

## **Supporting Information**

### **An Enzyme-Responsive and Photoactivatable Carbon-Monoxide Releasing Molecule for Bacterial Infection Theranostic**

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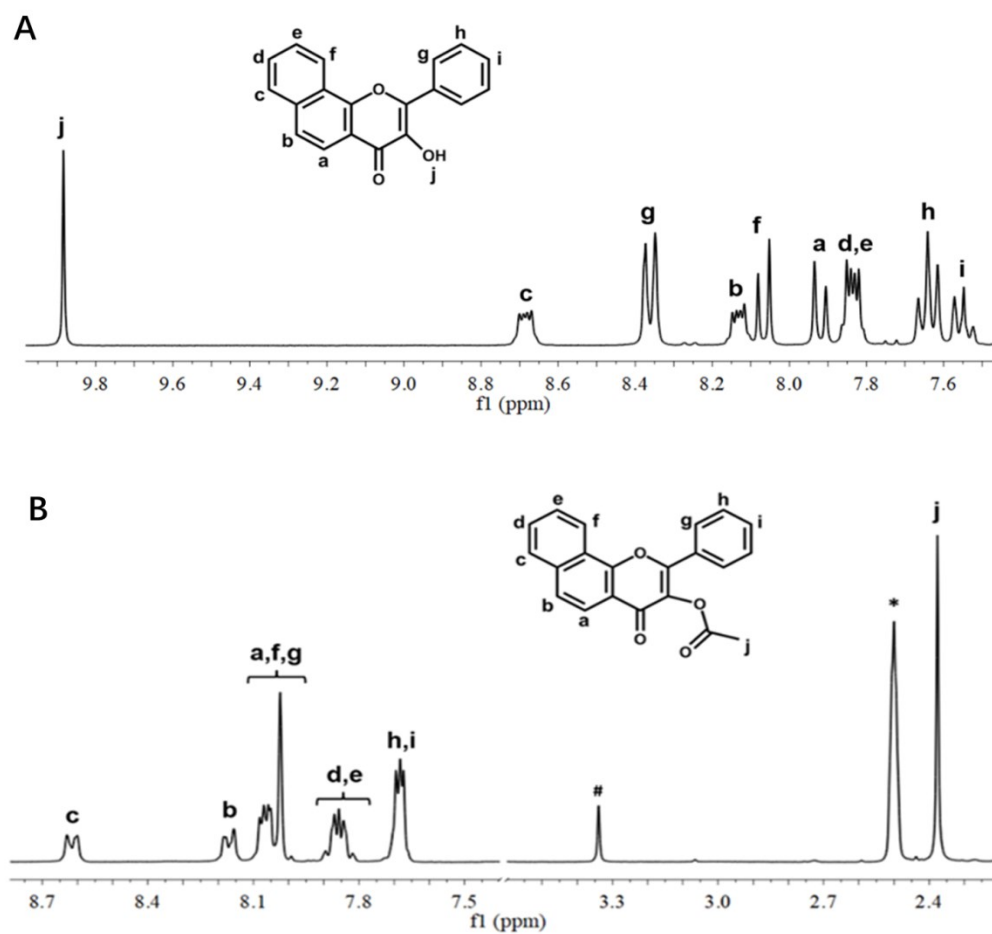
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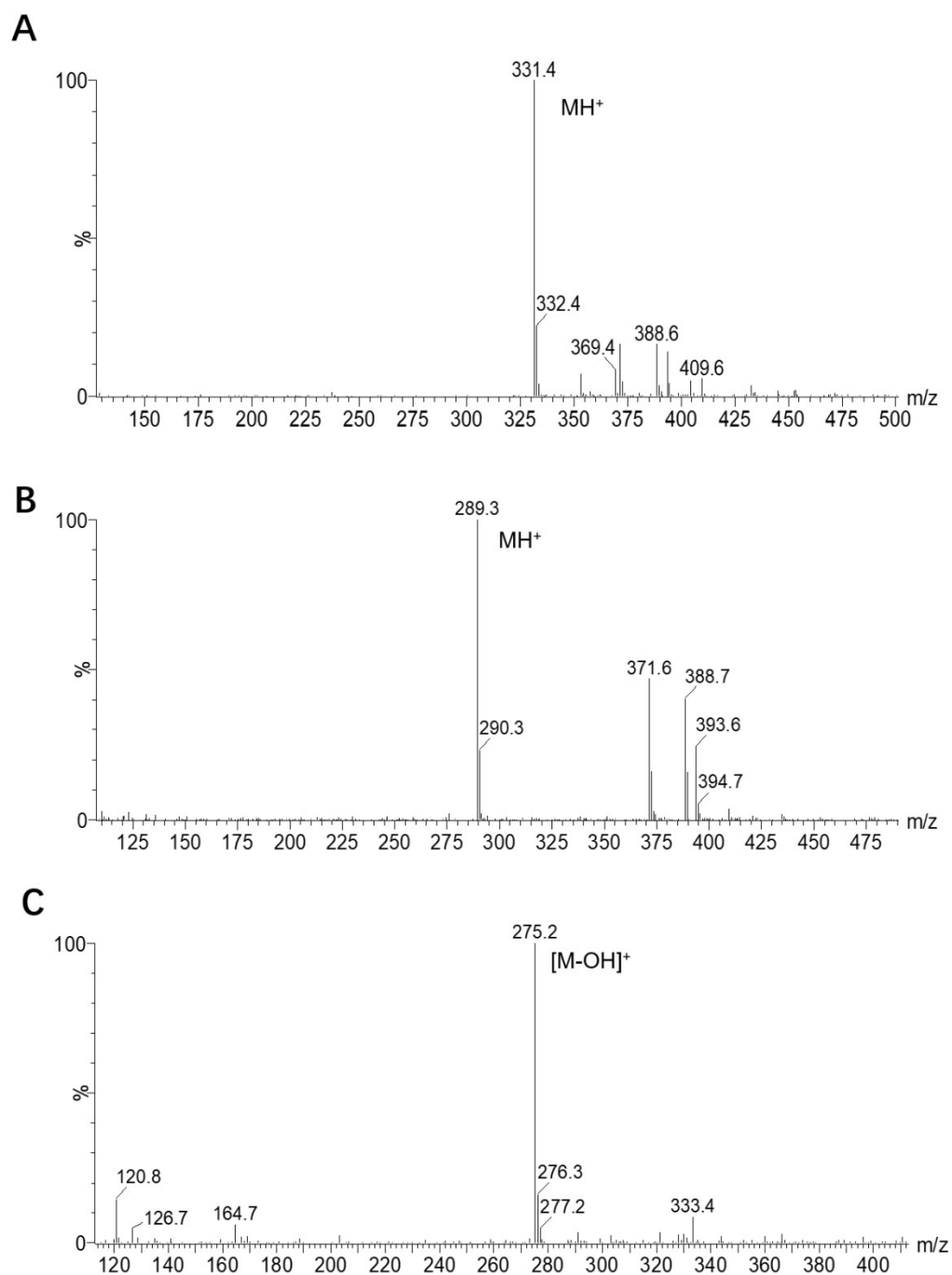
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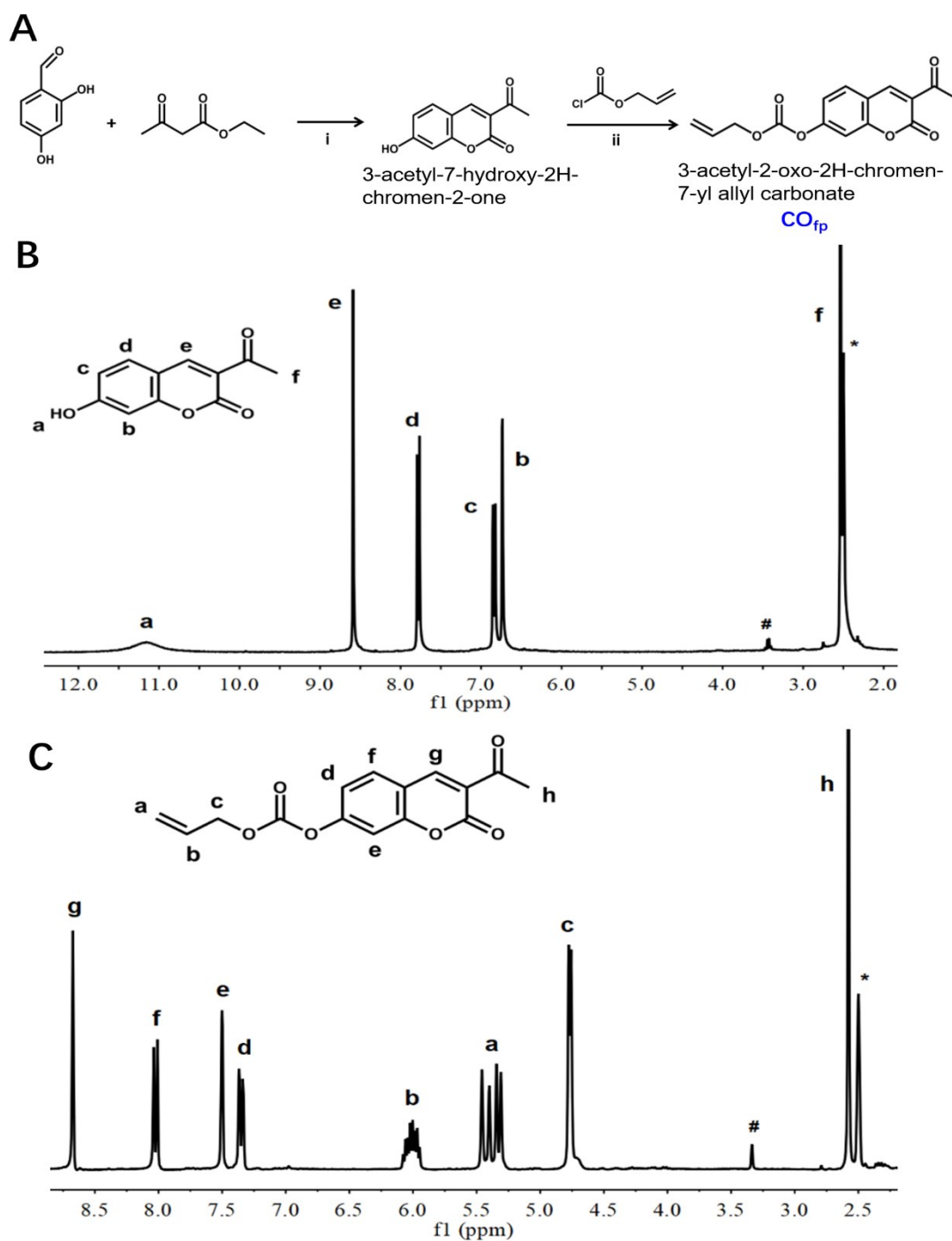
## SUPPLEMENTAL FIGURES AND SCHEMES



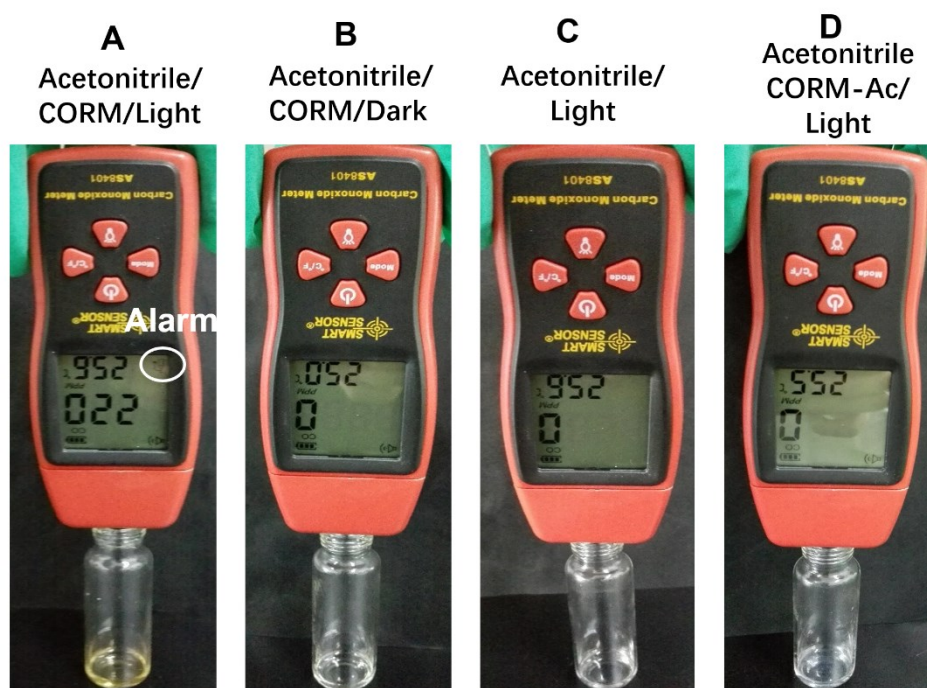
**Fig. S1.**  $^1\text{H}$  NMR spectra of (A) CORM and (B) CORM-Ac in  $\text{DMSO-d}_6$ . (The \* and # indicate the residual signal of the solvents, \*  $\text{DMSO-d}_6$ , #  $\text{H}_2\text{O}$ ).



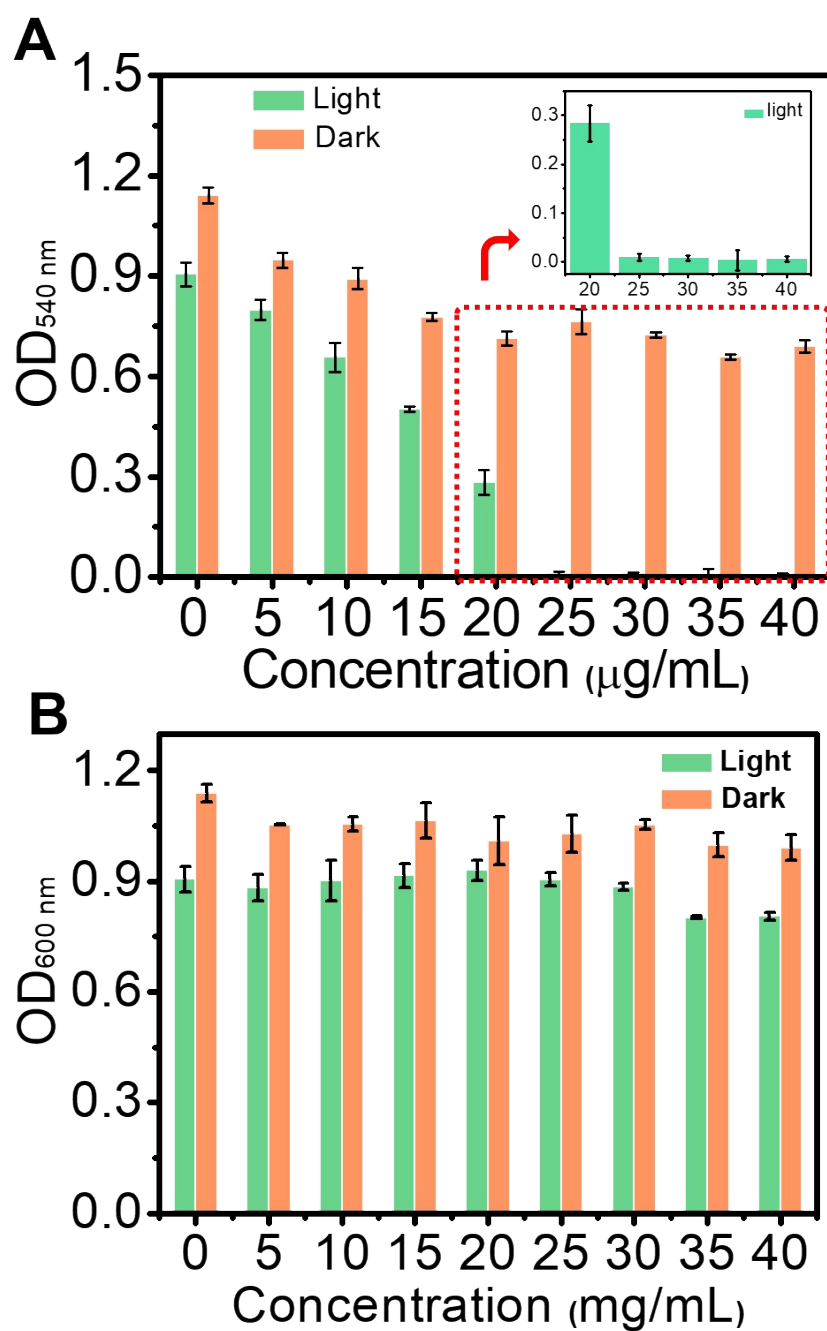
**Fig. S2.** ESI-MS spectra of (A) CORM-Ac, (B) CORM, and (C) photolysis production of CORM (iCORM).



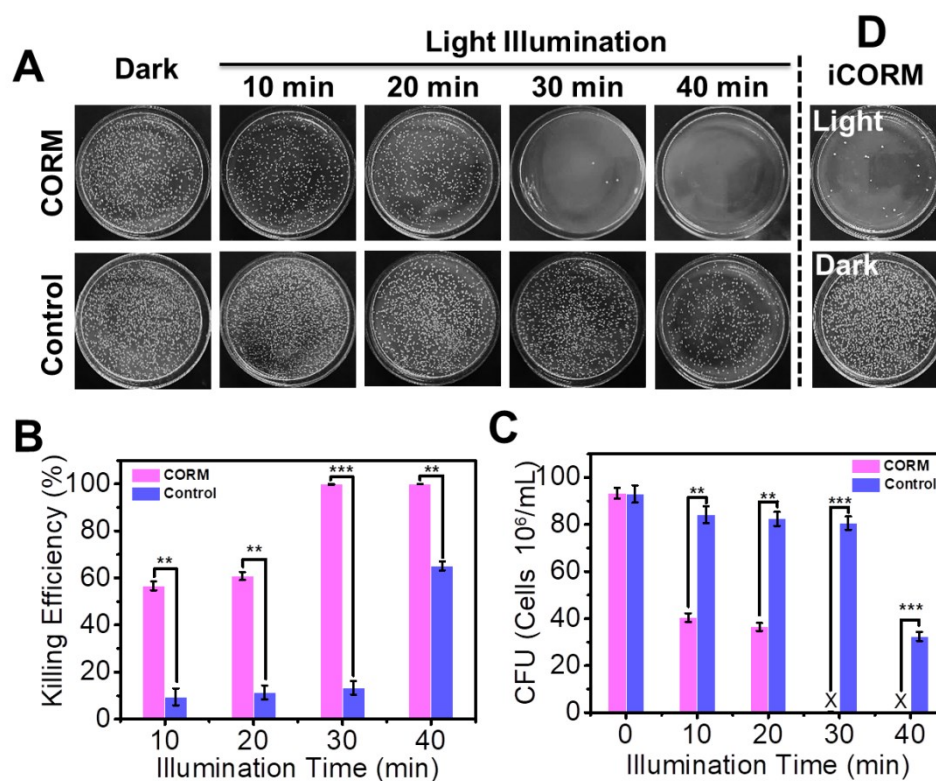
**Fig. S3.** (A) Synthetic route of CO fluorescent probe ( $CO_{fp}$ ). Reagents and conditions: i) EtOH, piperidine, RT, 12 h. ii) allyl chloroformate, triethylamine, DMF, 0 °C, 24 h.  $^1H$  NMR spectra of (B) 3-acetyl-7-hydroxy-2H-chromen-2-one and (C) 3-acetyl-2-oxo-2H-chromen-7-yl allyl carbonate ( $CO_{fp}$ ) in DMSO- $d_6$ . (The \* and # indicate the residual signal of the solvents, \* DMSO- $d_6$ , # H $_2$ O.)



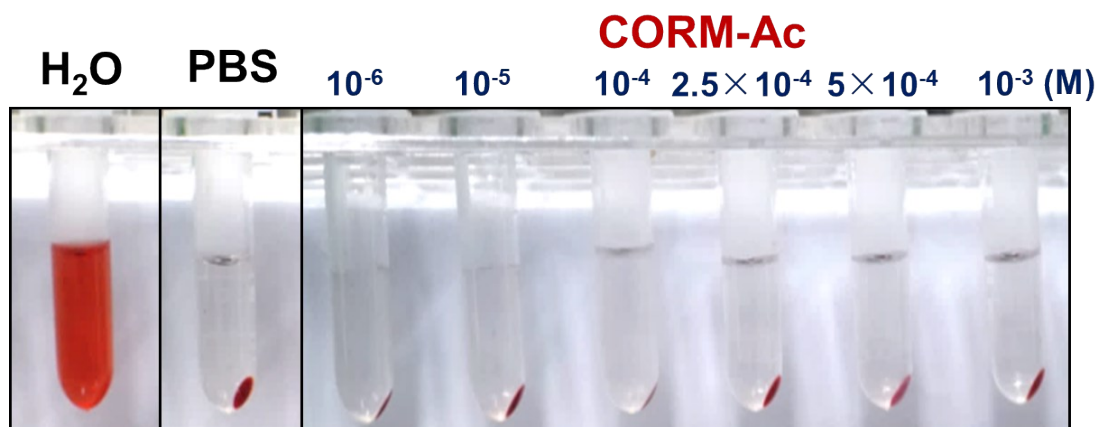
**Fig. S4.** The measurement of released CO from CORM by a commercially available CO detector under various treatments of (A) Illumination of CORM in acetonitrile for 12 h, (B) without illumination, (C) illumination of acetonitrile for 12 h, and (D) illumination of CORM-Ac in acetonitrile for 12 h.



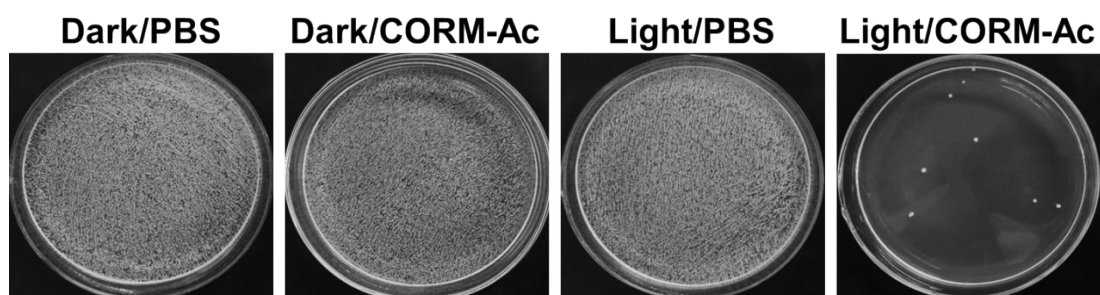
**Fig. S5.** The influence of (A) CORM and (B) DMSO concentrations on the viability of *S. aureus* in the presence of 30 min illumination under a sunlamp or not. (Error bars: standard deviation, n = 3.)



**Fig. S6.** The influence of illumination time against *S. aureus* viability. (A) Photographs of bacterial colony-forming units, (B) quantitative analysis and (C) killing efficiencies upon different illumination times. CORM (30  $\mu\text{g mL}^{-1}$ ) was added into *S. aureus* ( $10^6$  cells  $\text{mL}^{-1}$ ) suspension, the solution was kept in the dark, illuminated for 10 min, 20 min, 30 min, 40 min. (D) the bactericidal activities of iCORM-containing solution (30  $\mu\text{g mL}^{-1}$  of CORM illuminated for 12 h) in dark and 30 min of illumination. (× indicated undetectable CFU). (\* $p < 0.05$ , \*\* $p < 0.01$ , \*\*\* $p < 0.001$ ). (Error bars: standard deviation,  $n = 3$ .)

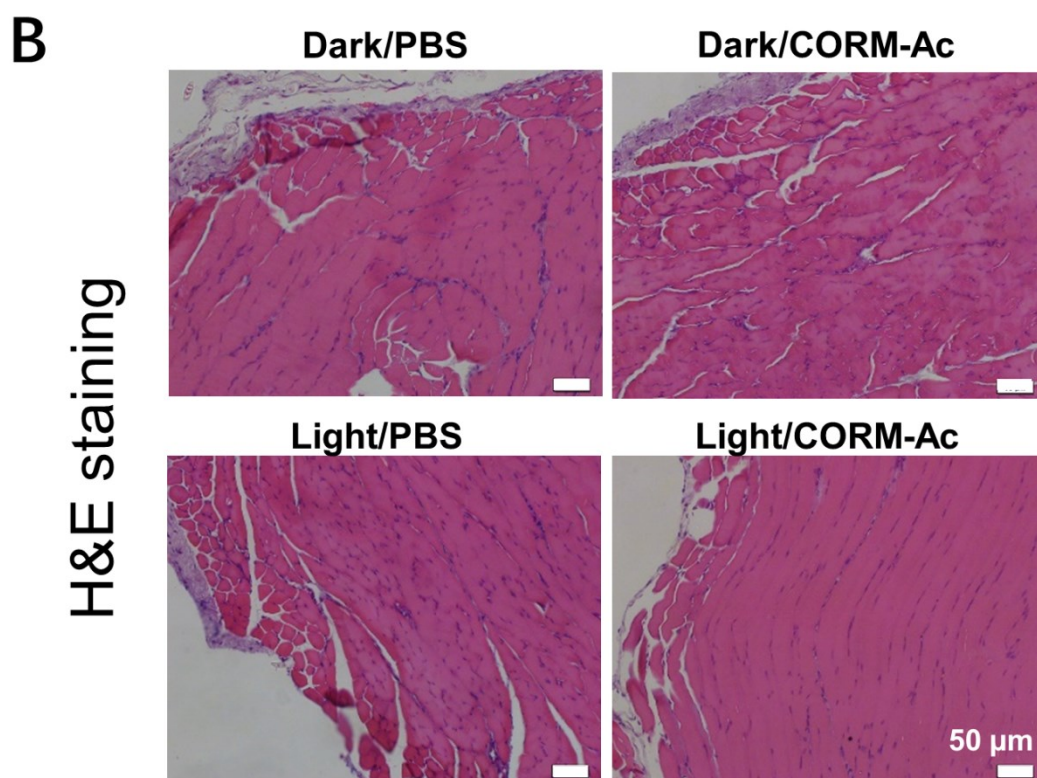
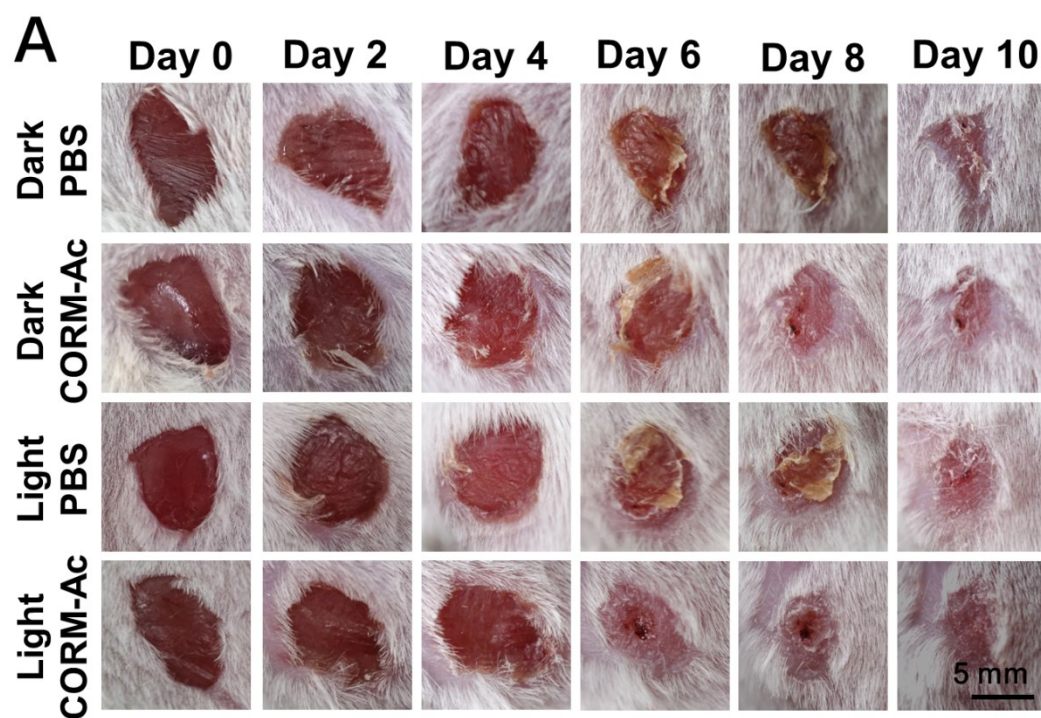


**Fig. S7.** Hemolysis images of erythrocyte suspension co-incubated with varied concentrations of CORM-Ac solution.



**Fig. S8.** *S. aureus* colonies grown on agar plate separated from the tissues with various treatments on days 5.





**Fig. S9.** (A) Representative wound closure images of un-infected wounds upon various treatments after healing for 0-10 days and (B) H&E staining images of wound sections for 10 days healing.