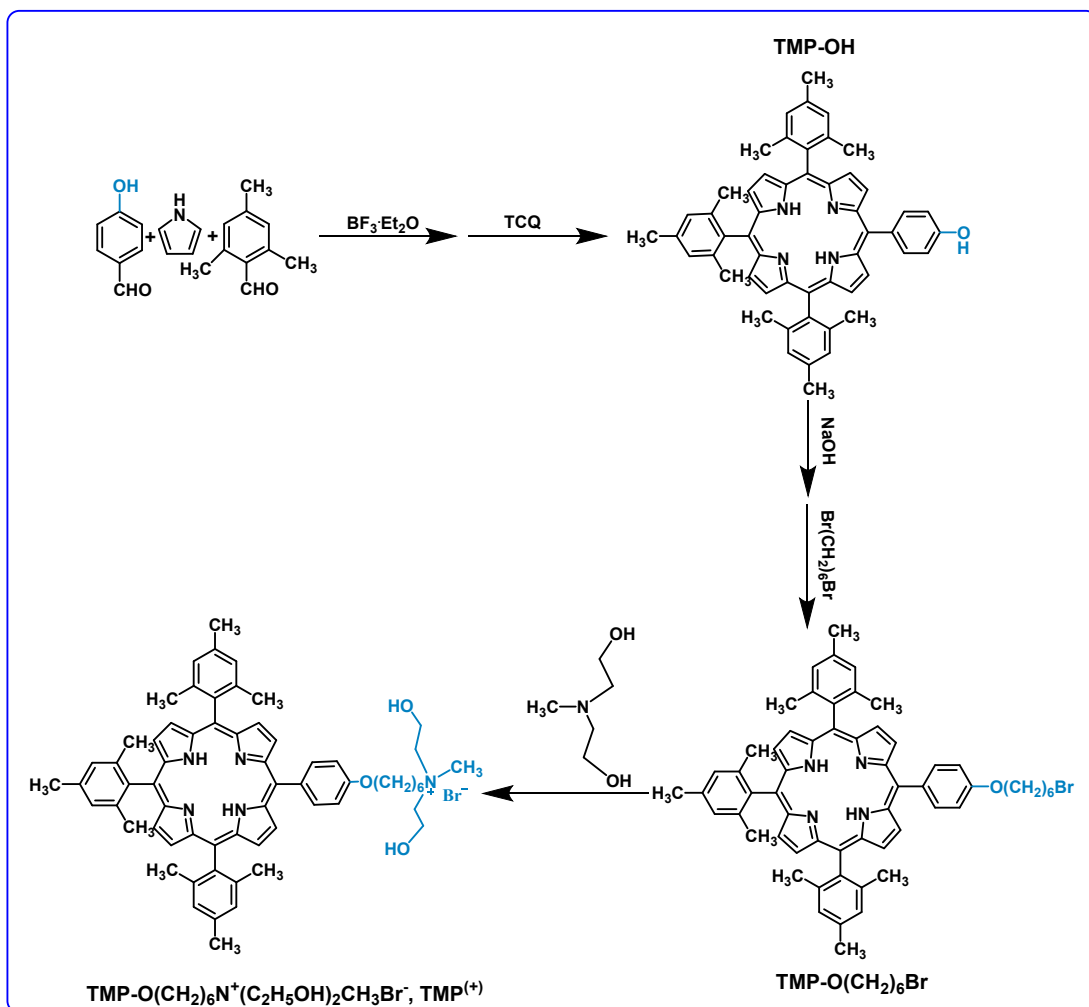


## Supporting Information

# Novel cation-loaded porphyrin nanofiber membranes for bacterial infections



## Supplementary Figures

### *5-(4-Hydroxyphenyl)-10, 15, 20-trimesitylporphyrin, TMP-OH*

$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  8.83 (d, 2H,  $J = 4.5$  Hz, pyrrole H), 8.71 (d, 2H,  $J = 4.6$  Hz, pyrrole H), 8.67 (s, 4H, pyrrole H), 8.04 (d, 2H,  $J = 8.3$  Hz, phenyl H), 7.30 (s, 6H, phenyl H), 7.10 (d, 2H,  $J = 8.3$  Hz, phenyl H), 5.32 (s, 1H, -OH), 2.65 (d, 9H,  $J = 4.0$  Hz, *p*- $\text{CH}_3$ ), 1.89 (s, 19H, *o*- $\text{CH}_3$ ), -2.51 (br, s, 2H, -NH).  $^{13}\text{C}$  NMR (DEPT, 151MHz,  $\text{CDCl}_3$ )  $\delta$ (ppm): 135.44 (s, porphyrin carbon), 127.88(s, porphyrin carbon), 113.54(s, porphyrin carbon), 21.63(d, - $\text{CH}_3$ ), 21.41(s, - $\text{CH}_3$ ). ESI-MS  $m/z$  calcd. for  $\text{C}_{53}\text{H}_{49}\text{N}_4\text{O}$ ,  $[\text{M}+\text{H}]^+$ , 757.3902; found: 757.3901.

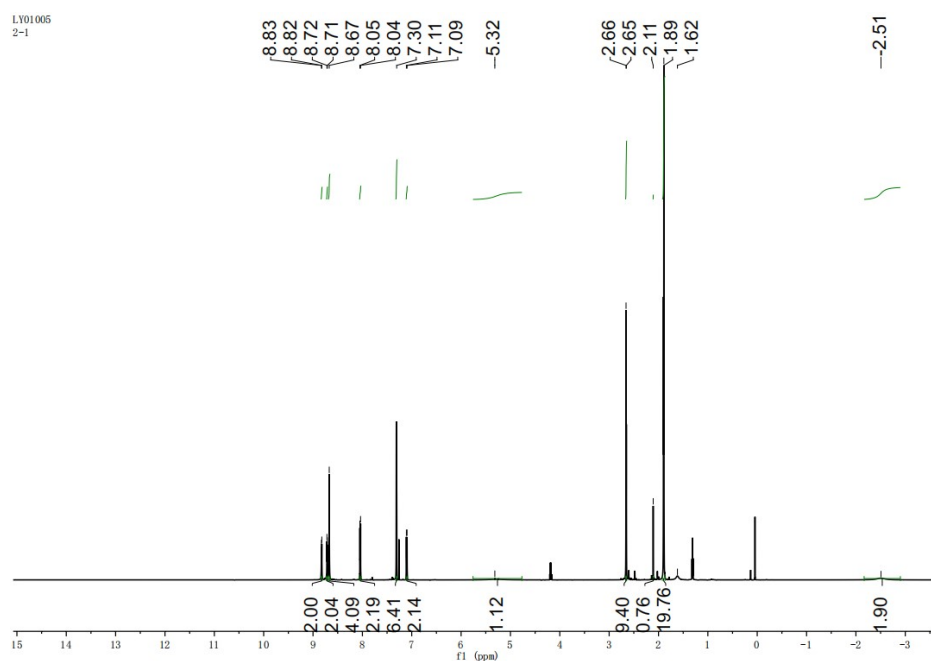


Figure S1  $^1\text{H}$  NMR of **TMP-OH**

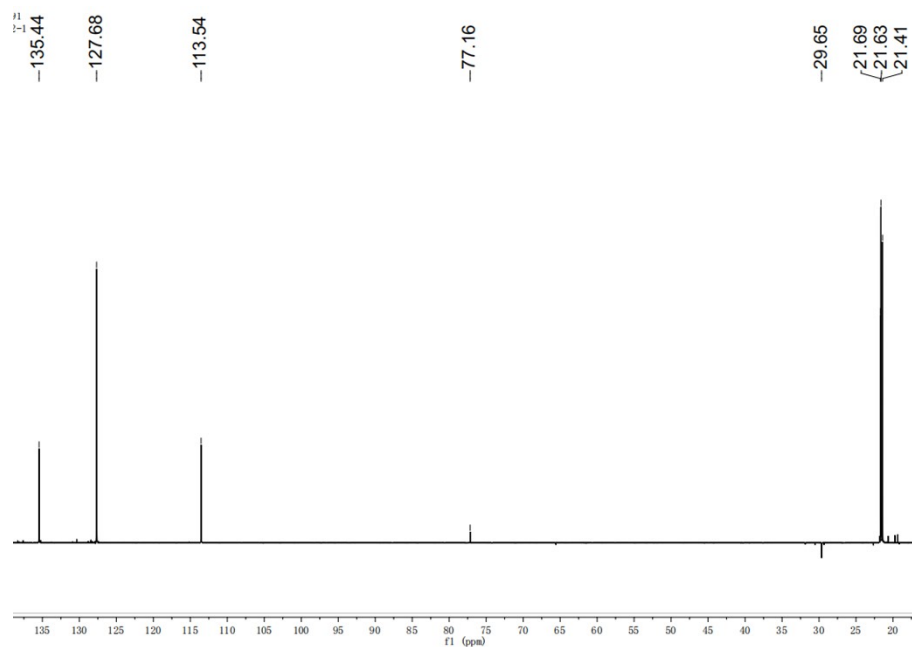


Figure S2  $^{13}\text{C}$  NMR(DEPT) of **TMP-OH**

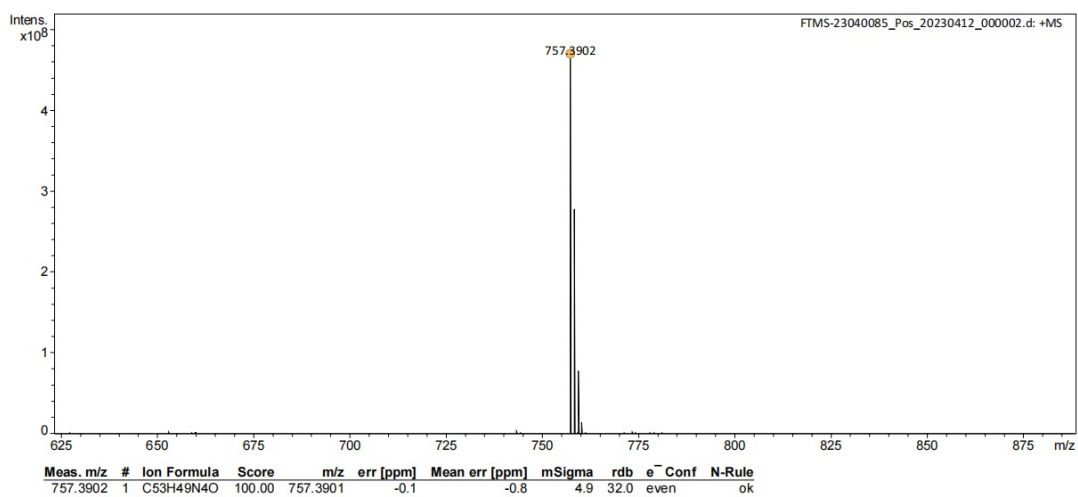


Figure S3 MS of **TMP-OH**

**5-[4-(6-Bromo-1-hexoxy) phenyl]-10, 15, 20-trimesitylporphyrin, TMP-O(CH<sub>2</sub>)<sub>6</sub>Br**

<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 8.83 (d, 2H, *J* = 4.5 Hz, pyrrole H), 8.69 (d, 2H, *J* = 4.6 Hz, pyrrole H), 8.64 (s, 4H, pyrrole H), 8.11 (d, 2H, *J* = 8.4 Hz, phenyl H), 7.28 (d, 8H, *J* = 8.8 Hz, phenyl H), 4.27 (t, 2H, *J* = 6.4 Hz, -OCH<sub>2</sub>-), 3.75 (t, 2H, *J* = 6.5 Hz, -CH<sub>2</sub>Br), 2.64 (d, 9H, *J* = 4.1 Hz, *p*-CH<sub>3</sub>), 2.01 (d, 2H, *J* = 14.3 Hz, -OCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Br), 1.87 (d, 19H, *J* = 4.3 Hz, *o*-CH<sub>3</sub>), 1.71 (s, 4H, -OCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Br), 1.59 (s, 2H, -OCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Br), -2.52 (br, s, 2H, -NH). <sup>13</sup>C NMR(DEPT, 151MHz, CDCl<sub>3</sub>) δ(ppm): 135.37 (s, porphyrin carbon), 127.67(s, porphyrin carbon), 112.6(s, porphyrin carbon), 67.97(s, -OCH<sub>2</sub>-), 33.83(s, -OCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Br), 32.6(s, -OCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Br), 29.29(s, -OCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Br), 28.02(s, -OCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Br), 25.46(s, -OCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Br), 21.63(d, -CH<sub>3</sub>), 21.42(s, -CH<sub>3</sub>). ESI-MS *m/z* calcd. for C<sub>59</sub>H<sub>60</sub>BrN<sub>4</sub>O, [M+H]<sup>+</sup>, 919.3947; found: 919.3945.

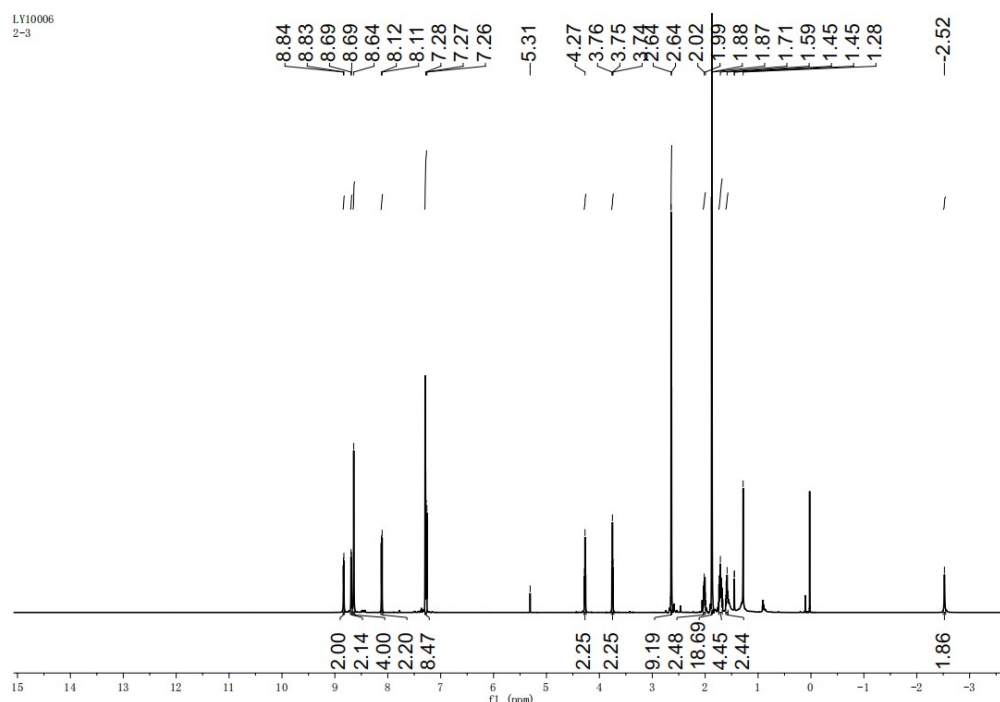


Figure S4 <sup>1</sup>H NMR of TMP-O(CH<sub>2</sub>)<sub>6</sub>Br

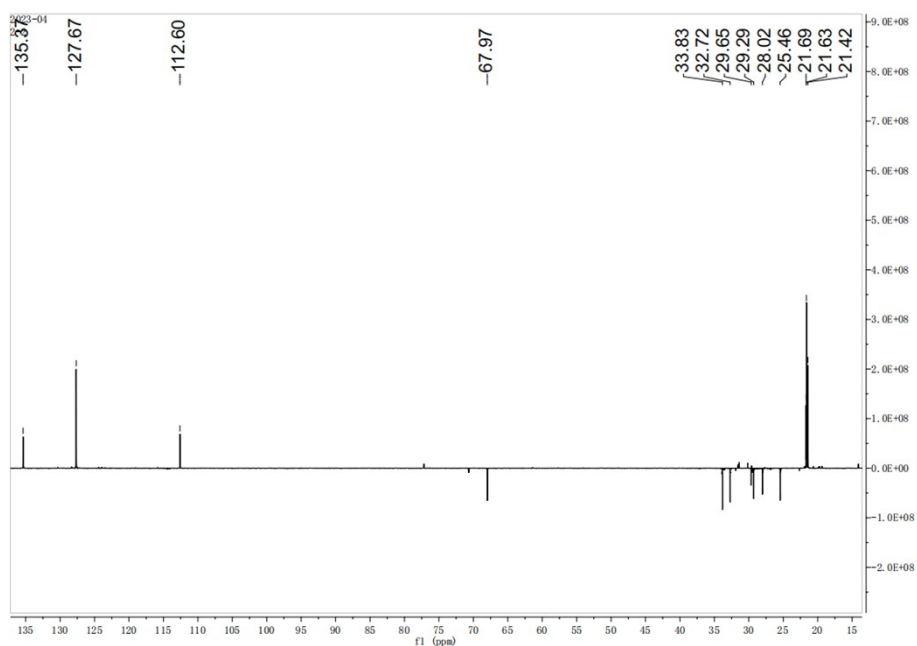


Figure S5  $^{13}\text{C}$  NMR (DEPT) of  $\text{TMP-O}(\text{CH}_2)_6\text{Br}$ .

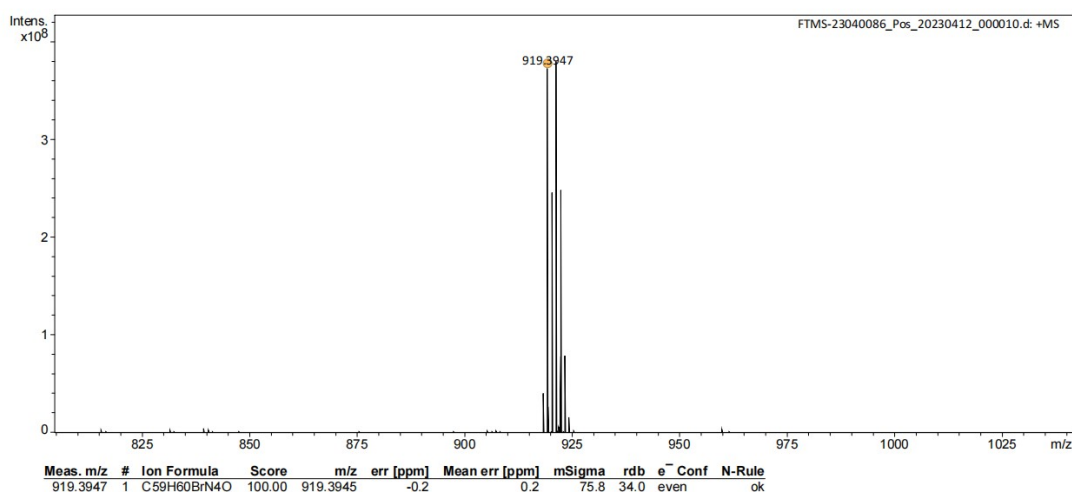


Figure S6 MS of  $\text{TMP-O}(\text{CH}_2)_6\text{Br}$ .

***N, N-bis-(2-hydroxyethyl)-N-(6-(4-(10,15,20-trimesitylporphyrin-5-yl) phenoxy) hexan)-N-methanaminium bromide,  $\text{TMP-O}(\text{CH}_2)_6\text{N}^+(\text{C}_2\text{H}_5\text{OH})_2\text{CH}_3\text{Br}$ ,  $\text{TMP}^{(+)}$ :***  
 $^1\text{H}$  NMR (600 MHz,  $d_6$ -DMSO)  $\delta$  8.79 – 8.42 (m, 8H, pyrrole H), 8.03 (s, 2H, phenyl H), 7.26 (s, 8H, phenyl H), 5.25 (s, 2H, -OH), 4.18 (s, 2H,  $-\text{OCH}_2-$ ), 3.80 (s, 4H,  $-\text{CH}_2\text{OH}$ ), 3.42 (s, 6H,  $-\text{NCH}_2-$ ), 3.06 (s, 3H,  $-\text{NCH}_3$ ), 2.43 (s, 9H,  $p$ - $\text{CH}_3$ ), 1.69 (s, 27H,  $-\text{CH}_3$ ,  $-\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{N}-$ ), -2.75 (br, s, 2H, -NH).  $^{13}\text{C}$  NMR(DEPT, 151MHz,  $d_6$ -DMSO)  $\delta$ (ppm): 135.03 (s, porphyrin carbon), 127.61(s, porphyrin carbon), 112.63 (s, porphyrin carbon), 67.33(s,  $-\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{N}-$ ), 63.03(s,  $-\text{N-CH}_2\text{CH}_2\text{OH}$ ), 62.19 (s, -

OCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>N-), 54.59(s, -N-CH<sub>2</sub>CH<sub>2</sub>OH), 48.82(s, -N-CH<sub>3</sub>), 28.42(s, -OCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>N-), 25.41(s, -OCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>N-), 24.99(s, -OCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>N-), 21.38(s, -OCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>N-), 21.07(s, -CH<sub>3</sub>), 20.95(s, -CH<sub>3</sub>), 20.78(s, -CH<sub>3</sub>). [M-Br]<sup>+</sup> ([TMP-O(CH<sub>2</sub>)<sub>6</sub>N<sup>+</sup>(C<sub>2</sub>H<sub>5</sub>OH)<sub>2</sub>CH<sub>3</sub>]) : 958.5629, found: 958.5638.

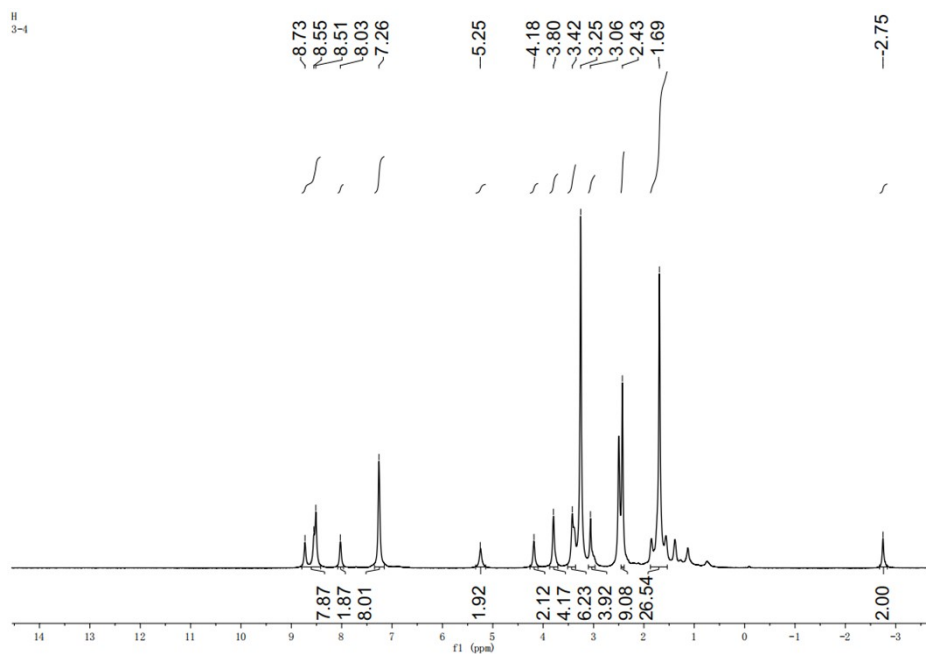


Figure S7 <sup>1</sup>H NMR of TMP-O(CH<sub>2</sub>)<sub>6</sub>N<sup>+</sup>(C<sub>2</sub>H<sub>5</sub>OH)<sub>2</sub>CH<sub>3</sub>Br<sup>-</sup>

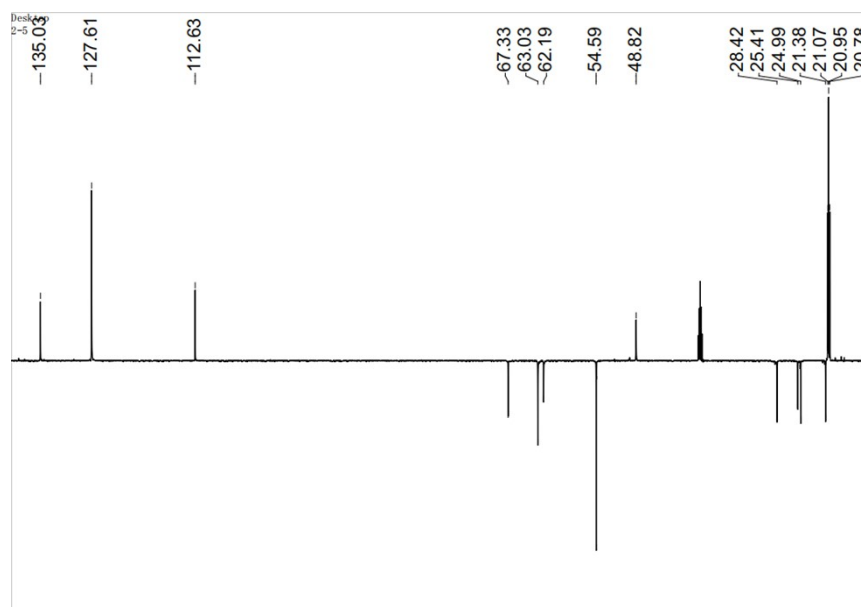


Figure S8 <sup>13</sup>C NMR (DEPT) of TMP-O(CH<sub>2</sub>)<sub>6</sub>N<sup>+</sup>(C<sub>2</sub>H<sub>5</sub>OH)<sub>2</sub>CH<sub>3</sub>Br<sup>-</sup>

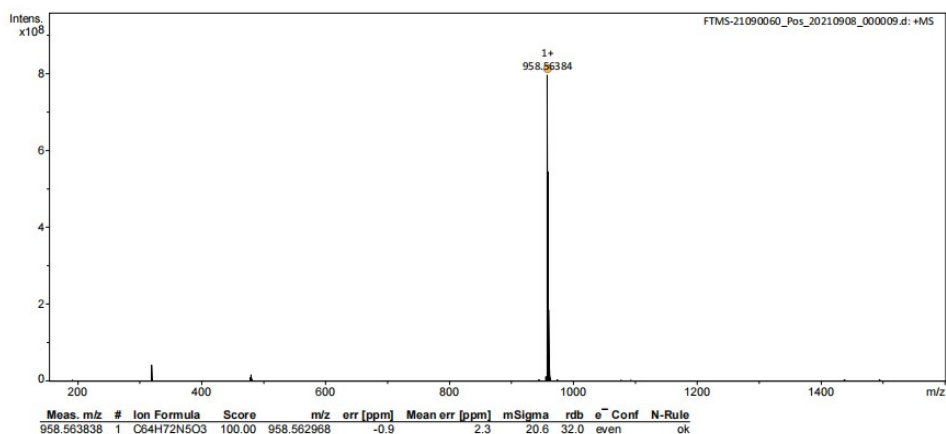


Figure S9 MS of  $\text{TMP-O(CH}_2)_6\text{N}^+(\text{C}_2\text{H}_5\text{OH})_2\text{CH}_3\text{Br}^-$

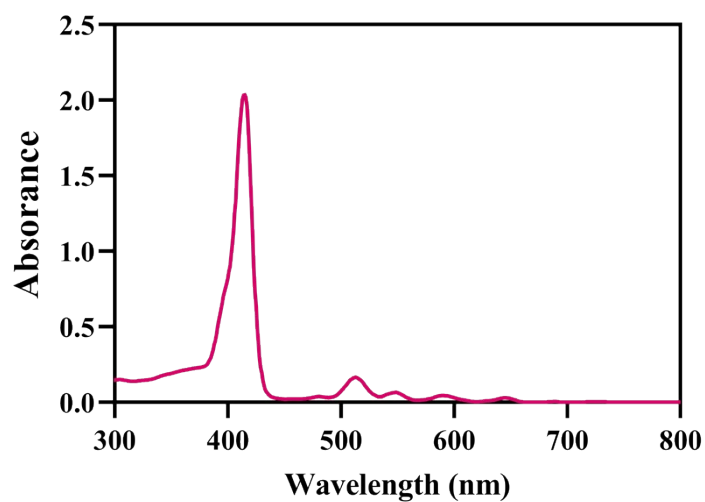


Figure S10 UV-Vis spectra of  $\text{TMP-O(CH}_2)_6\text{N}^+(\text{C}_2\text{H}_5\text{OH})_2\text{CH}_3\text{Br}^-$

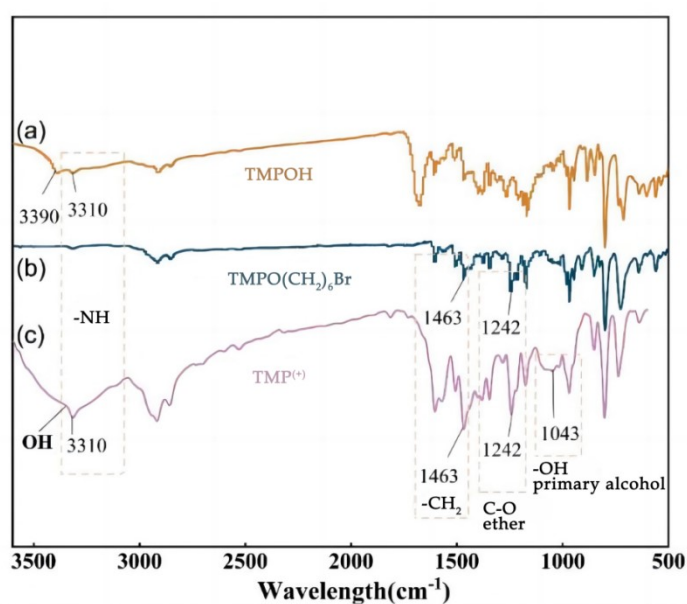


Figure S11 FT-IR spectrum: (a)  $\text{TMP-OH}$ ; (b)  $\text{TMP-O(CH}_2)_6\text{Br}$ ; (c)  $\text{TMP}^{(+)}$

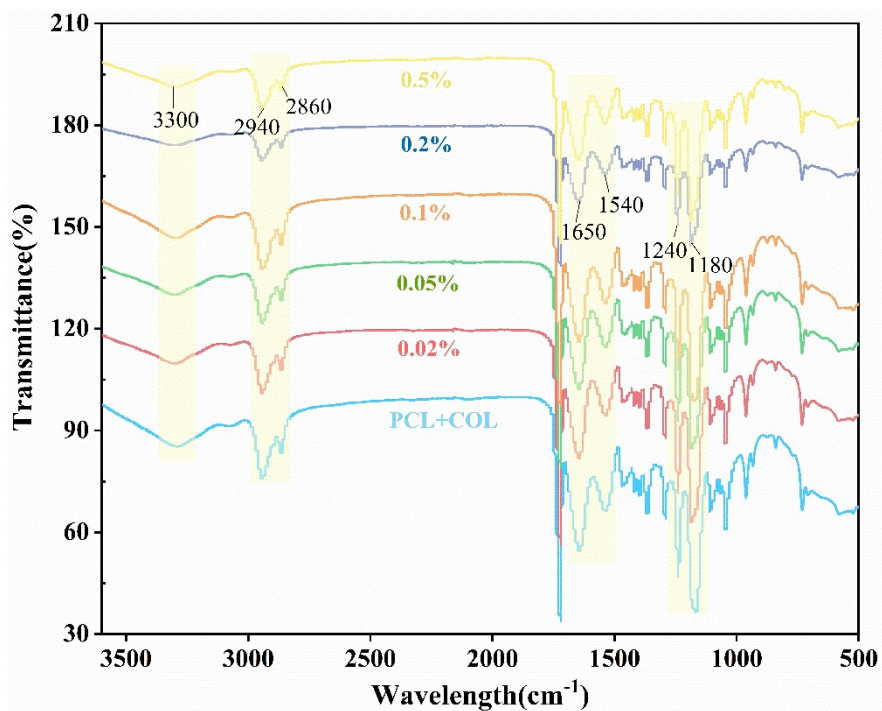
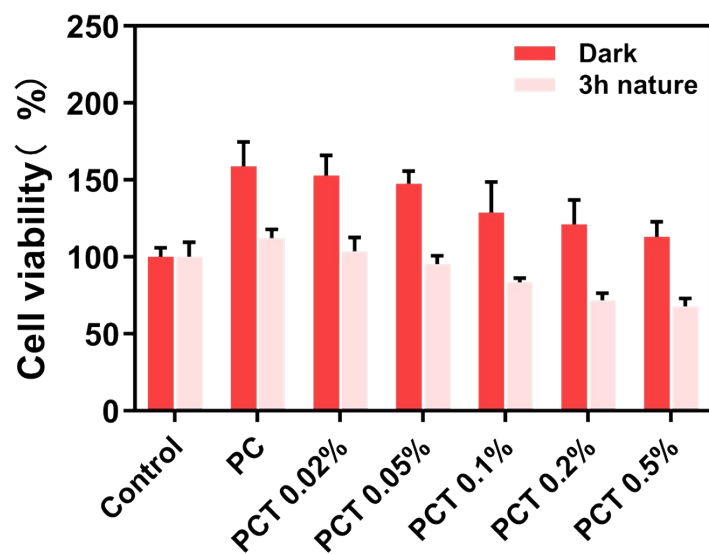


Figure S12 The FT-IR spectrum of nanofiber film containing different concentrations of **TMP<sup>(+)</sup>**.



**Fig. S13** Cell viability of L929 cells when contacting PC and PCT nanofiber membranes with or without light irradiation for 24 h.



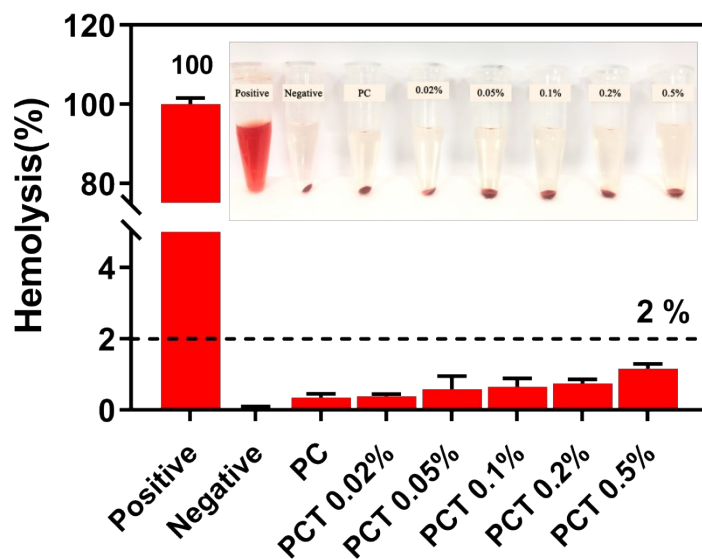


Fig. S14 Photographs and quantitative results of hemolysis of mouse red blood cell under positive group, negative group, PC and PCT nanofiber membranes conditions.

### Supplementary Tables

Light \ Group	PC	PCT 0.02%	PCT 0.05%	PCT 0.1%	PCT 0.2%	PCT 0.5%	PCP 0.5%
Dark	100	93.94	76.52	70.08	63.26	56.44	96.33
Laser	100	77.53	50.06	36.74	34.48	2.85	13.59

Table S1 Mean bacterial survival rate of nano-fiber membrane containing **TMPOH (PCP 0.5%)** before modification and **TMP<sup>(+)</sup>** at different concentrations on *S. aureus*.

Light \ Group	PC	PCT 0.02%	PCT 0.05%	PCT 0.1%	PCT 0.2%	PCT 0.5%	PCP 0.5%
Dark	100	78.01	66.91	57.13	28.73	25.83	97.82
Laser	100	58.83	58.67	39.17	7.67	6.17	15.41

Table S2 Mean bacterial survival rate of nano-fiber membrane containing **TMPOH (PCP 0.5%)** before modification and **TMP<sup>(+)</sup>** at different concentrations on *E. coli*.

<b>groups \ days</b>	<b>3 days (%)</b>	<b>7 days (%)</b>	<b>10 days (%)</b>	<b>14 days (%)</b>
<b>Blank</b>	14.79	73.64	84.57	89.09
<b>3M</b>	25.11	74.14	89.11	91.74
<b>PC</b>	29.12	74.43	91.68	93.15
<b>PCT</b>	41.97	76.02	93.35	95.61
<b>PCTL</b>	46.84	81.14	94.57	97.21

Table S3 The wound area ratio at the indicated time points for **Blank, 3M, PC, PCT, PCTL**.