Supporting Information

Post-functionalization of Sulfur Quantum Dots and Their Aggregation Dependent Antibacterial Activity

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EXPERIMENTAL SECTION:

1. Materials and methods: All the reagents and solvent were purchased from the commercial sources (Sigma Aldrich and SRL India Pvt. Ltd.) and used without further purification. Bruker spectrometer of 400 MHz was used to measure the NMR spectra and TMS (Me_4Si) was used as an internal standard. The NMR data were reported as: δ (ppm), represents the chemical shift value with respect to tetramethyl silane. The multiplicity of a peak was represented as: s = singlet, d = doublet, t = triplet, q = quartet, br = broad, m = multiplet. High resolution mass spectra were recorded on XEVO G2-XS QTof instrument. AFM images were acquired using JPK Instrument and processed by using JPK software. UV-Visible spectra were recorded on UV-3600 Shimadzu UV-Vis-NIR Spectrophotometer. Photoluminescence spectra were recorded on Thermo Scientific Varioskan Flash Multimode Reader. Zeta potential and hydrodynamic diameter of the functionalized SQDs were recorded by Malvern Zetasizer Nano instrument. TEM image of quantum dot was acquired using a FEI Tecnai T20 super twin microscope, operating at 200 kV. High resolution imaging and STEM-EDS mapping was acquired in FEI Titan microscope at an acceleration voltage of 300 kV. The bacterial TEM image and STEM-EDS mapping was acquired by JOEL JEM-2100F instrument. SEM images of bacteria were recorded by using Ultra55 FE-SEM Karl Zeiss EDS instrument. The X-ray photoelectron spectroscopy (XPS) measurements were carried out using a Thermo K-Alpha spectrometer.

2. Scheme of synthesis of ligands:

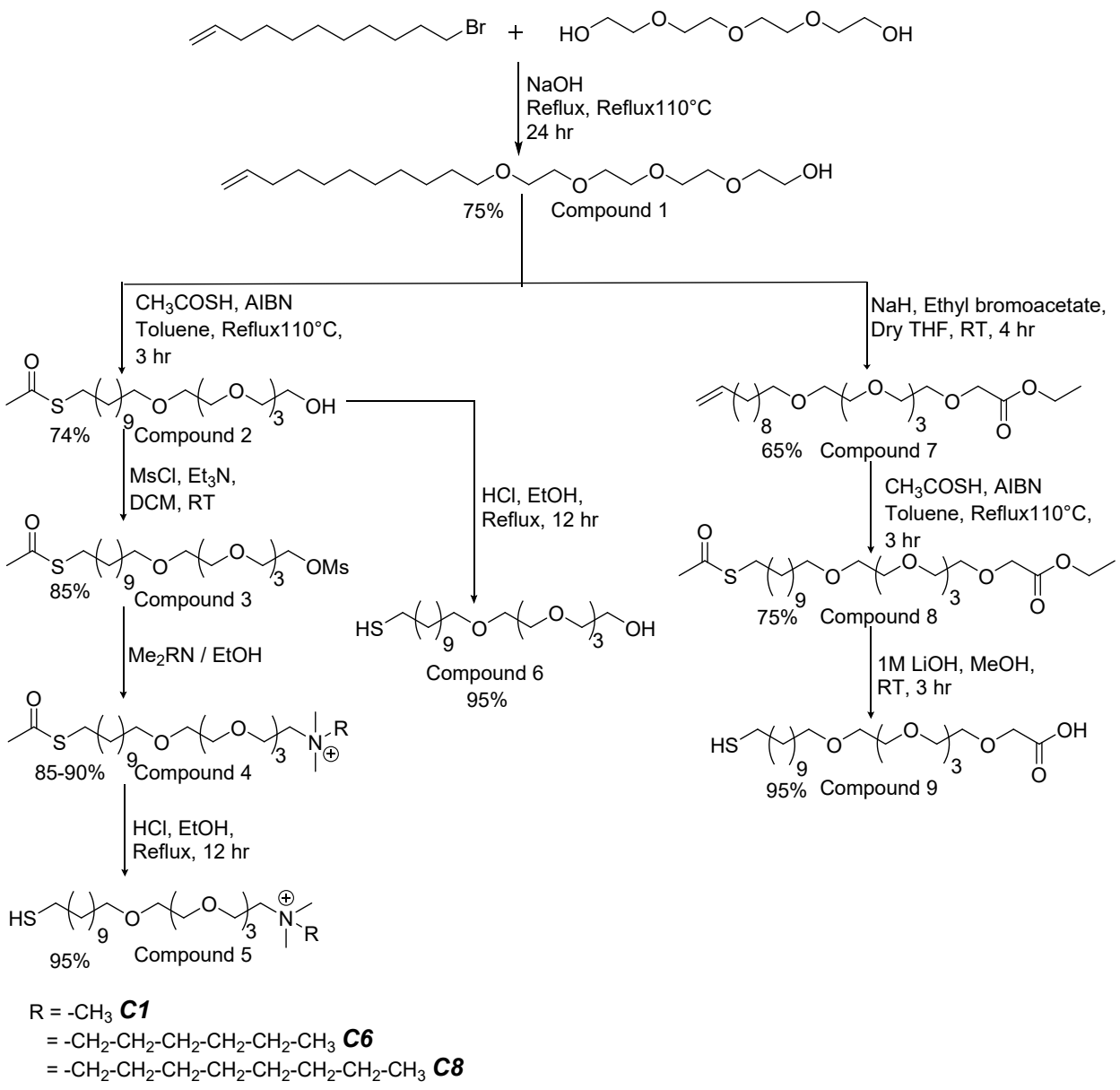


Figure S1. Scheme of synthesis of lignds.

Synthesis of compound 1: Sodium hydroxide (21.4 mmol) and tetraethyleneglycol (106.5 mmol) were taken in a round bottom flask and the mixture was stirred for 30 minutes at 110°C under argon atmosphere. After that 11-bromoundec-1-ene (21.4 mmol) was added slowly and the reaction was allowed to stir for another 24 hours. After the completion of the reaction, the crude product was extracted by washing with hexane (six times). The crude contains both the

monoalkylated and dialkylated product. The monoalkylated product was purified through column chromatography with a yield of 75%. The product was confirmed by ^{1}H-NMR spectra.

Synthesis of compound 2: Compound 1 was dissolved in dry toluene and to it, AIBN (0.3 equivalence) and thiol acetic acid (11.44 mmol) were added. The reaction mixture was refluxed at 110°C for 3 hours. After completion of the reaction, the crude reaction mixture was washed with saturated sodium bicarbonate solution (3 times). The organic layer was concentrated and then subjected to column purification. The product was confirmed by ^{1}H-NMR spectra. The overall yield of the reaction was 74%.

Synthesis of Compound 3. In a round bottom flask the compound 2 was dissolved in DCM and put over ice. To it triethylamine (8.802 mmol) was added, and the reaction mixture was allowed to stir for 15 minutes. Then methane sulfonyl chloride (6.6 mmol) was added dropwise, and the reaction mixture was stirred for overnight at room temperature. After completion of the reaction, the crude reaction mixture was washed with dilute HCl (0.1 M, 2 times) and then with saturated sodium bicarbonate solution (3 times). The organic layer was dried over anhydrous sodium sulfate and concentrated in vacuum. The crude reaction mixture was purified through column chromatography and was confirmed through ^{1}H-NMR spectra. The overall yield of the reaction was 85%.

Synthesis of Compound 4. The compound 3 was dissolved in 15 ml ethanol in three different round bottom flasks. Then, separately trimethylamine (for R=CH_3), N,N-Dimethylhexylamine (for R=C_6H_{13}) and N,N-Dimethyloctylamine (for R=C_8H_{17}) were added in those RB. The reaction mixtures were stirred under an argon atmosphere at room temperature for R=CH_3 and refluxed for R=C_6H_{13} and R=C_8H_{17}. The disappearance of starting material in TLC confirms the formation of the product. The product thus formed was purified by trituration of the crude product in hexane: ether (1:1) for three times. The overall yield of the reactions was 85-90 %. At the end, the products were characterised through ^{1}H NMR spectra.

Synthesis of Compound 5 (Positive C1, C6 and C8 Ligand). The compound 4 was dissolved in 20 ml ethanol and to it 1 ml of HCl was added. The reaction mixture was refluxed for 12 hours. After the completion of the reaction, the solvent was evaporated, and the crude was subjected to

solvent precipitation using hexane and diethylether (1:1). The final product was confirmed through ^{1}H NMR and HRMS spectra with overall yield of 95%. (For R=CH_3, R=C_6H_{13} and R=C_8H_{17}).

Synthesis of compound 6. In a round-bottomed flask, Compound 2 was dissolved in 20 ml ethanol and to it, 1 ml of HCl was added. The reaction mixture was refluxed for 12 hours. After the completion of the reaction, the solvent was evaporated, and the crude was subjected to column purification. The product was confirmed by ^{1}H NMR with an overall yield of 95%.

Synthesis of compound 7. In a round-bottomed flask, 10 ml of dry THF was taken and to it, sodium hydride (6.92 mmol) was added and the RB was kept at 0°C under an argon atmosphere. Next, compound 2 (5.77 mmol) was dissolved in dry THF and added to the reaction mixture under argon atmosphere. The reaction mixture was allowed to stir for 15 minutes. Subsequently, ethylbromoacetate was added dropwise to the reaction mixture under cold conditions and left to stir for 4 hr. After completion of the reaction, excess sodium hydride was quenched by adding few drops of water. The crude mixture was then concentrated using a rotatory evaporator and redissolved in ethyl acetate. The ethyl acetate was then washed three times with brine solution and concentrated with a rotatory evaporator. The crude mixture was subjected to column purification. The purified product was confirmed through ^{1}H NMR with an overall yield of 65%.

Synthesis of compound 8. The synthetic procedure is similar for the synthesis of compound 2. After column purification, the product was confirmed through ^{1}H NMR. The overall yield of the reaction was 75 %.

Synthesis of compound 9. In a round bottom flask compound 8 (1.96 mmol) was taken and dissolved in methanol. To it, 5 ml of 1M lithium hydroxide solution was added and stirred at room temperature for 4 hr. After the completetation of the reaction, the solution was cooled to 0°C and the pH was adjusted to 2 by the addition of 1M HCl. Later, the solvent was evaporated, and the crude was redissolved in ethyl acetate. The ethyl acetate was then washed with brine for three times and concentrated. The crude mixture was subjected to column purification and the product was confirmed by ^{1}H NMR.

Compound 5 C1 (R= -CH_3): ^{1}H-NMR (400 MHz, $CDCl_3$): δ 4.0156 (bs, 2H, -CH_2-N+-), 3.868-3.599 (14H, -O-CH_2-CH_2-O-), 3.482-3.449 (t, 2H, -CH_2-**CH_2**-O-), 3.397 (s, 9H, -N+ $(CH_3)_3$), 2.913 (s, 3H, CH_3-SO_3-), 2.726- 2.539 (m, 2H, -CH_2-SH), 1.711-1.574 (m, 4H, -CH_2-), 1.397-1.295 (m, 14H, -CH_2).

Compound 5 C6 (R= -C_6H_{13}): ^{1}H-NMR (400 MHz, $CDCl_3$): δ 3.958 (b, 2H, -O-**CH_2**-CH_2-N-), δ 3.765 (b, 2H, -O-CH_2-**CH_2**-N-), 3.610-3.551 (m, 12H, -O-CH_2-CH_2-O-), 3.473-3.407 (m, 4H, -CH_2-N $(CH_3)_2$-**CH_2** & -CH_2-**CH_2**-O-), 3.289 (s, 6H, -N$(CH_3)_2$-), 2.832 (s, 3H, CH_3-SO_3-), 2.681-2.497 (m, 2H, -**CH_2**-SH), 1.737-1.2549 (m, 24 H, -CH_2-), 0.882 (b, 3H, -CH_3-).

Compound 5 C8 (R= -C_8H_{17}): ^{1}H-NMR (400 MHz, $CDCl_3$): δ 3.924 (b, 2H, -O-**CH_2**-CH_2-N-), δ 3.759 (b, 2H, -O-CH_2-**CH_2**-N-), 3.613-3.518 (m, 12H, -O-CH_2-CH_2-O-), 3.456-3.375 (m, 4H, -CH_2-N $(CH_3)_2$-**CH_2** & -CH_2-**CH_2**-O-), 3.273 (s, 6H, -N$(CH_3)_2$-), 2.740 (s, 3H, CH_3-SO_3-), 2.650-2.448 (t, 2H, -CH_2-SH), 1.705-1.225 (m, 28 H, -CH_2-), 0.836-0.819 (b, 3H, -CH_3-).

Compound 6 : ^{1}H-NMR (400 MHz, $CDCl_3$): δ 3.741-3.582 (m, 16H, -O-CH_2-CH_2-O-), 3.464-3.430 (t, 2H, - CH_2-CH_2-O-), 2.545-2.490 (m, 2H, -**CH_2**-SH), 1.619-1.557 (m, 4H, -CH_2-), 1.367-1.265 (m, 14H, -CH_2).

Compound 9: ^{1}H-NMR (400 MHz, $CDCl_3$): δ 4.155 (s, 2H,-O-CH_2-CO-), 3.745-3.580 (m, 16H, -O-CH_2-CH_2-O-), 3.471-3.438 (t, 2H, -CH_2-**CH_2**-O-), 2.693-2.490 (m, 2H, -**CH_2**-SH), 1.681-1.556 (m, 4H, -CH_2-), 1.265 (m, 14H, -CH_2).

3. Preparation and functionalization of sulfur quantum dots (SQDs): Sulfur quantum dots (SQDs) were prepared by a bottom up hydrothermal method using sublime sulfur, *p*-phenylenediamine as a precursor and tetraethylene glycol as a stabilizer. Briefly, 200 mg sublime sulfur, 200 mg *p*-phenylenediamine and 2 ml of tetraethylene glycol were added to 25 ml of water. The mixture was then transferred to a 25 mL teflon-lined stainless-steel for autoclave and heated at 200 °C for 24 hours. After completion of the reaction, the SQD was purified through column

chromatography by using ethyl acetate and hexane mixture. The purified SQDs were characterized through different characterization techniques and proceeded for functionalization.

To achieve the surface functionalization of SQD, 3 mg of ligand was added to 1 mg of SQD in water and stirred at room temperature for 48 hours. After 48 hours, the solution was washed repeatedly with DCM (6 times) to remove all the unbound ligands. Subsequently, the functionalized materials were characterized by different characterization techniques to confirm the effective surface functionalization. We have measured the concentration of SQD by lyophilizing the stock solution and followed by measured the extinction coefficient using UV-Vis spectra at different weight concentrations (Figure S14a). By using the extinction coefficient value, the concentration of the functionalized materials was evaluated. This methods provides higher accuracy for evaluating the MIC and MBC values.

4. Determination of MIC and MBC: Two gram-positive (*Methicillin-resistant Staphylococcus aureus* (MRSA)*, Enterococcus faecalis* (*E. faecalis*)) and two gram-negative bacterial strains (*Pseudomonas aeruginosa* (PA)*, Escherichia coli* (E.coli)) were chosen to check the antibacterial efficacy of functionalized SQDs compared to the unfunctionalized one. At first, the freeze-dried bacterial species were revived by incubating at 37°C on a nutrient agar plate. To prepare the primary stock, the bacterial colonies formed on the agar plate were cultured overnight (10 -12 hr) in Luria broth media (LB, HiMedia – 20 g/L). Later, 100 µL of primary stock was added to 10 mL fresh LB media and incubated at 37°C until it reaches the mid-log phase (OD_{620nm}~0.3), and then optical density was adjusted by diluting in LB to 0.01 (10^6 to 10^7 bacteria/ mL) for further experiments. For evaluating the minimum inhibitory concentrations (MIC), 100 µL of the bacterial solutions were added to 100 µL of different concentrations of functionalized SQDs in 96 well plate and then the optical density of the solutions were measured for a period of 16 hr by using a microplate reader equipped with shaker and incubator (37 °C). The concentration of functionalized SQDs at which no growth of bacterial curve was observed was known as MIC. After 16 hr, the treated solutions were then streaked on a nutrient agar plate and incubated for another 12 hr. The minimum concentration at which no colony formation on the agar plate was observed is termed MBC concentration.

5. Live/dead assay using fluorescence microscopy: The different bacteria-killing abilities of the functionalized SQDs were assessed by staining the bacteria with calcein-AM (green) and propidium iodide (red). Briefly, MRSA bacteria was harvested by centrifugation at 5000 rpm and resuspended in PBS. The bacterial solution having OD=0.2 was incubated with 500 ng/ml (MIC of C1@SQD) concentration of functionalized SQDs at 37°C for 1 hr. After treatment, the bacterial solution was washed two times with PBS and then stained with 4 μM of calcein-AM and propidium iodide for 30 minutes. Thereafter the extra dye was removed by centrifugation and resuspended in PBS buffer. Subsequently 10 μL of the stained bacterial solution was drop-casted on a clean glass slide and visualized in confocal microscope.

6. Estimation of Oxidative Stress: Oxidative stress generated by functionalized SQDs was estimated by Ellman's assay. Briefly, 0.8 mM GSH was prepared in 50 mM bicarbonate buffer with pH 8.6 and was added to functionalized SQDs so that the final concentration of GSH becomes 0.4 mM. Parallelly, two controls were taken: positive control where 10 mM H_2O_2 was added to GSH and negative control where no material was added. The solutions were then incubated at 37°C for 1 hr. At the end of 1 hr, 100 μL of the solution was added to 100 μL of 2 mM DTNB (5,5′- dithiobis(2-nitrobenzoic acid)) in a 96-well plate. DTNB solution was prepared in 50 mM TRISHCl buffer (pH 8.3). The absorbance of the resulting solution was measured at 412 nm and

$$\left(1-\frac{A_{412}\ of\ the\ sample\ at\ particular\ time}{A_{412}\ of\ the\ negative\ control\ at\ 0\ minute}\right)_{\times 100\ \%}$$

the percentage loss of glutathione was calculate by the formula given below.

To assess the effectiveness of SQD in generating hydroxyl radicals, we introduced isopropyl alcohol (0.4 mM) into the Ellman's assay procedure (Figure. b). Isopropyl alcohol (IPA) is recognized for its ability to quench hydroxyl radicals within a solution. However, under our experimental conditions, we did not observe any change in glutathione level compared to the control.

7. Estimation of membrane depolarization ability of functionalized SQDs: The membrane depolarization ability of the functionalized SQDs was measured following the reported method. At first, the bacteria was harvested by centrifugation at 5000 rpm for 5 min from the mid-log phase culture. The pellet was then washed with a 1:1 mixture of HEPES buffer (5 mM) of pH 7.2 and

glucose (5 mM). After washing, it was again resuspended in a 1:1:1 mixture of 5 mM HEPES buffer, 5 mM glucose and 100 mM KCl solution. Subsequently, 98 µl of the bacterial solution having OD 0.2 was added to 2 µL of 5 mM $DISC_3(5)$ dye and was incubated for 30 minutes. Later, 100 µl of functionalized SQDs having a concentration of 8 µg/ml was added to the bacterial solution (final concentration 4 µg/ml) and the change in the fluorescence was monitored for the next 2 minutes (excitation wavelength was 622 nm and an emission wavelength was 670 nm). The Enhancement in fluorescence intensity with the addition of functionalized SQDs with respect to control quantifies the membrane depolarization ability.

8. Intracellular ROS Study with DCFDA Probe: At first, bacteria were harvested from the mid-log phase culture and resuspended in PBS buffer. Subsequently, 100 mM DCFDA dye was prepared in dimethylsulfoxide (DMSO) and 20 µL of this was added to 1 ml bacterial solution having OD 0.1. The mixture was kept at 37°C for 30 minutes. After that, 100 µL of the bacterial solution was added to 100 µL of functionalized SQDs (final concentrations 400 ng/ml) and the change in fluorescence intensity was measured with an excitation wavelength of 485 nm and an emission wavelength of 527 nm. An increase in fluorescence intensity signifies intracellular ROS generation.

9. Hemolysis assay: For the hemolysis assay, 2.0 mL of freshly drawn human blood from a healthy donor was centrifuged at 5000 rpm for five minutes. The supernatant was pipetted out and the precipitated RBCs were resuspended in cold PBS. After repeated washing for two times, the RBCs were redispersed in 2 mL of cold PBS. Consequently, 1 ml of this was dissolved in 24 ml of PBS (final volume 25 mL). From this stock, 300 µL of the solution was added to 300 µL of different concentrations of functionalized SQDs and incubated for 1 hr at 37°C (final RBCs conc 2%). 0.1% of Triton X-100 was used as a positive control and PBS was used as a negative control. After 1 hr, the samples were centrifuged at 5000 rpm for 5 minutes and 200 µL of supernatant was taken out. Subsequently, the absorbance was measured at 570 nm and the percentage of hemolysis was calculated by comparing the positive and negative control.

10. Cytotoxicity assay: At first, human cervical cancer cell (HeLa) lines were grown in Dulbecco's modified Eagle's medium (DMEM, Gibco) supplemented with 10% fetal bovine

serum (FBS, Gibco) at 37 °C in 5% CO_2. Then, cells with a seeding density of approximately 10000 cells / well were seeded in 96-well plate for 24 h in a 37°C humidified incubator (5% CO_2). Thereafter, the medium was withdrawn and washed with DPBS buffer. Subsequently, 100 µL of fresh medium containing the functionalized SQDs were added and incubated for another 24 hours. Thereafter the cell viability was checked by MTT dye (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide). Upon incubation for 4 hr with the dye, the viable cell converts the dye to insoluble formazan. The formazan crystals were then dissolved in 100 µL of DMSO and the relative cell viability was obtained by measuring the absorbance at 570 nm.

11. SEM sample preparation for bacterial imaging: For SEM sample preparation, MRSA bacteria having OD=0.01 (in PBS) were incubated with the functionalized SQDs at 37°C for 3 hr. The concentration of SQDs were adjusted according to their MIC values. After incubation, the unbound materials were removed by centrifugation at 5000 rpm for 5 min. Thereafter, the treated bacterial pellets were resuspended in 3% glutaraldehyde in PBS and incubated for 1 hour. After incubation, the solution was centrifuged to collect the cells and was dehydrated using different ethanol gradients (30, 50, 70 and 100 %). Subsequently 10 µL of the solution was drop-casted on a silicon wafer and sputtered with gold prior to imaging in SEM.

12. TEM sample preparation for bacterial imaging: MRSA bacteria were harvested at the mid-log phase (OD_{620nm}~0.3) and were washed with PBS buffer thrice and then resuspended in DI water. Subsequently, the bacterial solutions were treated with functionalized SQDs according to their MIC concentrations and incubated at 37°C for 1 hour. After 1 hour, the unbound material was removed by centrifugation. Then 10 µL of the treated bacterial solution was drop casted in UV treated carbon-coated copper for 10 minutes. After 10 minutes the solution was blotted by using a blotting paper and negative staining was performed using 0.5% uranyl acetate and used for TEM imaging.

13. *In vivo* antibacterial study: The protocols for the care and management of the animals followed the guidelines established by the national organization, the 'Committee for the Purpose of Control and Supervision of Experiments on Animals (CPCSEA),' and received approval from the Animal Ethics Committee at the Indian Institute of Science (IISc), Bengaluru, under proposal

number CAF/Ethics/894/2022. The *in vivo* experiments were carried out on female BALB/c mice. In this study, at first mice were anesthetized with a mixture of xylazine and ketamine. The xylazine and ketamine solution was prepared by adding 80:20 ratio in PBS, and then 100 µL/10-gram dose was injected through IP. Then the circular wound was created (8 mm diameter) through scalpel method using sterile surgical scissors. Thereafter, the mice were infected by 10 µl of bacterial suspension (10^7 CFU/ml, 0.1 OD) containing Methicillin-resistant *Staphylococcus aureus.* After 1 hour of inoculation the wounds were treated according to the MBC value of the functionalized SQDs on day 1 and day 3. PBS buffer was used as a negative control and vancomycin was used as a positive control. The concentration of SQD and vancomycin used in this study were 10 µg/ml and 20 µg/ml respectively. The reduction in the wound size of the mice of different groups were monitored on day 3, day 5, day 7 and day 10. Parallelly, the bactericidal effect of the treated materials on the wound was evaluated by estimating the number of colony formation on the agar plate. At first, the swab stick was rubbed on the wounds area and homogenized in PBS buffer. The solutions were then streaked on the agar plate and incubated at 37°C for 12 hr. The photographs of the agar plates are shown in Figure S21. After 10^{th} day the blood of the mice was collected and then the mice were sacrificed to harvest the major organs for the histological evaluation. The wound tissue and major organs were stained with H&E (Hematoxylin and eosin stain) for the evaluation of wound maturity and toxicity. After 10^{th} day, the amounts of collagen deposition on the healed tissue were evaluated by Masson's trichrome staining. In addition, the inflammatory response upon treatment with the functionalized SQDs were evaluated by TNF-α and IL-6 immune response by staining with diaminobenzidine (DAB).

Additional Figures

14. ^{1}HNMR Spectra of compound 5 (R= -CH_3)

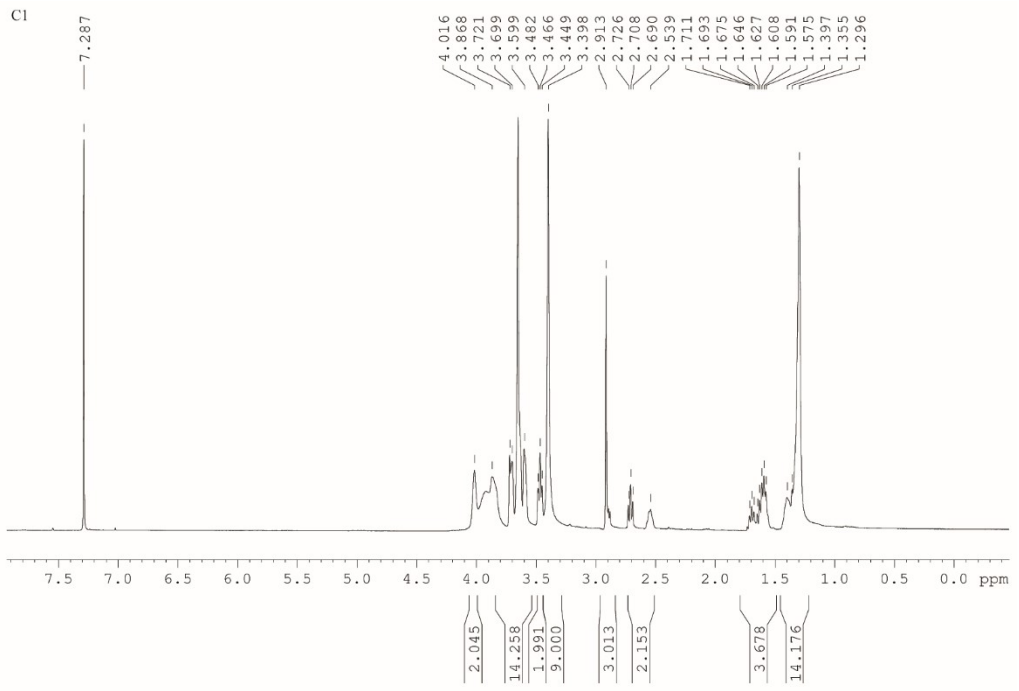


Figure S2. ^{1}H NMR spectra of positive C1 ligand.

15. HRMS spectra of compound 5 (R= -CH_3)

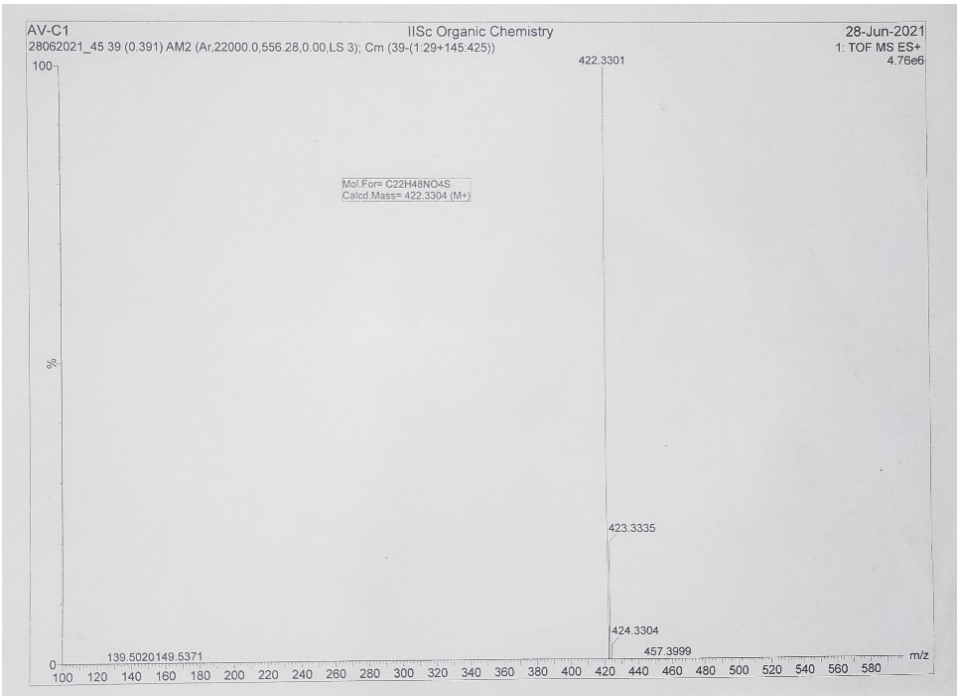


Figure S3. HRMS spectra of positive C1 ligand.

16. ^{1}HNMR Spectra of compound 5 (R= -C_6H_{13})

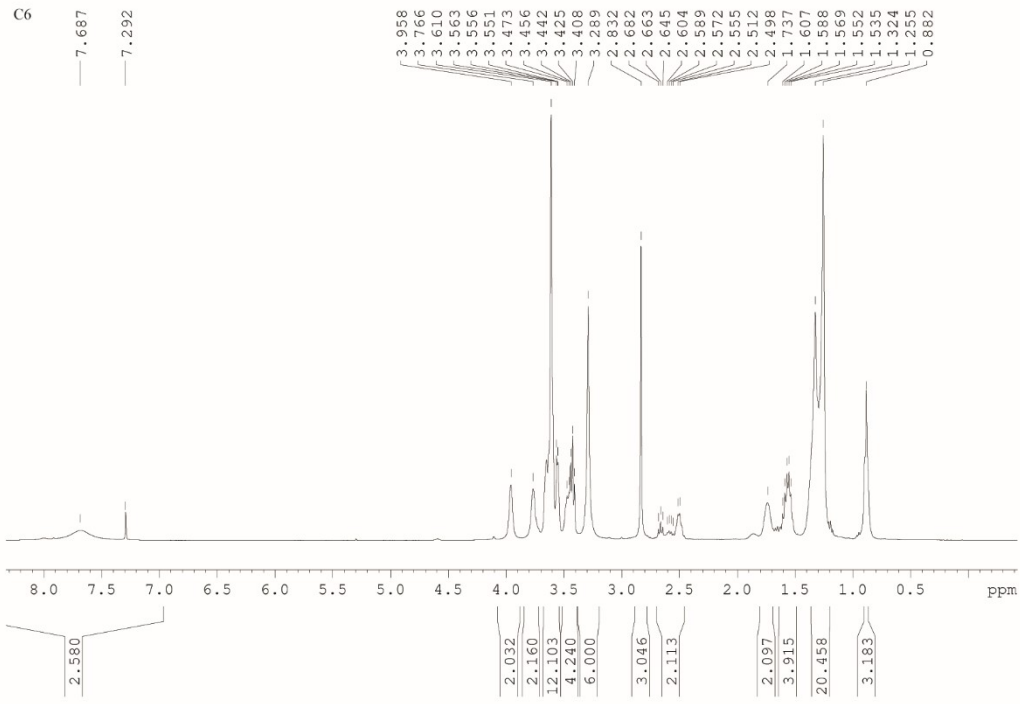


Figure S4. ^{1}H NMR spectra of positive C6 ligand.

17. HRMS spectra of compound 5 (R= - C_6H_{13})

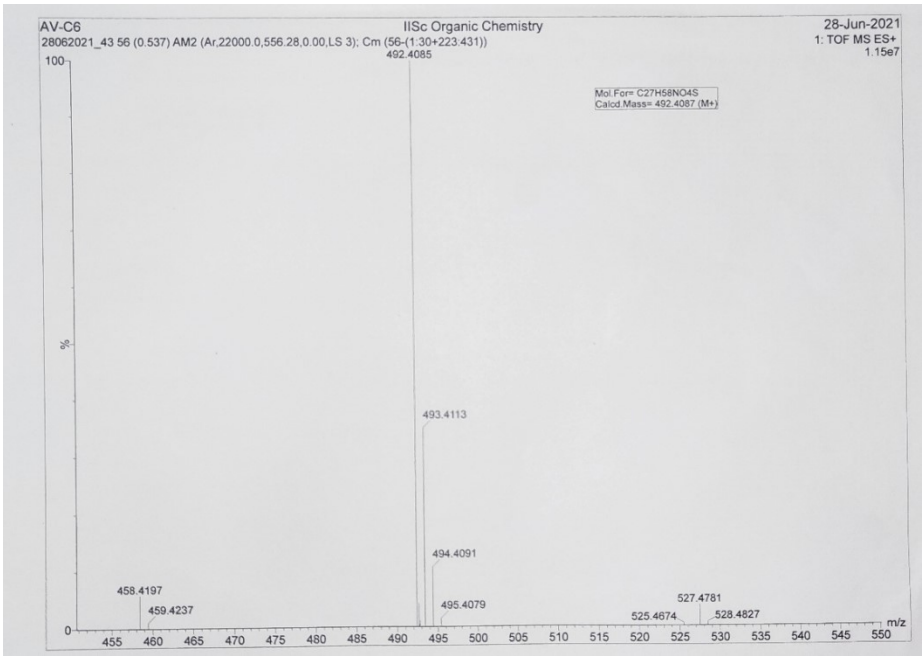


Figure S5. HRMS spectra of positive C6 ligand.

18. ^{1}HNMR Spectra of compound 5 (R= -C_8H_{17})

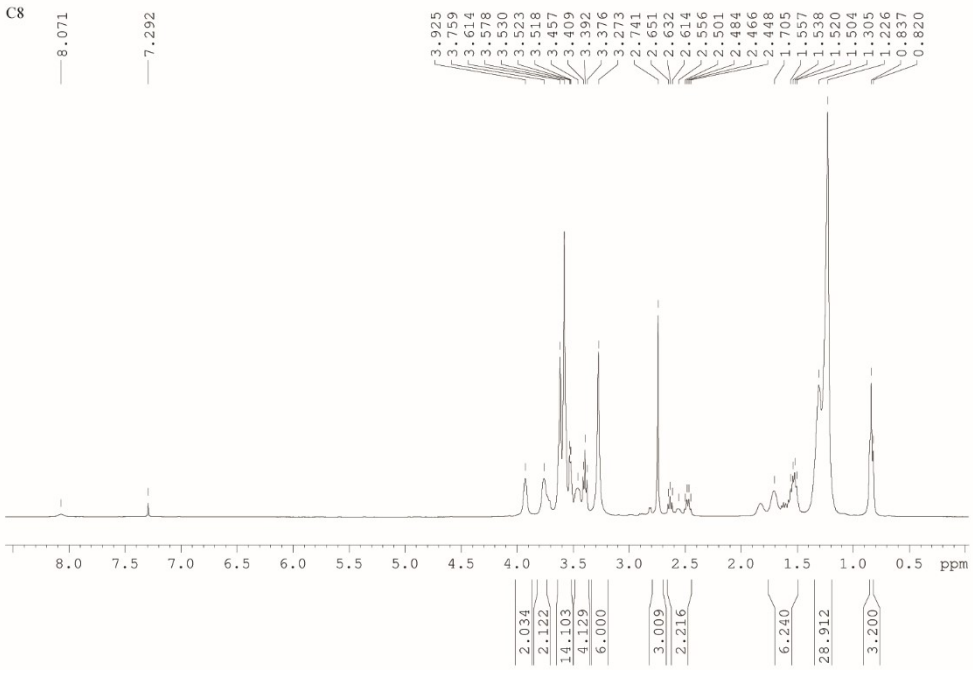


Figure S6. ^{1}H NMR spectra of positive C6 ligand.

19. HRMS spectra of compound 5 (R= - C_8H_{17})

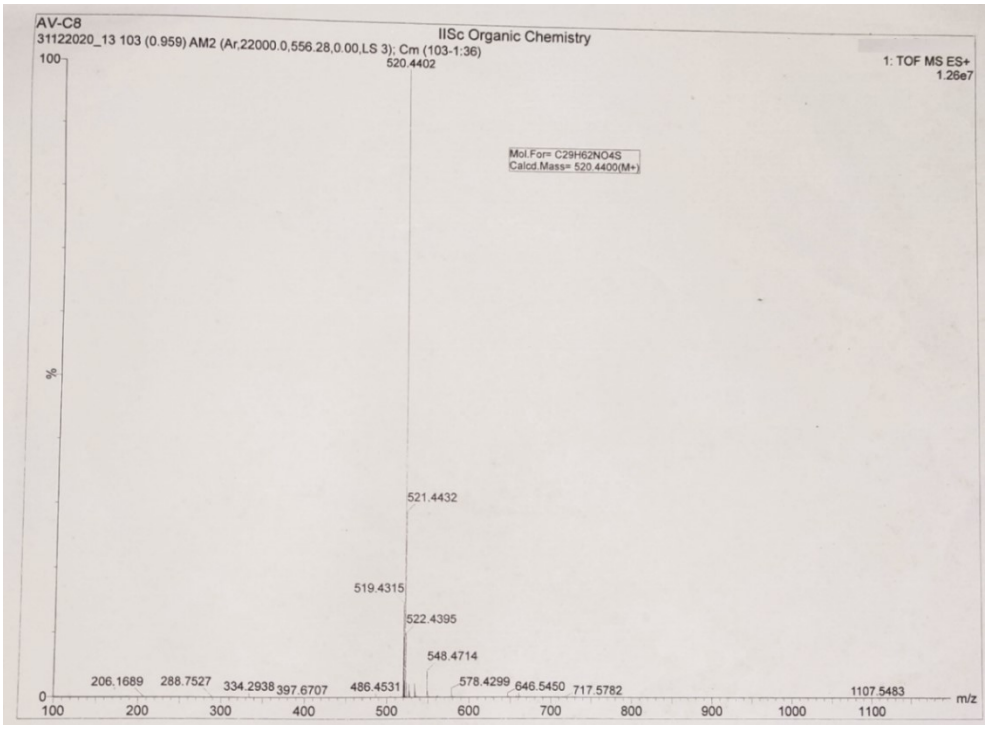


Figure S7. HRMS spectra of positive C8 ligand.

20. ^{1}HNMR Spectra of compound 6.

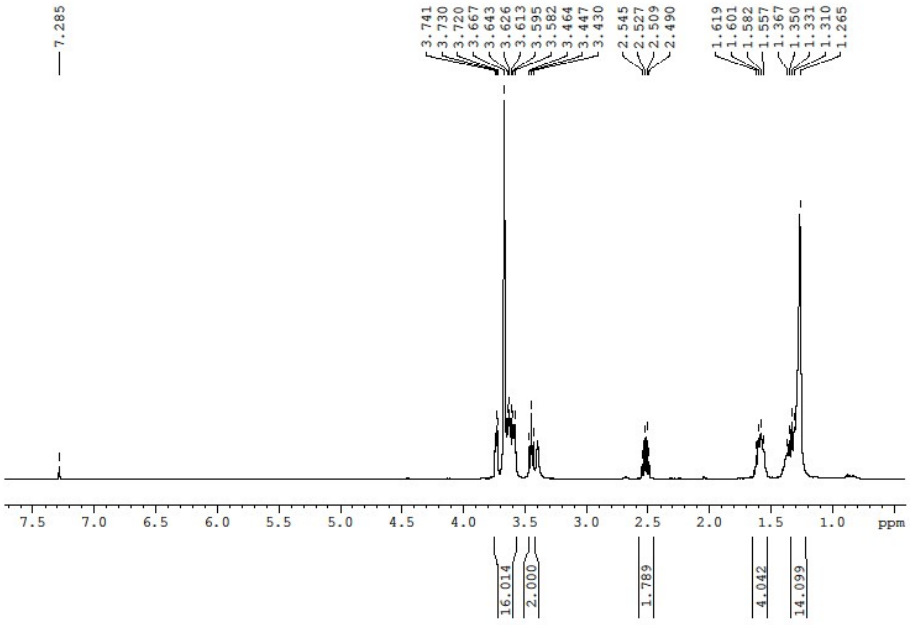


Figure S8. ^{1}H NMR spectra of neutral ligand.

21. HRMS spectra of compound 6.

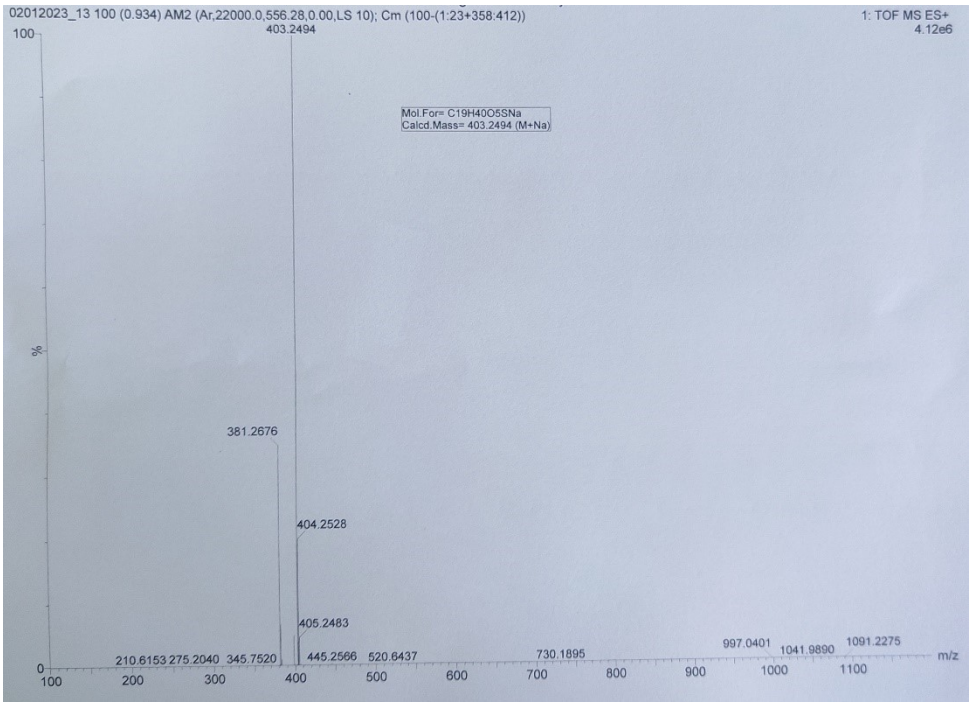


Figure S9. HRMS spectra of neutral ligand.

22. ^{1}HNMR Spectra of compound 9.

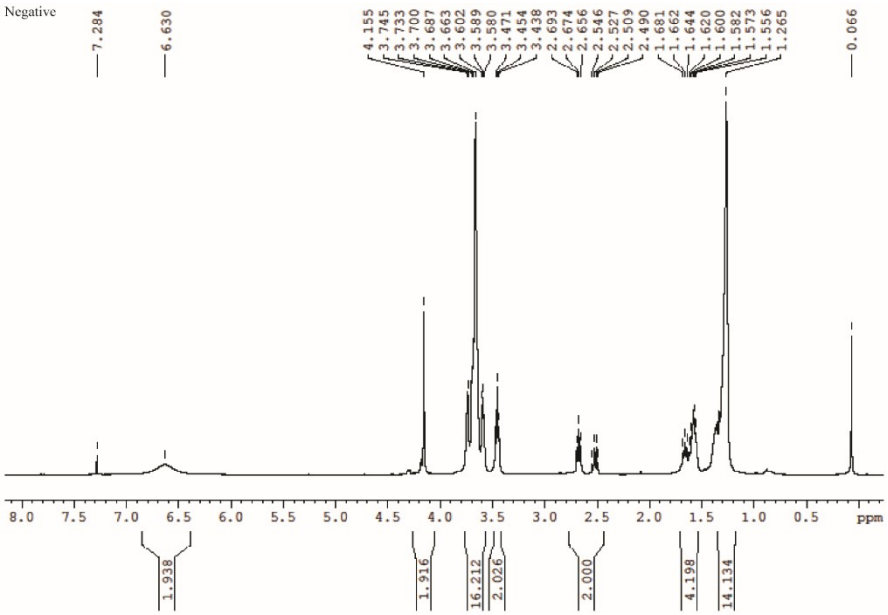


Figure S10. ^{1}H NMR spectra of negative ligand.

23. HRMS spectra of compound 9.

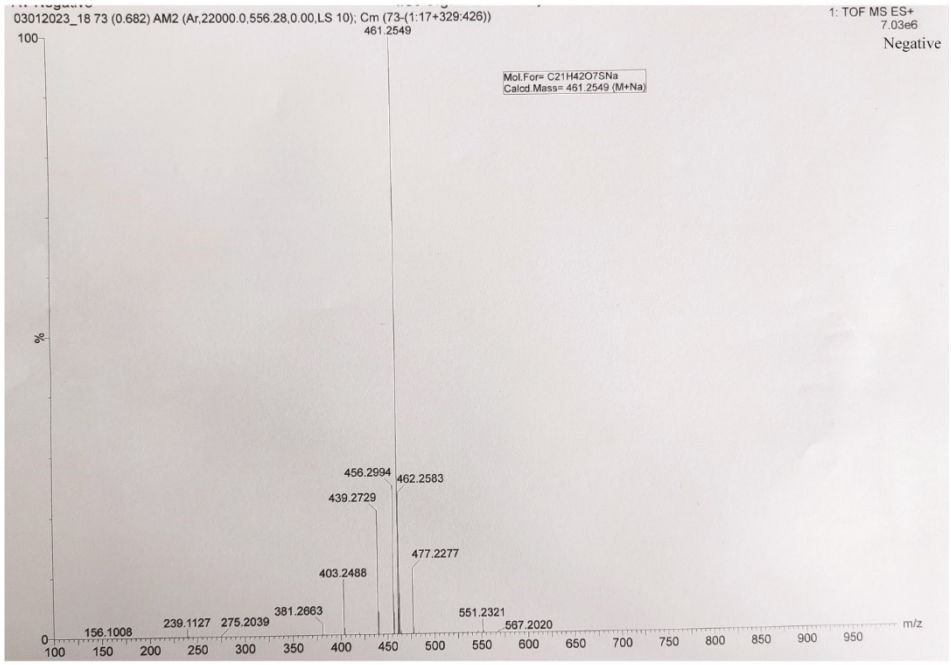
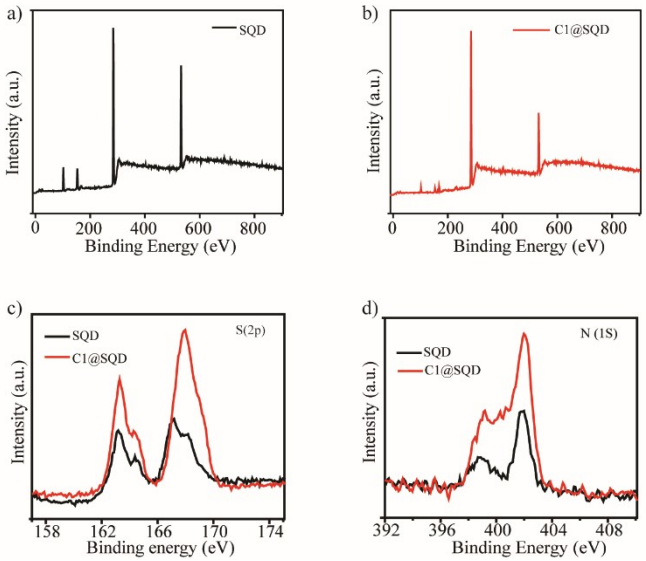


Figure S11. HRMS spectra of negative ligand.



24. XPS spectra of SQD and functionalized SQD.

Figure S12. (a) Full range XPS spectra of SQDs. (b) Full range XPS spectra of C1@SQD. (c) XPS spectra of S (2p) of SQD and C1@SQD. (d) XPS spectra of N (1s) of SQD and C1@SQD.

25. IR spectra.

Figure S13. IR spectra of SQD and functionalized SQD.

26. UV-Vis spectra of functionalized SQDs.

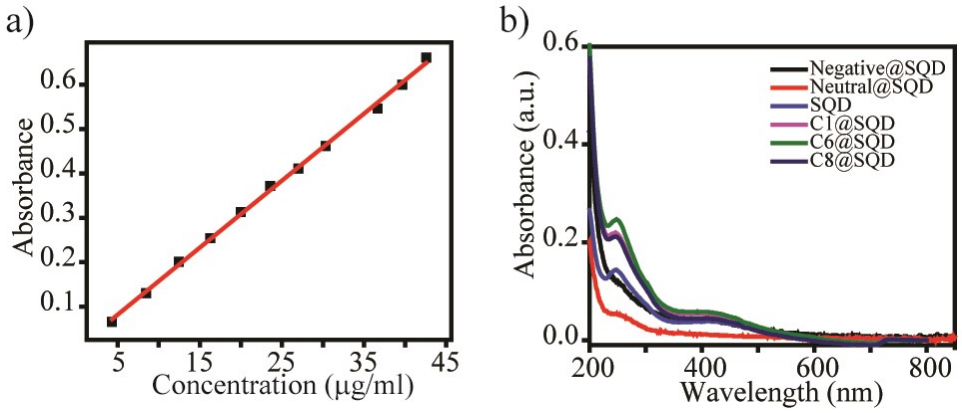
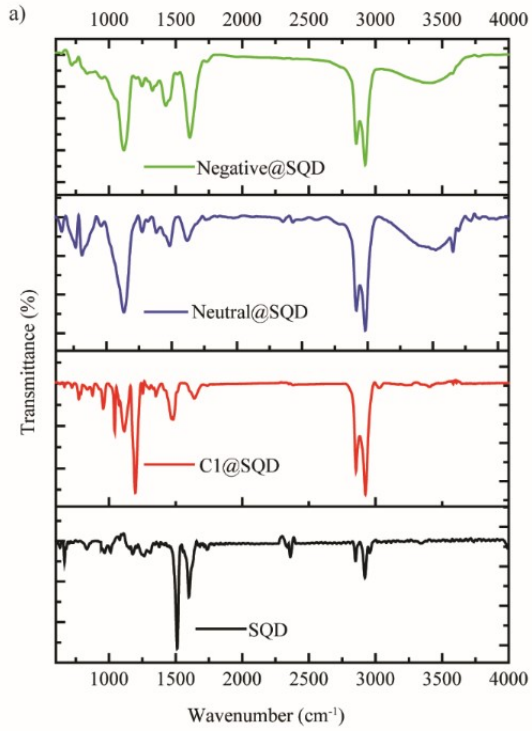


Figure S14. (a) Absorbance of SQDs at various concentration at 420 nm. The linear fitting was used to determine the extinction coefficient of SQD. The extinction coefficient is 0.0151 $\mu g^{-1}mLcm^{-1}$(b) UV-vis spectra of functionalized SQDs.



27. Antibacterial activity of functionalized SQD against E. faecalis and E. coli.

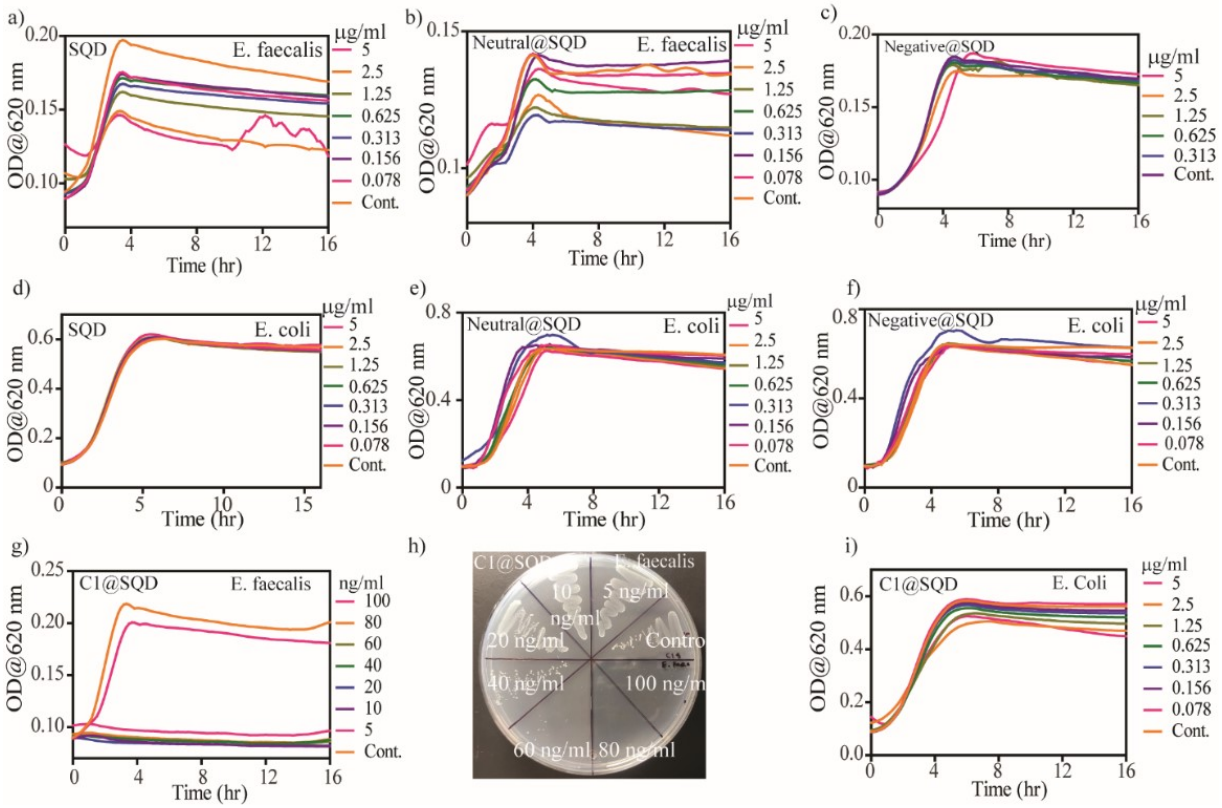
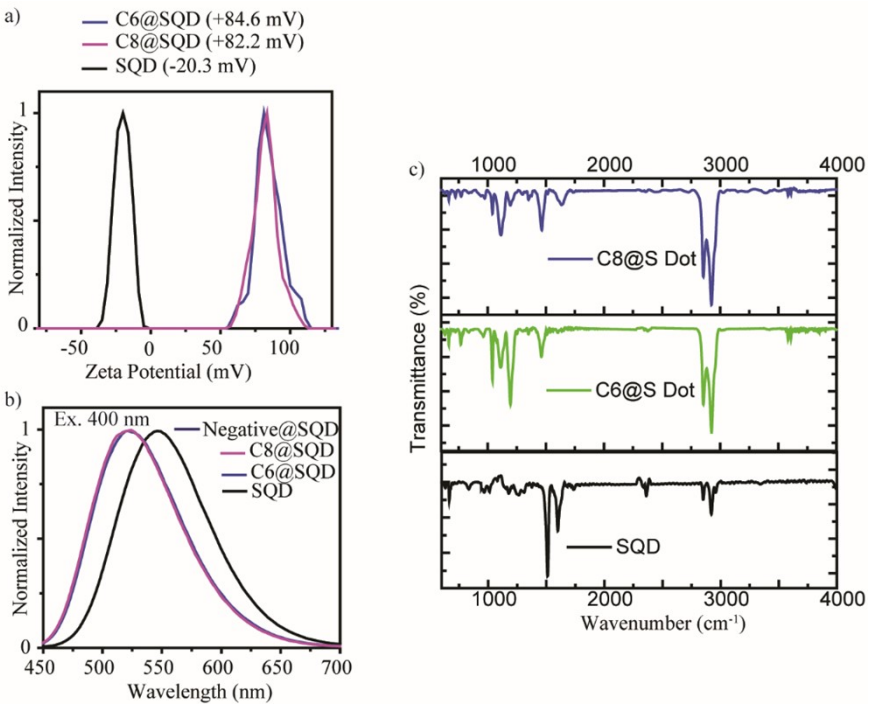
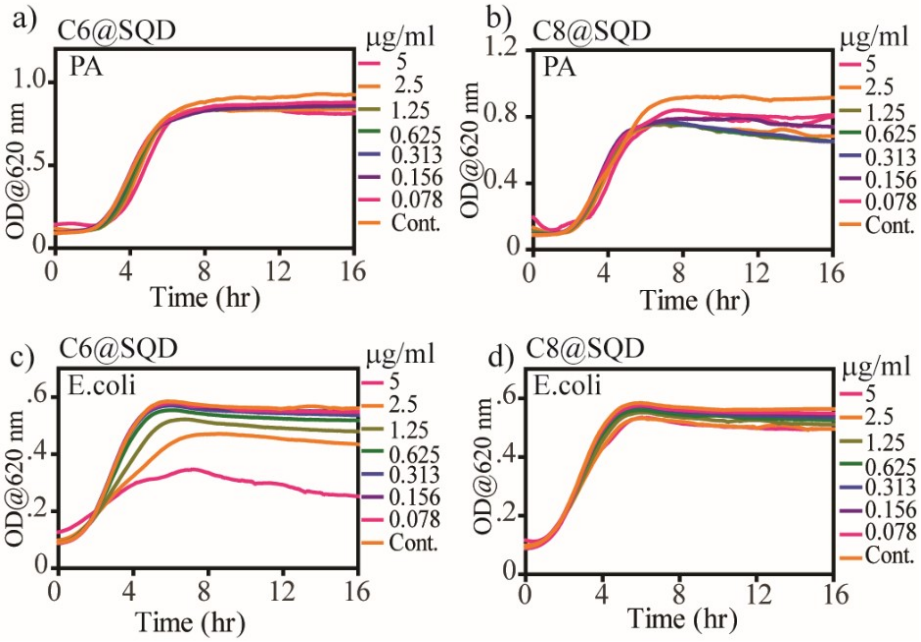


Figure S15. Growth kinetic curve of E. faecalis in presence of (a) only SQD, (b) Neutral@SQD, (c) Negative@SQD,. Growth kinetic curve of E.Coli in presence of (d) only SQD, (e) Neutral@SQD, (f) Negative@SQD . (g) Growth kinetic curve of E. faecalis in presence of C1@SQD. (h) Colony forming ability of E. faecalis after treating with C1@SQD. (i) Growth kinetic curve of E.coli in presence of C1@SQD.



28. Zeta potential, fluorescence and IR spectra of C6@SQD and C8@SQD.

Figure S16. (a) Zeta potential of SQD, C6@SQD and C8@SQD. (b) Fluorescence emission spectra of SQD, C6@SQD and C8@SQD (excitation 400 nm).



29. Antibacterial efficacy of C6@SQD and C8@SQD against PA and E.coli.

Figure S17. Growth kinetic curve of PA in presence of different concentration of (a) C6@SQD, (b) C8@SQD. Growth kinetic curve of E.coli in presence of different concentration of (c) C6@SQD, (d) C8@SQD.

30. Antibacterial efficacy of C6@SQD and C8@SQD against E. faecalis.

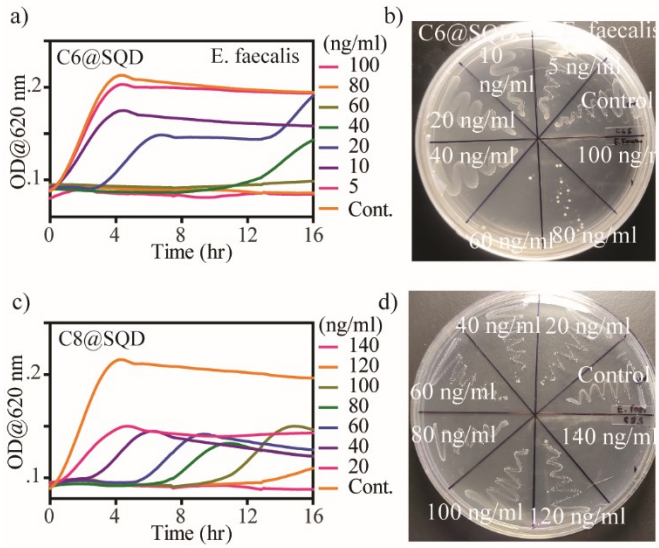


Figure S18. Growth kinetic curve of E. faecalis in presence of different concentration of (a) C6@SQD, (c) C8@SQD. Colony forming ability of MRSA after treating with different concentration of (b) C6@SQD, (d) C8@SQD.

31. ROS generations by SQD.

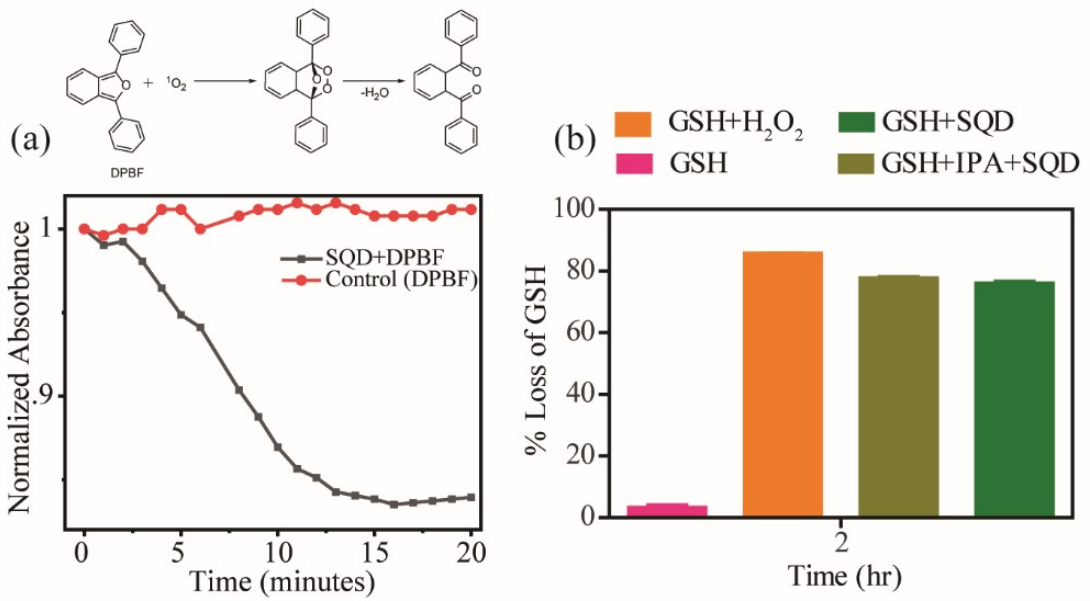
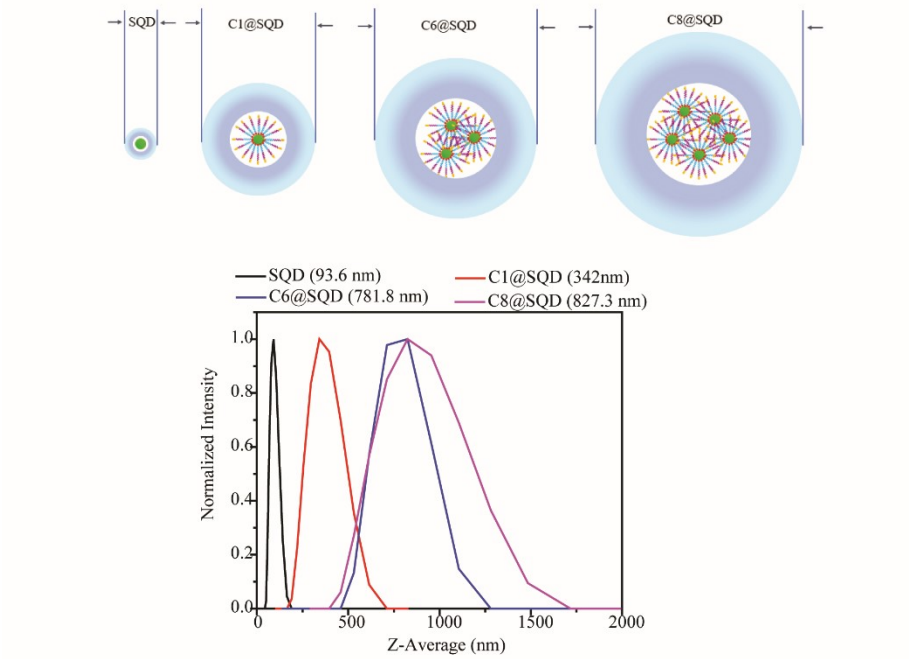
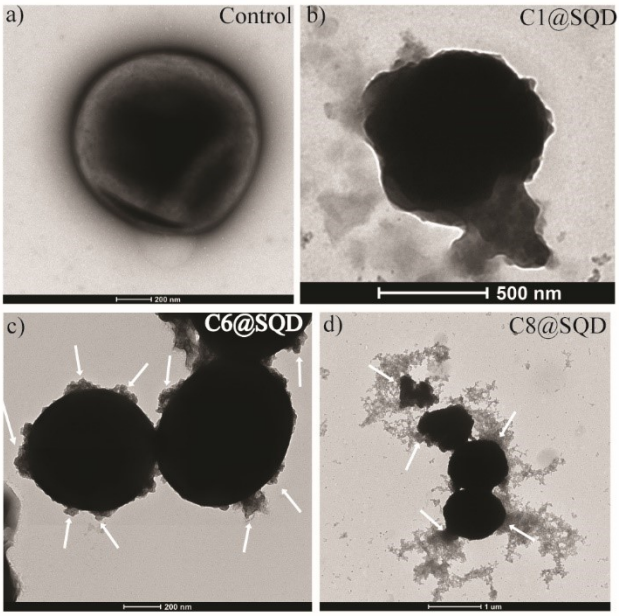


Figure S19. (a) Singlet oxygen generation efficacy of SQDs estimated through DPBF. (b) Evaluation of hydroxyl radical generation efficacy of SQDs quantified by adding hydroxyl radical quencher isopropyl alcohol (IPA) in Ellman's assay.



32. Hydrodynamic diameter (D_h) of functionalized SQDs.

Figure S20. DLS measurement of functionalized SQDs.



33. TEM image of MRSA bacteria treated with functionalized SQDs.

Figure S21. TEM image of MRSA bacteria (a) control MRSA, (b) MRSA bacteria treated with C1@SQD, (c) MRSA bacteria treated with C6@SQD, (d) MRSA bacteria treated with C8@SQD. White arrow indicates the aggregation of material on bacterial surface. Relatively lower level of aggregation of material was observed on bacterial surface treated with C6@SQD and a higher level of aggregation was observed on bacterial surface treated with C8@SQD.

34. Photograph of agar plates during the treatment.

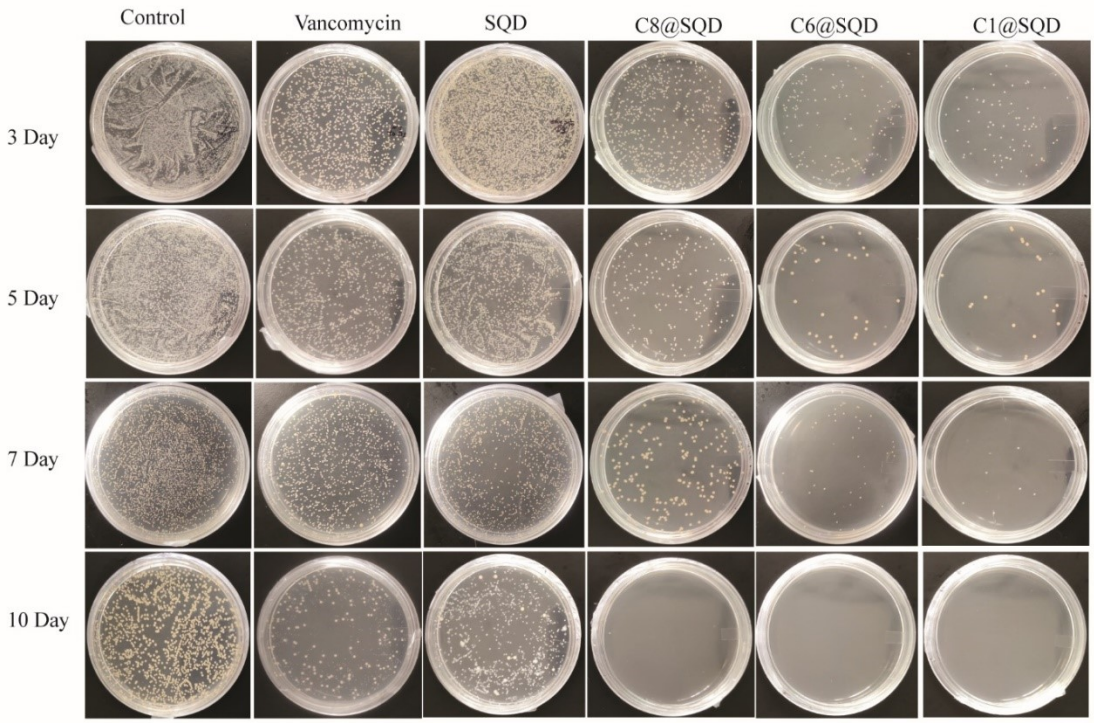


Figure S22. Photograph of agar plates during the treatment on days 3, 5, 7 and 10 days.

35. Biochemical parameters of the infected mice on 10th day.

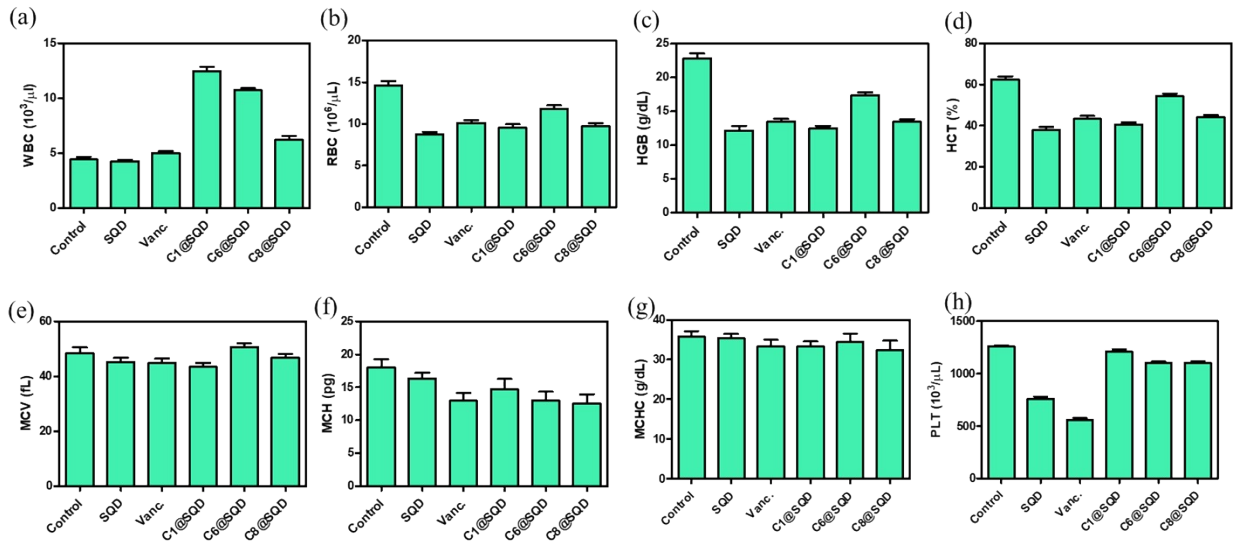


Figure S23. Hematological indicators of (a) white blood cells (WBC), (b) red blood cells (RBC), (c) hemoglobin (HGB), (d) hematocrit (HCT), (e) mean corpuscular volume (MCV), (f) mean corpuscular hemoglobin (MCH), (g) MCHC, (i) platelets (PLT).