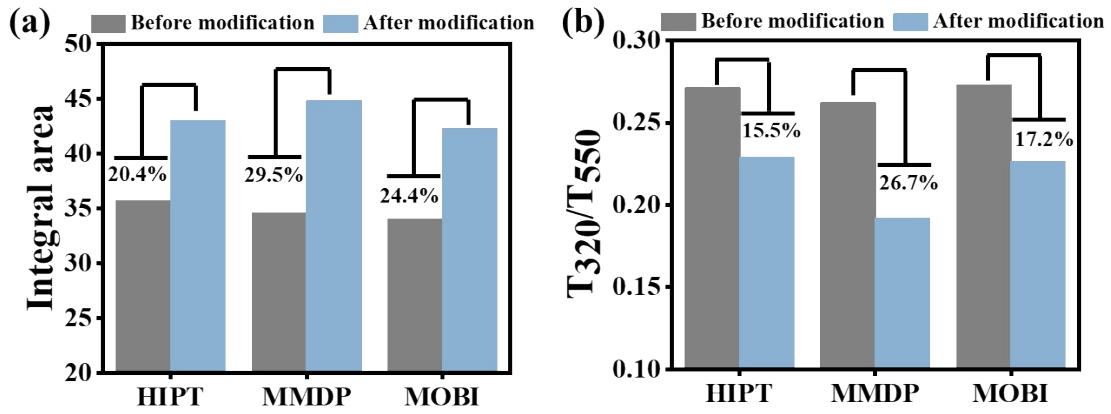

Figure S18. Quantitative analysis of the UV enhancement. (a) Integral area values of UV absorption curve (shown in Figure 3e-3g) from 290 to 400nm. (b) The ratio of transmittance at 320 nm and 550 nm in UV transmittance curve (shown in Figure 3h-3j).

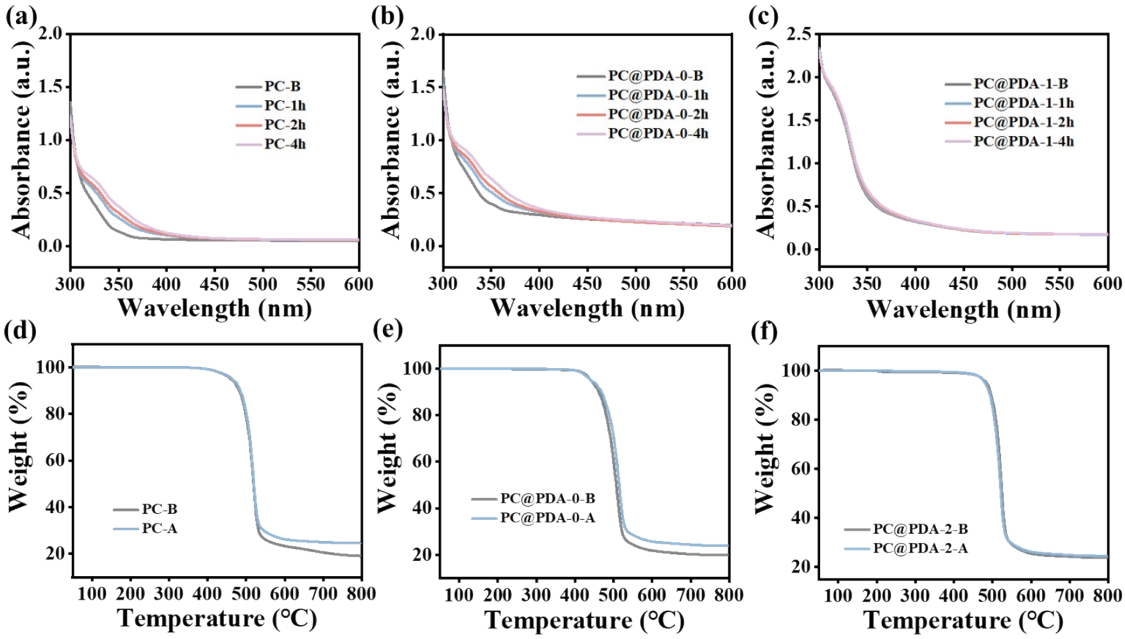

Figure S19. UV protection of MMDP-doped PDA coatings. (a)-(c) UV-Vis absorption spectra of naked PC and PDA coated PC (PC@PDA-0 and PC@PDA-2) after UV irradiation for different times, respectively, (a) naked PC, (b) PC@PDA-0, (c) PC@PDA-2. (d)-(f) TGA curves of naked PC and PDA coated PC (PC@PDA-0 and

PC@PDA-2) after UV irradiation for different times, respectively, (d) naked PC, (e) PC@PDA-0, (f) PC@PDA-2.

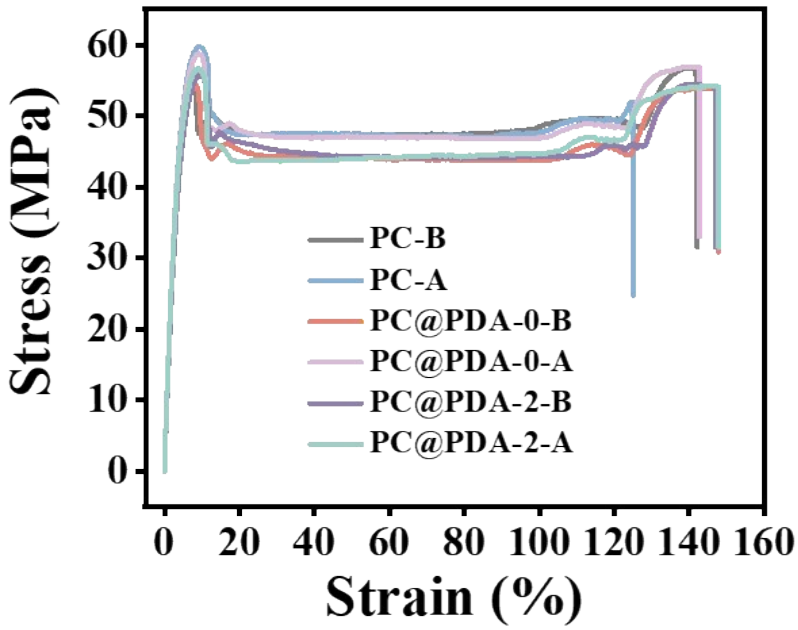

Figure S20. Stress-strain curves of naked PC and PDA coated PC (PC@PDA-0 and PC@PDA-2) before and after UV irradiation.

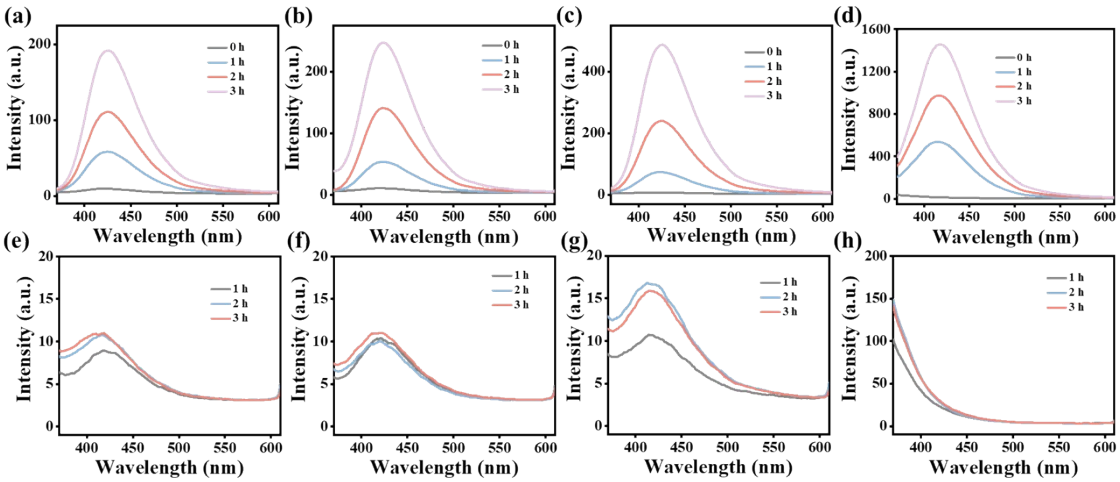

Figure S21. UV-trigged generation of hydroxyl radicals by PDA coatings. (a)-(d) Fluorescence spectra of HTA generated by different materials in the presence of UV,

respectively, (a) Water, (b) Fabric-0, (c) Fabric-1, (d) Fabric-2. (e)-(f) Fluorescence spectra of HTA generated by different materials in dark, respectively, (e) Water, (f) Fabric-0, (g) Fabric-1, (h) Fabric-2.

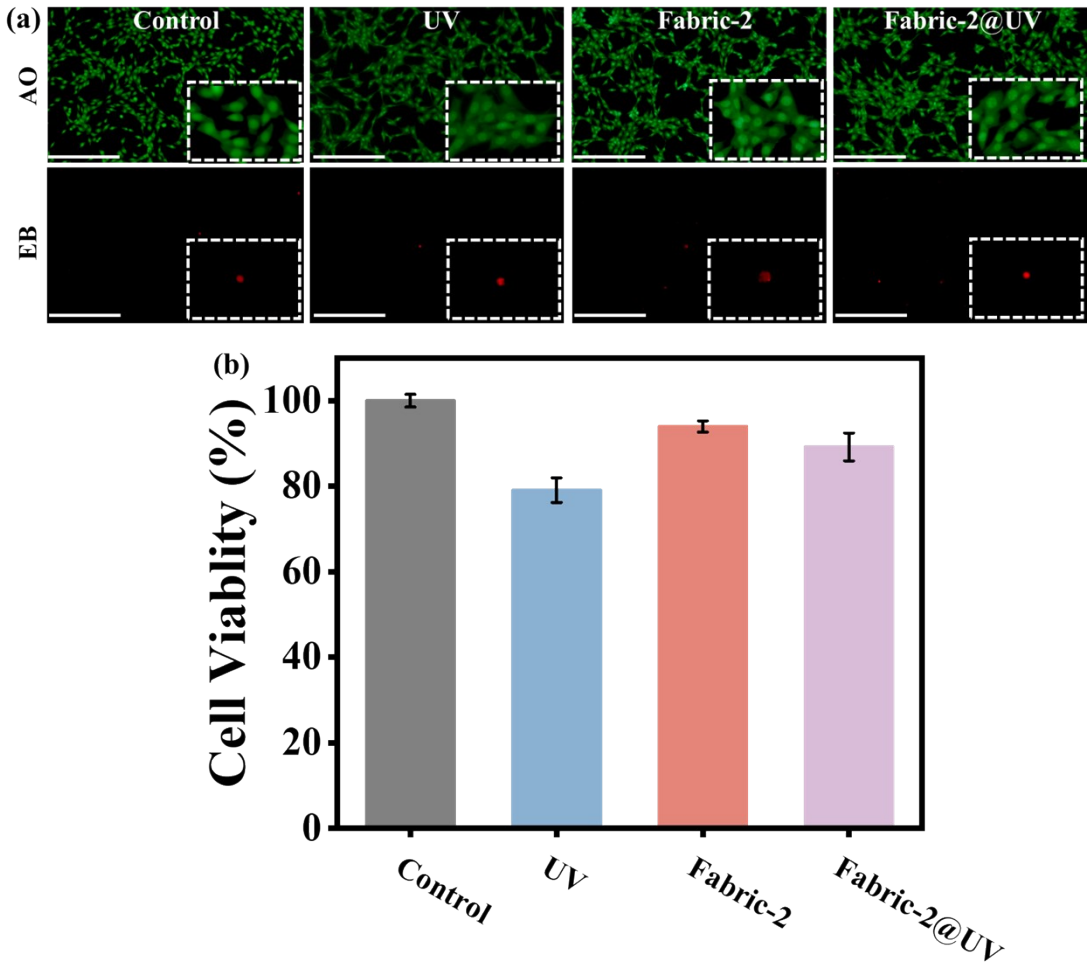

Figure S22. Biocompatibility assessment. (a) The results of AO/EB staining of NIH-3T3 cells after virous treatment. (b) The Corresponding cell viability after virous treatments, scale bar, 100 μm.

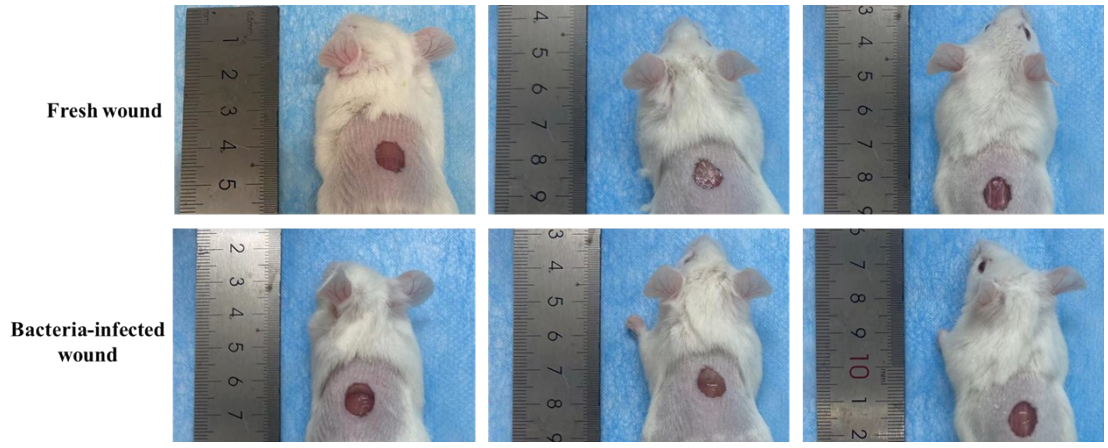

Figure S23. Photographs of a mouse model of a bacterially infected wound.

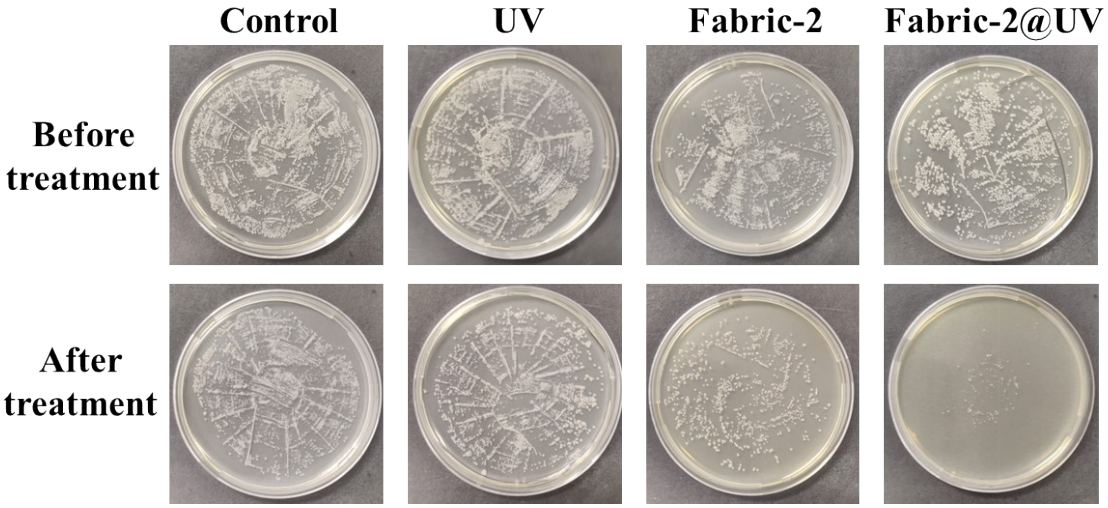

Figure S24. Survival of bacteria on infected wounds of mice before and after different treatments.

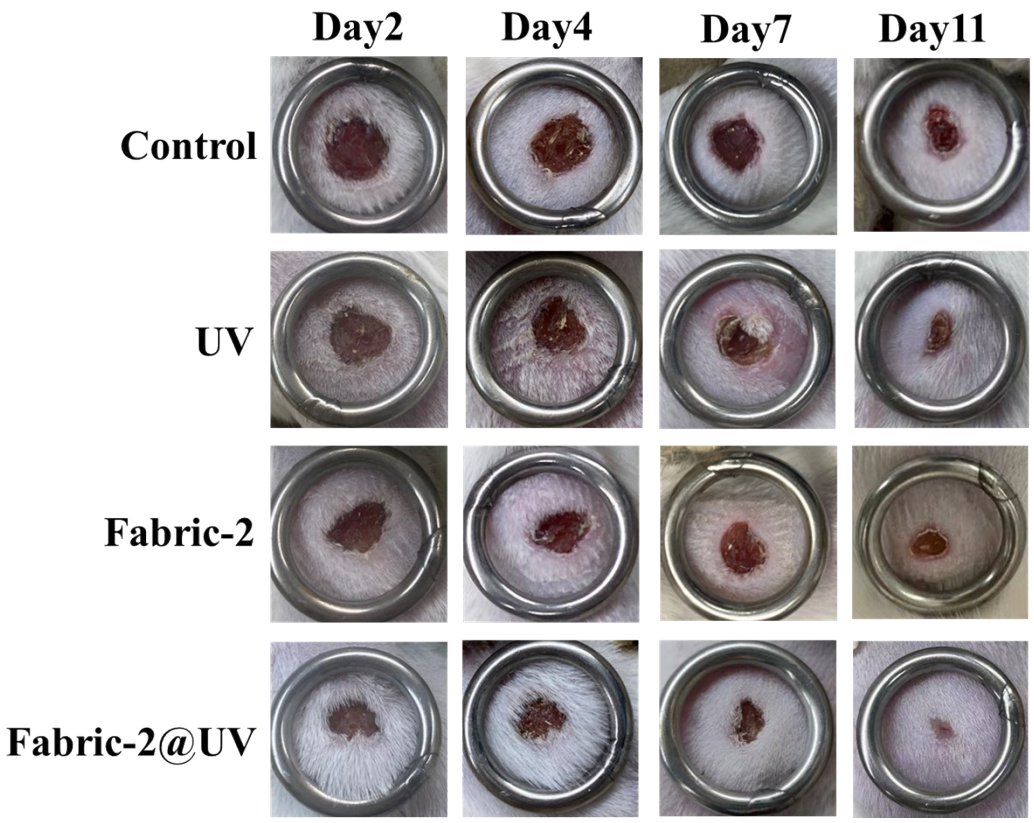

Figure S25. Photographs of the healing process at different time, the diameter of the ring was 14 mm.

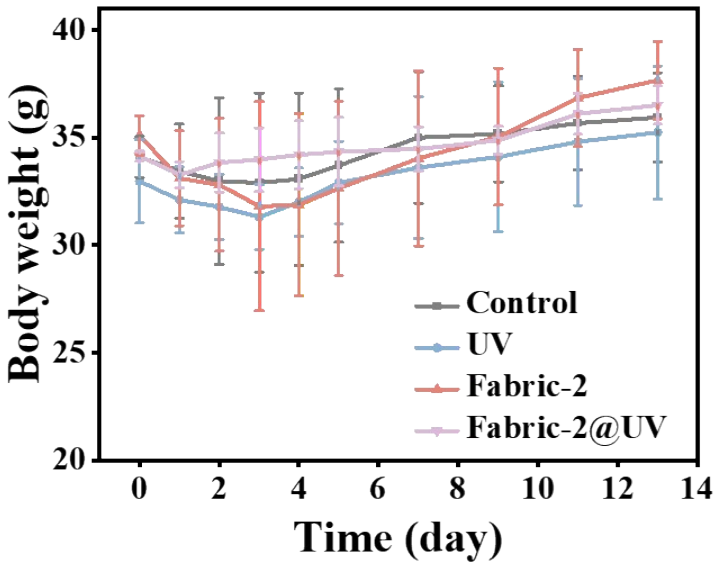

Figure S26. Body weight of mice with bacterially infected wound after the treatments.

Table S1. (a) Full names of important abbreviations. (b) Reaction parameters for the fabrication of PDA coatings. (c) Reaction parameters for the post-modification of PDA coatings.

(a)

Abbreviations	Full name
DA	Dopamine
PDA	Polydopamine
DHI	5,6-Dihydroxyindole
IQ	5,6-Dihydroxyindolequinone
PC	Polycarbonate
PVC	Polyvinyl chloride
PS	Polystyrene
PMMA	Polymethylmethacrylate
PET	Polyethylene glycol terephthalate
TH	Thiol heterocycles molecules
HIPT	1H-Imidazo[4,5-b]pyridine-2(3H)-thione
MMDP	2-Mercapto-5-methoxyimidazole[4,5-b]pyridine
MOBI	5-Methoxy-2-mercaptobenzimidazole

(b)

Sample	DA (mg)	HIPT (mg)	MMDP (mg)	MOBI (mg)	Substrate	Ethanol (mL)	Tris-HCl Buffer (200mM, pH=8.5, mL)	Temperature (℃)	Reaction time (h)
PC@PDA-0	8				PC	2	6	25	24
PC@PDA-1	5	10			PC	2	6	25	24
PC@PDA-2	8		8		PC	2	6	25	24
PC@PDA-3	6			12	PC	2	6	25	24
PC@PDA-4	10		5		PC	2	6	25	24
PC@PDA-5	7		14		PC	2	6	25	24
PVC@PDA-6	8				PVC	2	6	25	24
PVC@PDA-7	8		8		PVC	2	6	25	24
PS@PDA-8	8				PS	2	6	25	24
PS@PDA-9	8		8		PS	2	6	25	24
PMMA@PDA-10	8				PMMA	2	6	25	24
PMMA@PDA-11	8		8		PMMA	2	6	25	24
PET@PDA-12	8				PET	2	6	25	24
PET@PDA-13	8		8		PET	2	6	25	24
PC@PDA-14	8				PC	2	6	25	24
PC@PDA-15	8				PC	2	6	25	24
PC@PDA-16	8				PC	2	6	25	24
PC@PDA-17	8				PC	2	6	25	3
PC@PDA-18	8				PC	2	6	25	6
PC@PDA-19	8				PC	2	6	25	12
PC@PDA-20	8				PC	2	6	25	24
PC@PDA-21	8				PC	2	6	25	24
PC@PDA-22	8				PC	2	6	25	24
PC@PDA-23	8				PC	2	6	25	24
PC@PDA-24	8				PC	2	6	25	24
PC@PDA-25	8				PC	2	6	25	24
PC@PDA-26	8				PC	2	6	25	24

(c)

Sample	HIPT (mg)	MMDP (mg)	MOBI (mg)	Coating for Post modification	Ethanol (mL)	Tris-HCl Buffer (200mM, mL)	pH	Temperature (℃)	Reaction time (h)
PC@PM-14		8		PC@PDA-14	2	6	8.5	25	24
PC@PM-15		8		PC@PDA-15	2	6	9.5	25	24
PC@PM-16		8		PC@PDA-16	2	6	10.5	25	24
PC@PM-17		8		PC@PDA-17	2	6	10.5	25	24
PC@PM-18		8		PC@PDA-18	2	6	10.5	25	24
PC@PM-19		8		PC@PDA-19	2	6	10.5	25	24
PC@PM-20		8		PC@PDA-20	2	6	10.5	25	24
PC@PM-21		8		PC@PDA-21	2	6	10.5	25	24
PC@PM-22		8		PC@PDA-22	2	6	10.5	25	48
PC@PM-23		8		PC@PDA-23	2	6	10.5	42	24
PC@PM-24	8			PC@PDA-24	2	6	10.5	42	24
PC@PM-25		8		PC@PDA-25	2	6	10.5	42	24
PC@PM-26			8	PC@PDA-26	2	6	10.5	42	24

Table S2. The coordinates of the model structure after optimization.

	x	y	z
C	0.954280	0.757200	-0.000001
C	0.948870	-0.663630	-0.000002
C	-0.237850	-1.408200	-0.000002
C	-1.438270	-0.711190	0.000001
C	-1.458920	0.710540	0.000002
C	-0.279500	1.439170	0.000001
O	-2.714060	1.298160	0.000003
O	-2.669800	-1.339230	0.000000
C	2.331970	1.167400	-0.000009
C	3.091040	0.022490	0.000013
N	2.262600	-1.082900	-0.000004
H	-0.234330	-2.495060	-0.000004
H	-0.322290	2.525890	-0.000001
H	-2.598670	2.263530	-0.000001
H	-2.523530	-2.300420	0.000001
H	2.707460	2.182040	-0.000017
H	4.164640	-0.104210	0.000024
H	2.569580	-2.045490	-0.000005

DHI

	x	y	z
C	-0.289260	-1.471210	0.000011
C	-1.559230	-0.788470	-0.000001
C	-1.572800	0.786470	0.000000
C	-0.311910	1.498550	-0.000010
C	0.849920	0.784490	-0.000003
C	0.838500	-0.707830	0.000001
O	-2.671760	1.346590	0.000011
O	-2.650480	-1.366100	-0.000010
C	2.236500	1.171400	0.000000
C	2.971700	0.024820	0.000001
N	2.150780	-1.097410	0.000000
H	-0.264570	-2.555800	0.000005
H	-0.329100	2.583700	-0.000012
H	2.618370	2.181800	0.000009
H	4.045620	-0.104350	-0.000002
H	2.471540	-2.056700	0.000002

IQ

	x	y	z
C	0.582180	-0.738520	0.000032
C	0.629150	0.675640	0.000001
N	1.710440	1.448600	0.000009
C	2.864220	0.752940	0.000052
C	2.951150	-0.647440	0.000089
C	1.793440	-1.427990	0.000080
N	-0.733990	-1.179680	0.000008
C	-1.445970	-0.072800	-0.000035
N	-0.695180	1.076860	-0.000040
S	-3.208140	-0.103530	-0.000078
H	3.774420	1.346510	0.000059
H	3.930100	-1.115670	0.000125
H	1.830480	-2.513070	0.000108
H	-1.037540	2.030580	-0.000071
H	-3.381120	1.236640	-0.000138

HIPT

	x	y	z
C	-0.385520	1.073830	-0.000002
C	0.010910	-0.276240	0.000001
N	1.256170	-0.757540	0.000005
C	2.194130	0.190260	0.000006
C	1.937570	1.582370	0.000000
C	0.627510	2.040130	-0.000004
N	-1.772860	1.173040	-0.000003
C	-2.184590	-0.075560	-0.000006
N	-1.164570	-0.999250	-0.000004
S	-3.895730	-0.509010	0.000004
O	3.507160	-0.166700	0.000010
C	3.814610	-1.568780	-0.000007
H	2.777800	2.267370	-0.000001
H	0.401220	3.101870	-0.000007
H	-1.253870	-2.008510	-0.000005
H	-3.707740	-1.846780	-0.000006
H	4.904480	-1.624820	-0.000011
H	3.416820	-2.060640	0.893240
H	3.416820	-2.060620	-0.893260

MMDP

	x	y	z
C	0.206550	-0.542710	-0.000020
C	0.325960	0.866480	0.000019
C	-0.782920	1.704280	0.000073
C	-2.044590	1.104680	0.000089
C	-2.176530	-0.300890	0.000052
C	-1.056570	-1.137890	-0.000004
N	1.468500	-1.135940	-0.000071
C	2.304020	-0.117100	-0.000056
N	1.693800	1.107240	-0.000017
S	4.068130	-0.221290	-0.000100
O	-3.393530	-0.950680	0.000066
C	-4.581330	-0.157280	0.000083
H	-0.681500	2.784800	0.000098
H	-2.923020	1.737970	0.000128
H	-1.181490	-2.215760	-0.000033
H	2.145110	2.013920	-0.000019
H	4.094860	-1.569980	-0.000159
H	-5.410990	-0.867150	0.000073
H	-4.644180	0.472870	0.895860
H	-4.644180	0.472900	-0.895670

MOBI

	x	y	z
C	3.576660	-0.304100	-0.210810
C	2.801630	-1.317920	-0.753310
C	1.384460	-1.289410	-0.662160
C	0.717000	-0.249660	-0.006760
C	1.498210	0.798110	0.545480
C	2.911750	0.748530	0.429690
C	1.180720	1.999940	1.266250
C	2.372970	2.619950	1.553050
N	3.417580	1.869210	1.052690
O	3.344450	-2.399800	-1.417620
O	0.724070	-2.342200	-1.267730
C	-0.767470	-0.220020	0.058270
C	-1.504260	-1.230060	0.689320
C	-2.923730	-1.197140	0.730750
C	-3.632510	-0.151380	0.162940
C	-2.927240	0.896850	-0.460250
C	-1.510050	0.841210	-0.498920
O	-0.907830	-2.310210	1.308950
O	-3.533400	-2.260600	1.373910
C	-3.314370	2.104300	-1.136830
C	-2.158180	2.720340	-1.549420
N	-1.069010	1.954180	-1.182430
H	4.659700	-0.337250	-0.291020
H	0.195260	2.350590	1.538740
H	2.569910	3.544070	2.078160
H	4.397420	2.106780	1.124070
H	4.311690	-2.299580	-1.422140
H	-0.230040	-2.145760	-1.265880
H	-4.718780	-0.151590	0.209360
H	0.053990	-2.158740	1.333940
H	-4.495490	-2.125260	1.334990
H	-4.322330	2.463020	-1.296760
H	-2.013000	3.649400	-2.082760
H	-0.100150	2.225890	-1.276240

M1

	x	y	z
C	3.664100	0.635110	-0.163170
C	2.782640	1.635870	-0.703060
C	1.230230	1.374510	-0.686710
C	0.709260	0.130940	-0.118690
C	1.628800	-0.765560	0.379670
C	3.092500	-0.490670	0.344880
C	1.482910	-2.038280	1.028430
C	2.735440	-2.477090	1.343150
N	3.699410	-1.569800	0.931460
O	3.165110	2.706240	-1.181890
O	0.514030	2.253560	-1.167120
C	-0.738780	-0.132610	-0.126940
C	-1.256670	-1.368690	-0.712620
C	-2.804030	-1.655390	-0.686200
C	-3.690340	-0.662750	-0.130000
C	-3.153200	0.487180	0.369090
C	-1.683480	0.737520	0.361140
O	-0.546340	-2.217170	-1.250000
O	-3.183190	-2.733530	-1.149330
C	-3.753750	1.638200	0.988550
C	-2.742390	2.486880	1.318400
N	-1.508000	1.951510	0.969190
H	4.735340	0.804940	-0.163470
H	0.556720	-2.553450	1.229820
H	3.038900	-3.387440	1.842390
H	4.694840	-1.661930	1.086130
H	-4.756740	-0.862630	-0.114140
H	-4.808890	1.790880	1.161900
H	-2.783080	3.456770	1.795280
H	-0.633350	2.457130	1.008840

M2

	x	y	z
C	3.590350	-0.185360	0.181540
C	2.883740	-1.304720	0.599850
C	1.469120	-1.374370	0.491160
C	0.725440	-0.302400	-0.020090
C	1.440840	0.832940	-0.493360
C	2.855680	0.867570	-0.370780
C	1.054630	2.060300	-1.136890
C	2.205680	2.775090	-1.364020
N	3.291350	2.062300	-0.901230
O	3.503340	-2.408660	1.150050
O	0.878330	-2.533440	0.965830
C	-0.757250	-0.310890	-0.049350
C	-1.517300	-1.407540	-0.609960
C	-3.082720	-1.307740	-0.729790
C	-3.756900	-0.153480	-0.180040
C	-3.001520	0.819340	0.400150
C	-1.514700	0.722490	0.461230
O	-1.006820	-2.469690	-1.000300
O	-3.664830	-2.241000	-1.283320
C	-3.350860	2.062000	1.040840
C	-2.190530	2.637760	1.452550
N	-1.096430	1.838290	1.126910
H	4.672560	-0.147800	0.268950
H	0.054850	2.365720	-1.410000
H	2.345320	3.742470	-1.825620
H	4.256030	2.358080	-0.960280
H	4.459360	-2.235960	1.192050
H	0.188590	-2.781820	0.311720
H	-4.837760	-0.094750	-0.251580
H	-4.349990	2.449520	1.175570
H	-2.027210	3.570990	1.974390
H	-0.128550	2.105850	1.248780

M3

	x	y	z
C	-1.929950	-0.968580	-0.466690
C	-2.952380	-1.088490	0.510950
C	-3.496560	0.019970	1.168880
C	-3.008890	1.277250	0.844290
C	-1.983100	1.441030	-0.127150
C	-1.449040	0.325200	-0.780100
C	-1.610620	-2.293280	-0.907180
C	-2.428380	-3.150290	-0.208600
O	-3.468000	2.437610	1.430420
O	-1.575600	2.731810	-0.350390
S	-0.168560	0.539910	-2.008870
N	-3.237830	-2.429810	0.643310
C	1.286590	0.293090	-1.033260
N	1.269630	0.116610	0.323800
C	2.585660	-0.038090	0.712970
C	3.335660	0.066300	-0.484830
N	2.491030	0.272010	-1.566450
C	3.215630	-0.252460	1.931370
C	4.607000	-0.348510	1.869990
C	5.271850	-0.230060	0.638290
N	4.669600	-0.026530	-0.544520
H	-4.279420	-0.086370	1.914760
H	-0.870250	-2.570840	-1.644130
H	-2.502590	-4.227830	-0.248270
H	-4.144030	2.205310	2.090080
H	-0.892510	2.727280	-1.048180
H	-3.925990	-2.822070	1.271180
H	0.443880	0.097370	0.911090
H	2.667190	-0.338850	2.863790
H	5.185580	-0.515170	2.772650
H	6.356130	-0.307110	0.612130

M4

	x	y	z
C	2.352090	0.806840	-0.760820
C	3.160510	1.526180	0.158690
C	3.733250	0.926260	1.285650
C	3.483030	-0.420140	1.504880
C	2.666370	-1.171990	0.615870
C	2.114000	-0.565530	-0.515360
O	3.989530	-1.114650	2.582910
O	2.470560	-2.488400	0.953440
S	1.114880	-1.541360	-1.640270
C	-0.505920	-1.238320	-0.988980
N	-0.930100	0.019590	-0.623170
C	-2.242860	-0.110520	-0.230270
C	-2.545850	-1.475020	-0.400580
N	-1.433780	-2.163570	-0.871080
N	-3.054950	0.851520	0.219100
C	-4.277900	0.416850	0.520880
C	-4.715440	-0.925960	0.399210
C	-3.840650	-1.894040	-0.068080
O	-5.207990	1.293570	0.983170
C	-4.820620	2.669260	1.119420
C	1.927360	1.739720	-1.764980
C	2.479550	2.955720	-1.434590
N	3.225110	2.830030	-0.283200
H	4.352710	1.487470	1.979620
H	4.522930	-0.505830	3.122140
H	1.886770	-2.894350	0.283840
H	-0.377660	0.870130	-0.645550
H	-5.734940	-1.168020	0.676960
H	-4.147290	-2.930350	-0.170420
H	-5.709350	3.183110	1.489210
H	-4.000910	2.779840	1.836050
H	-4.519540	3.092050	0.156010
H	1.302390	1.532590	-2.622480
H	2.403690	3.911590	-1.933200
H	3.720840	3.580480	0.178770

M5

	x	y	z
C	2.649360	-0.991020	-0.385630
C	3.580910	-1.132640	0.676150
C	4.079490	-0.037040	1.389380
C	3.632660	1.228580	1.040020
C	2.696160	1.413190	-0.014100
C	2.213410	0.311070	-0.727360
O	4.047940	2.377620	1.679940
O	2.314700	2.709280	-0.254300
S	1.060540	0.556520	-2.071350
C	-0.487360	0.336030	-1.236560
C	2.354930	-2.307700	-0.866140
C	3.098850	-3.181240	-0.107940
N	3.838600	-2.478580	0.819140
N	-0.603490	0.201520	0.117680
C	-1.959550	0.073220	0.386230
C	-2.588730	0.146220	-0.879320
N	-1.634950	0.308260	-1.883330
C	-2.680040	-0.088460	1.564000
C	-4.070340	-0.177720	1.463100
C	-4.709230	-0.106050	0.205990
C	-3.978880	0.055740	-0.975260
O	-6.076880	-0.192400	0.042640
C	-6.891460	-0.256370	1.214220
H	4.792570	-0.159730	2.199870
H	4.679630	2.133520	2.378460
H	1.657580	2.708130	-0.976950
H	1.678270	-2.568860	-1.667590
H	3.162950	-4.259320	-0.150840
H	4.465310	-2.884590	1.500420
H	0.159630	0.191080	0.783230
H	-2.187810	-0.143380	2.529680
H	-4.652430	-0.303190	2.367760
H	-4.492040	0.111080	-1.929690
H	-7.923550	-0.270940	0.858360
H	-6.696620	-1.168120	1.792290
H	-6.740340	0.620790	1.855240

M6

	x	y	z
C	-2.515450	-0.752180	-0.042810
C	-3.540640	0.189820	-0.577740
C	-3.480990	1.543380	-0.480780
C	-2.344540	2.115370	0.199830
C	-1.254400	1.154890	0.812100
C	-1.413660	-0.284110	0.629760
C	-2.964230	-2.066800	-0.391200
C	-4.142300	-1.921740	-1.069180
N	-4.496580	-0.590230	-1.178300
S	-0.240160	-1.399670	1.365810
C	1.247520	-0.835770	0.589420
N	2.412730	-0.783040	1.309910
C	3.391290	-0.341740	0.443410
C	2.722830	-0.150050	-0.790780
N	1.382550	-0.481750	-0.672500
C	4.751350	-0.082590	0.565340
C	5.373290	0.369090	-0.598210
C	4.632370	0.530820	-1.782740
N	3.320630	0.282360	-1.909240
O	-2.163460	3.325370	0.335330
O	-0.316750	1.676370	1.409440
H	-4.240360	2.197350	-0.895470
H	-2.467410	-2.997700	-0.163740
H	-4.780610	-2.681520	-1.499830
H	-5.313270	-0.237020	-1.660040
H	2.514260	-0.964880	2.301690
H	5.290020	-0.219500	1.497380
H	6.433450	0.600120	-0.599950
H	5.138150	0.882410	-2.678750

HIPT-IQ

	x	y	z
C	-3.128990	-0.784830	0.036350
C	-4.180420	0.125390	0.575720
C	-4.180720	1.476170	0.444650
C	-3.085230	2.079430	-0.279740
C	-1.970830	1.152220	-0.897870
C	-2.064020	-0.286430	-0.678440
S	-0.868950	-1.370870	-1.429220
C	0.618970	-0.805570	-0.665300
N	0.665940	-0.255530	0.585980
C	1.997160	0.011020	0.845610
C	2.688110	-0.434710	-0.298880
N	1.803730	-0.936070	-1.236560
C	2.691290	0.573700	1.916400
C	4.067840	0.651580	1.769710
C	4.672260	0.175560	0.578980
N	4.023720	-0.360680	-0.447620
O	6.029270	0.302470	0.530500
C	6.695990	-0.151300	-0.655860
C	-3.512240	-2.106390	0.423630
C	-4.680300	-1.995340	1.128620
N	-5.088300	-0.680420	1.218900
O	-2.960880	3.292210	-0.443840
O	-1.066860	1.698900	-1.525050
H	-4.957010	2.108670	0.861360
H	-0.127510	-0.051530	1.182080
H	2.191390	0.928100	2.811880
H	4.696490	1.071310	2.546560
H	7.753550	0.062990	-0.491860
H	6.553600	-1.226600	-0.803470
H	6.339010	0.383880	-1.541400
H	-2.983270	-3.021120	0.203360
H	-5.274170	-2.772800	1.590210
H	-5.909980	-0.351600	1.709470

MMDP-IQ

	x	y	z
C	3.190000	-0.505930	-0.482690
C	4.082990	0.673830	-0.666690
C	3.955940	1.856970	-0.009440
C	2.881190	1.979110	0.943940
C	1.933290	0.743670	1.194100
C	2.155330	-0.473980	0.418600
O	2.645920	3.001530	1.588740
O	1.047470	0.876150	2.033720
S	1.173940	-1.922530	0.736260
C	-0.449240	-1.275520	0.443080
C	3.669920	-1.511960	-1.383670
C	4.743250	-0.981950	-2.041280
N	5.002310	0.309490	-1.617360
N	-1.479700	-1.608800	1.279850
C	-2.614100	-0.988500	0.780370
C	-2.170320	-0.301000	-0.374640
N	-0.808810	-0.511320	-0.568790
C	-3.940800	-0.953070	1.198430
C	-4.837150	-0.207100	0.432400
C	-4.406770	0.477640	-0.727130
C	-3.073420	0.439930	-1.141560
O	-5.250200	1.219470	-1.526950
C	-6.626180	1.314080	-1.154680
H	4.619370	2.698300	-0.177480
H	3.261610	-2.502020	-1.518780
H	5.367520	-1.429490	-2.802860
H	5.728030	0.912530	-1.982400
H	-1.403530	-2.126250	2.147140
H	-4.273240	-1.479940	2.087080
H	-5.874150	-0.161470	0.740900
H	-2.762250	0.972080	-2.034500
H	-7.095980	1.942200	-1.914100
H	-7.110470	0.329870	-1.148860
H	-6.745610	1.784560	-0.170990

MOBI-IQ

References

1 Y. Wang, J. Su, T. Li, P. Ma, H. Bai, Y. Xie, M. Chen and W. Dong, *ACS Appl. Mater. Interfaces*, 2017, **9**, 36281-36289.