

# Supporting Information

## One-Pot Preparation of Cetylpyridinium Chloride-Containing Nanoparticles for Biofilm Eradication

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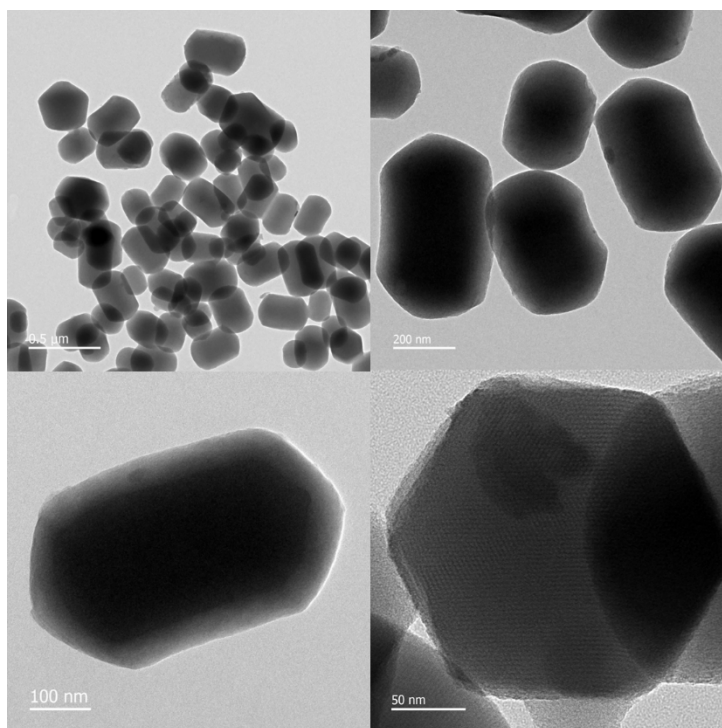
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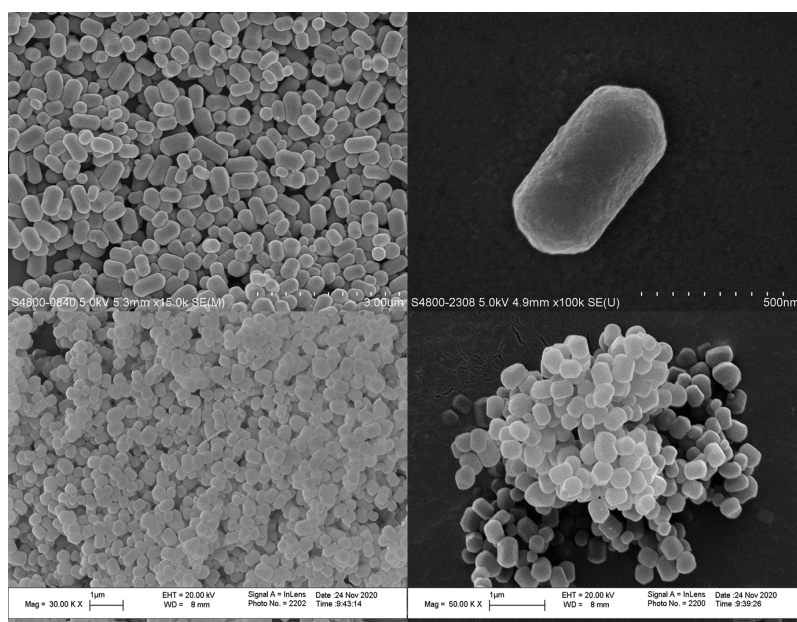
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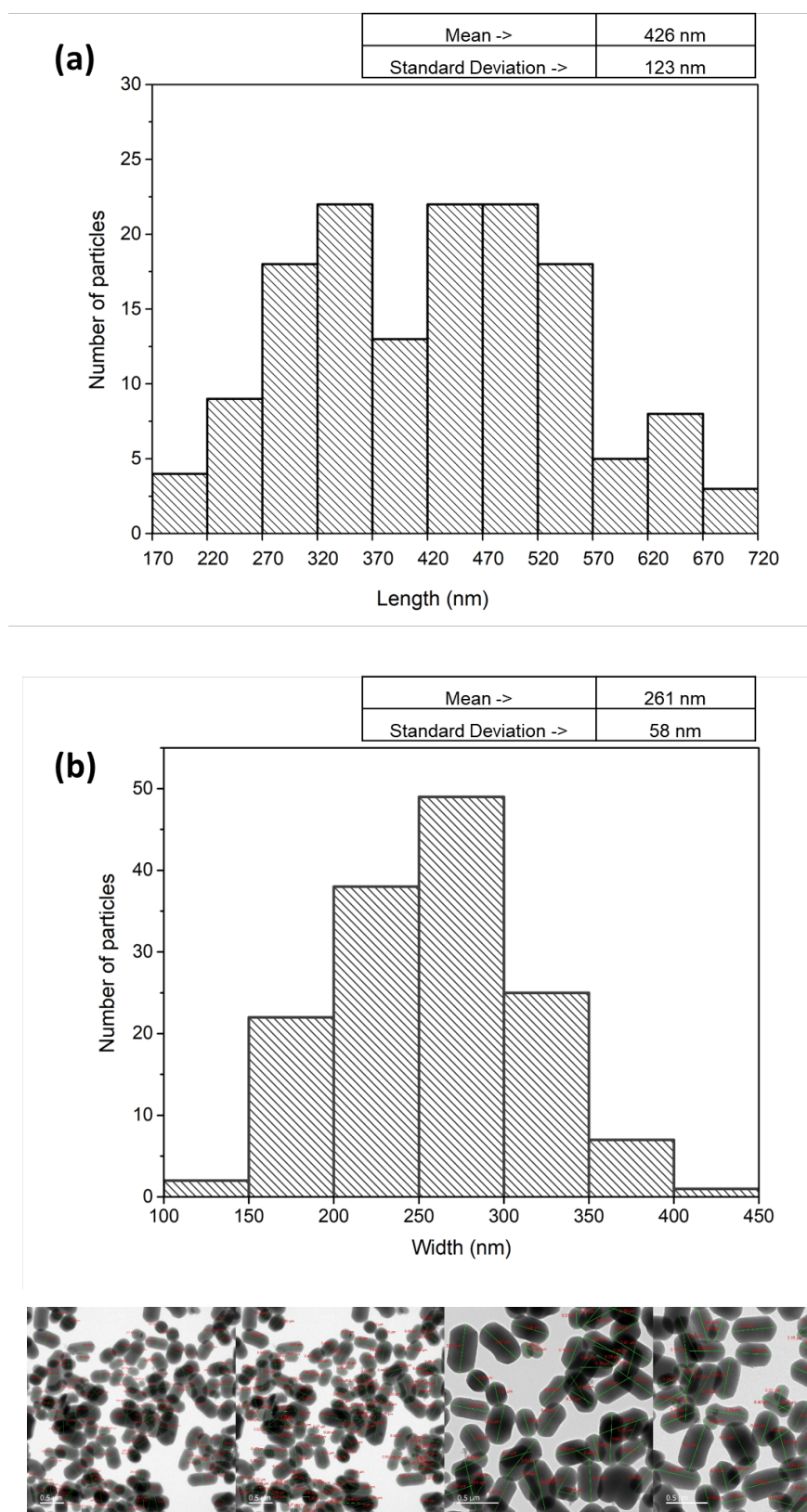
‡ These authors contributed equally to this work.



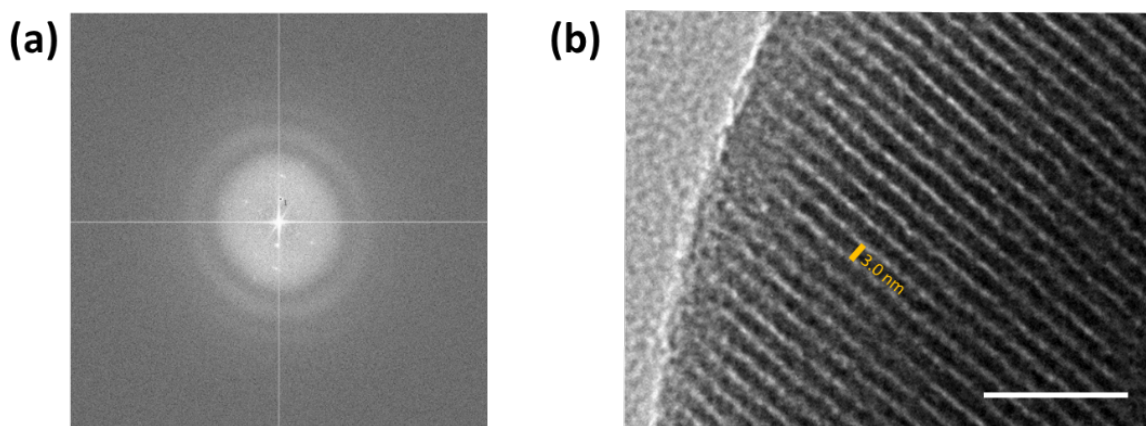
**Figure S1.** Additional transmission electron microscopic (TEM) images of CPC-MSN at different magnifications.



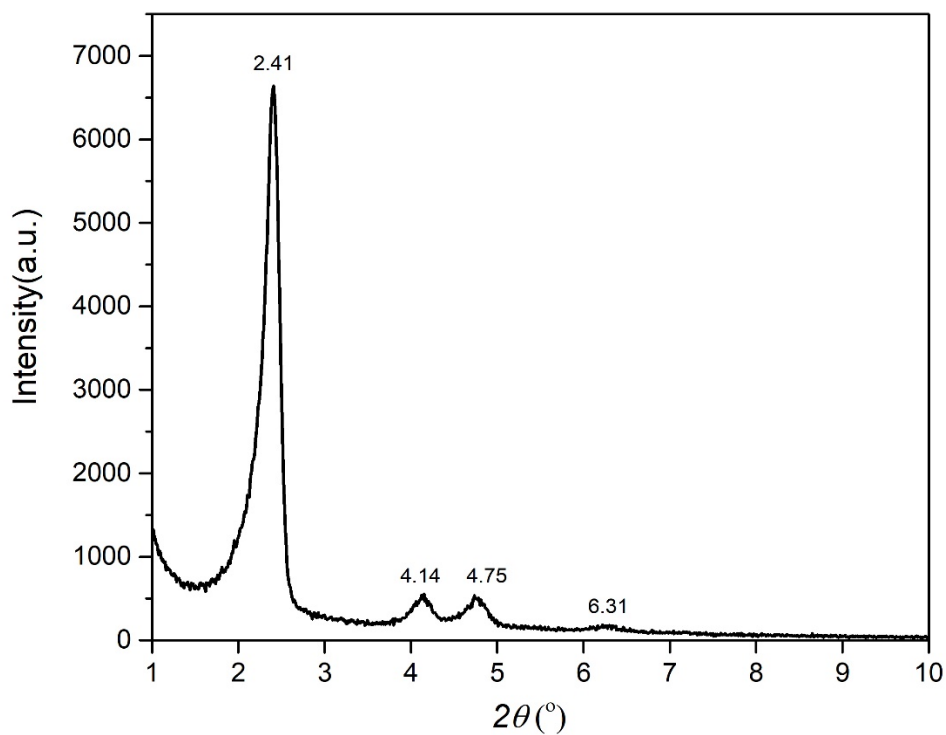
**Figure S2.** Additional scanning electron microscopic (SEM) images of CPC-MSN at different magnifications.



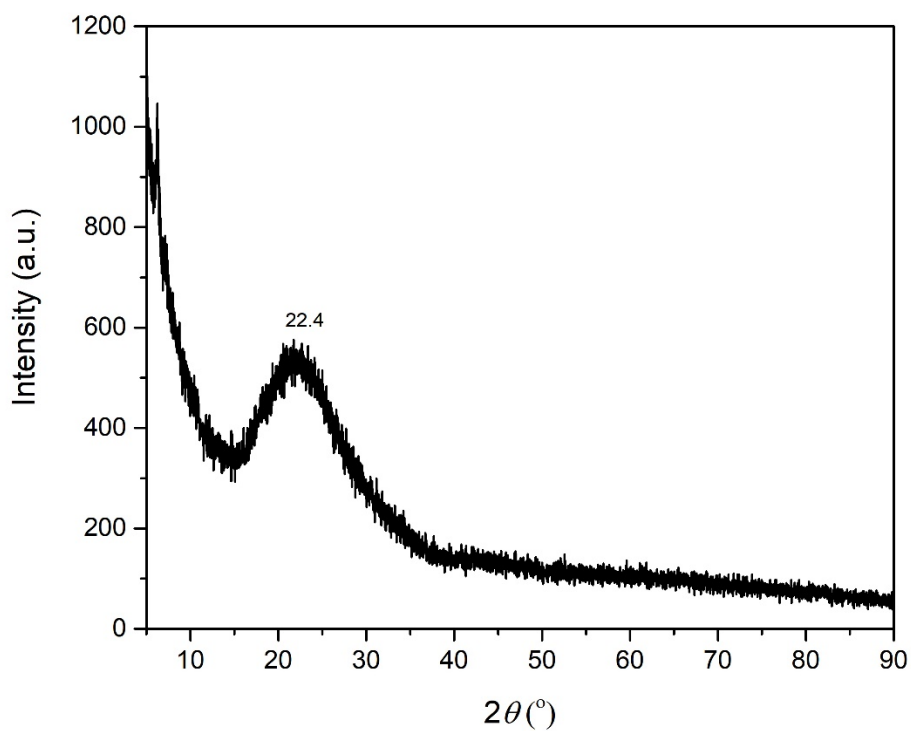
**Figure S3.** Size distribution of CPC-MSN (estimated from TEM images). (a) Length; (b) Width. Number of particles measured = 145.



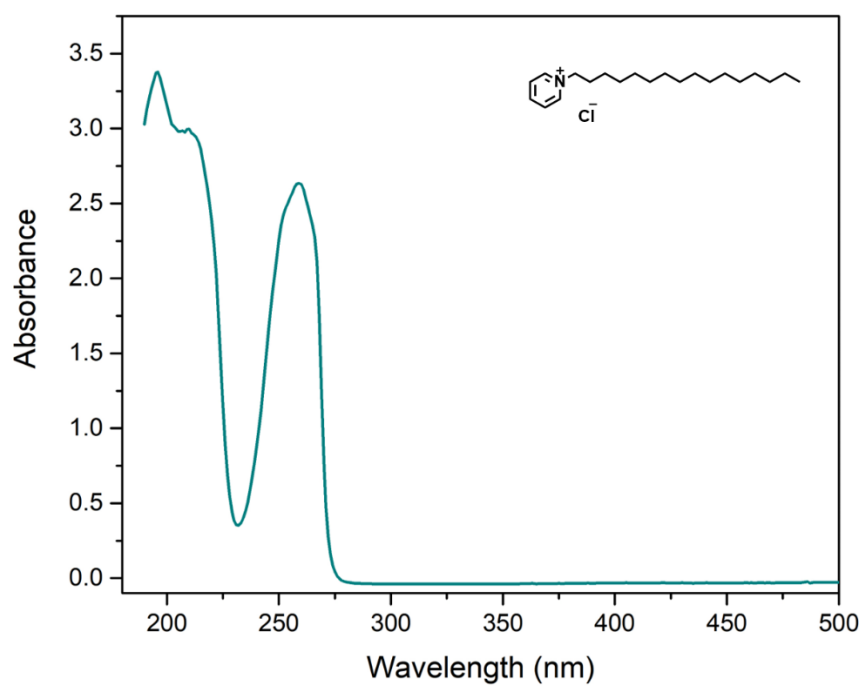
**Figure S4.** (a) Diffraction pattern of CPC-MSN through Fast Fourier Transform (FFT) analysis. (b) Enlarged TEM image showing the channels. Scale bar = 20 nm.



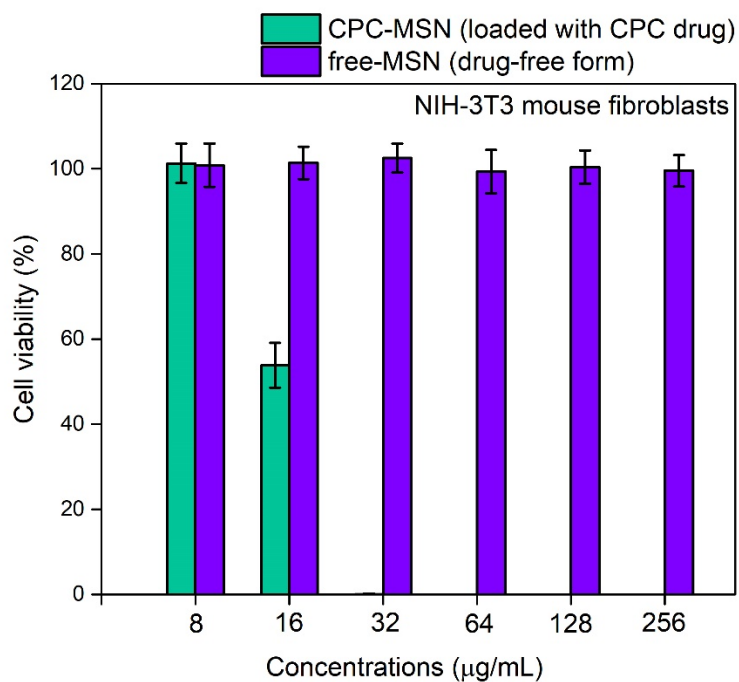
**Figure S5.** Small-angle X-ray powder diffraction (SAXRD) pattern of CPC-MSN.



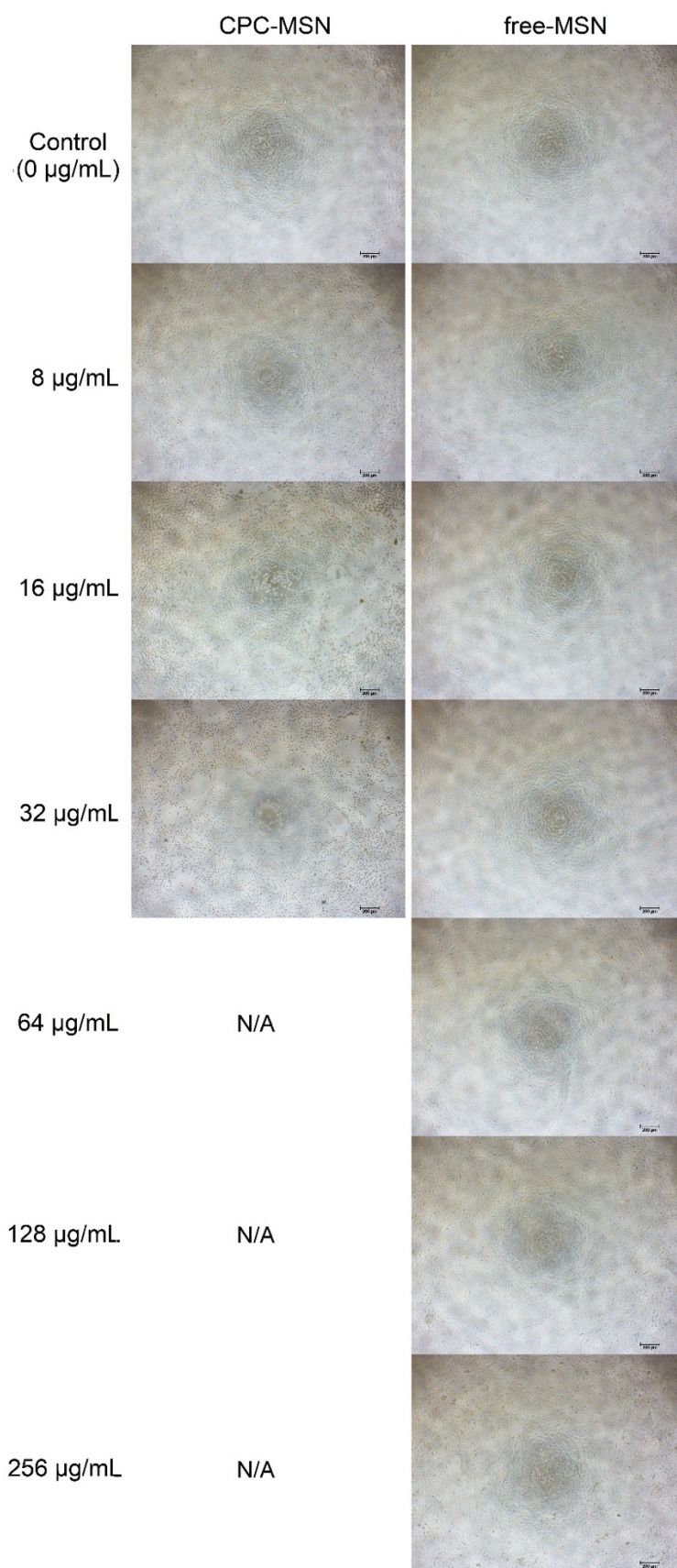
**Figure S6.** Wide-angle X-ray powder diffraction (WAXRD) pattern of CPC-MSN.



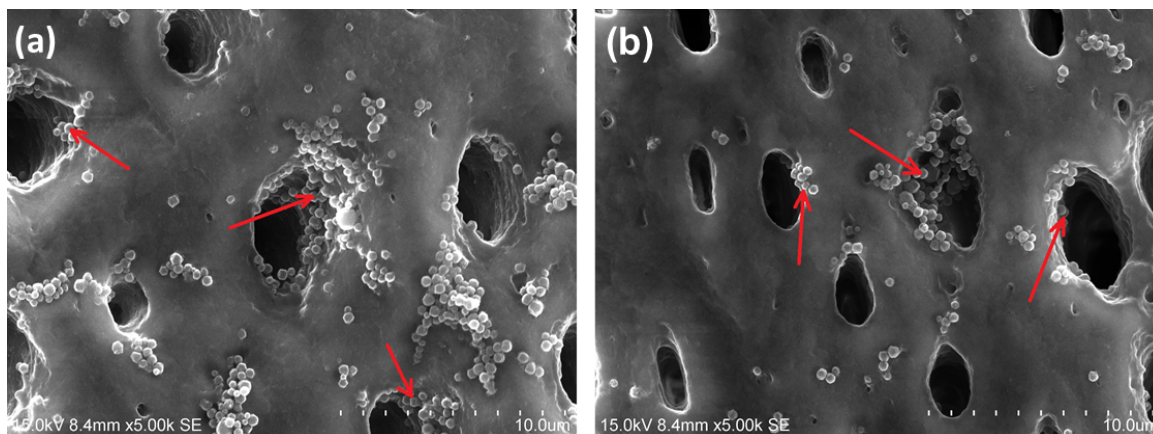
**Figure S7.** UV-Vis spectrum of 1 mM cetylpyridinium chloride (CPC) in H<sub>2</sub>O. Molar extinction coefficient was estimated as 6573 M<sup>-1</sup> cm<sup>-1</sup> at 260 nm.



**Figure S8.** The cell viability of NIH/3T3 mouse fibroblasts after 24 h treatment with **CPC-MSN** (loaded with CPC drug) and **free-MSN** (drug-free form) was assessed using CCK-8 by measuring the absorbance of the supernatant at 450 nm wavelength. Three independent experiments in triplicate were performed.



**Figure S9.** The bright-field cell images (NIH/3T3 cells) after treatment with **CPC-MSN** (loaded with CPC drug) 8–32  $\mu\text{g/mL}$  and **free-MSN** (drug-free form) 8–256  $\mu\text{g/mL}$ . Magnification  $\times 4$ , scale bar = 200  $\mu\text{m}$ .

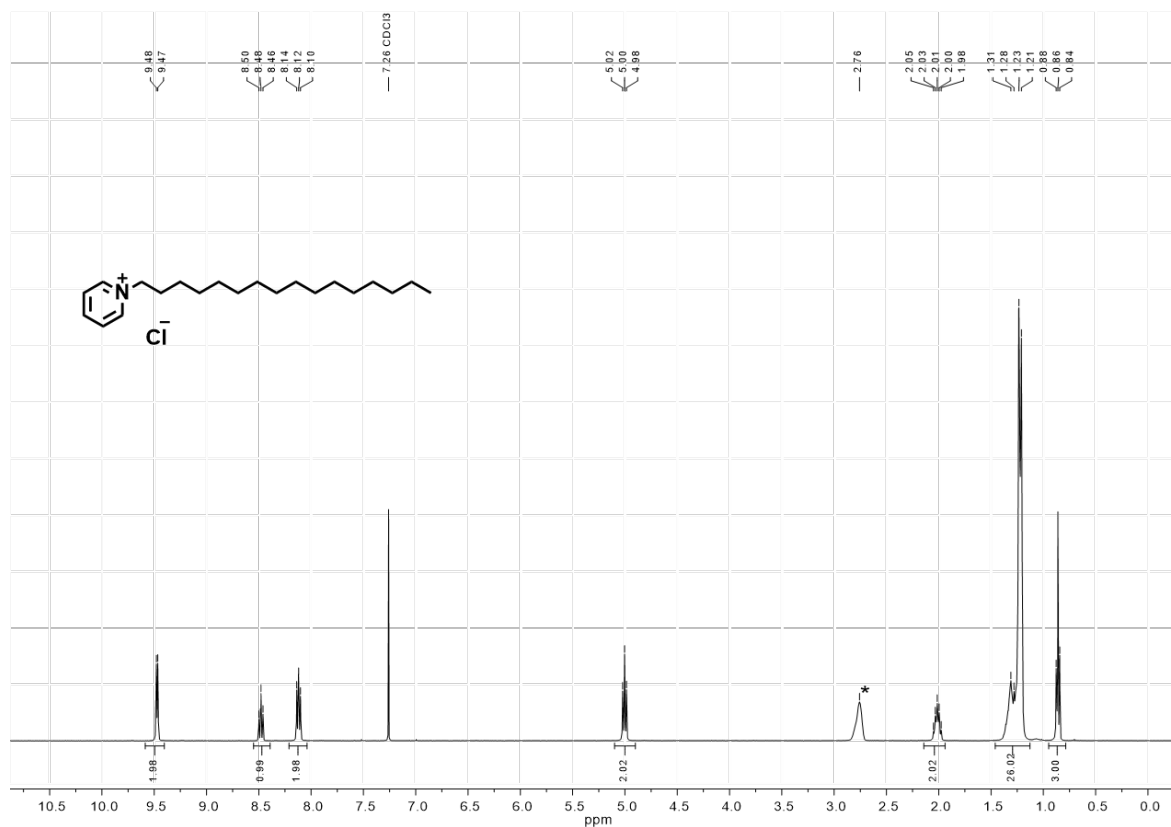


**Figure S10.** Additional scanning electron microscopic (SEM) images for dental tubule penetration by CPC-MSN. Arrows pointing to CPC-MSN inside dental tubules. Scale of (a) and (b) = 10  $\mu\text{m}$ .

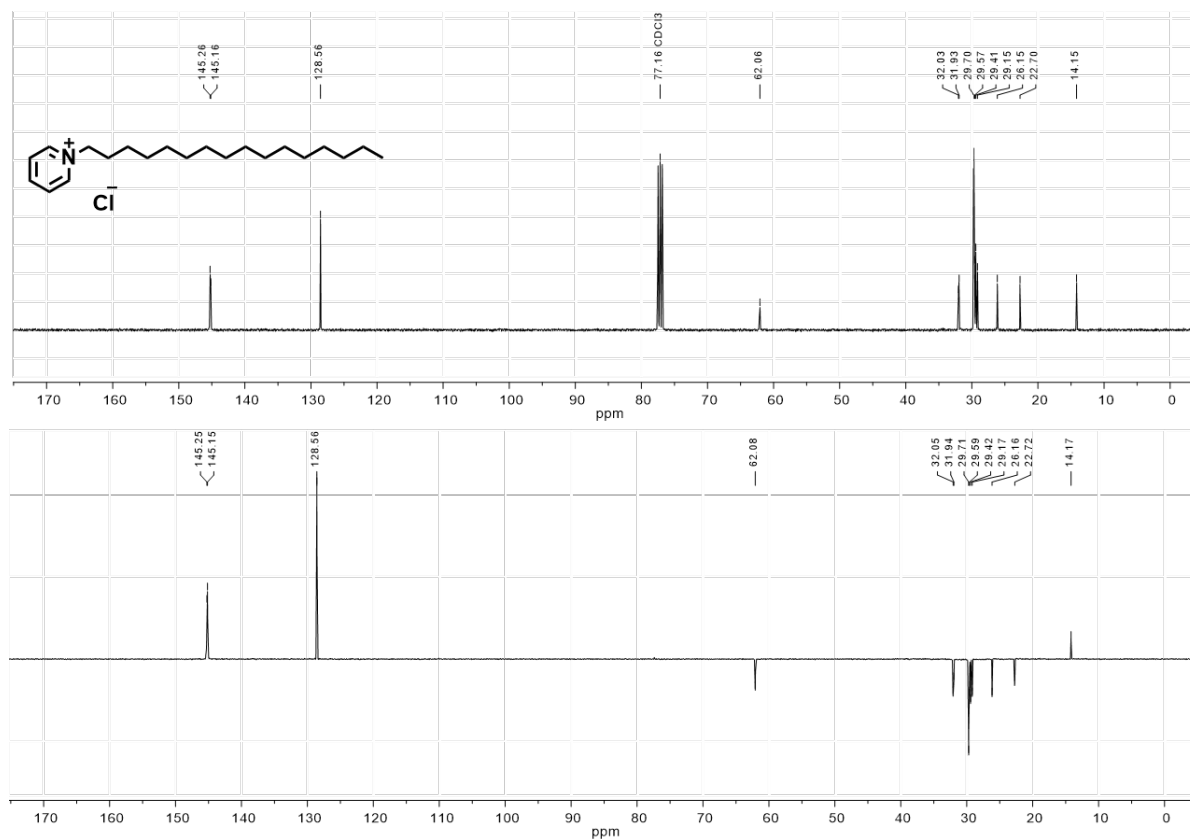
**Table S1.** NMR characterization of CPC drug used in this study:

|                                       |  |
|---------------------------------------|--|
| <b><math>^1\text{H}</math> NMR</b>    | $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ , 298K) $\delta$ 9.47 (d, $J = 5.6$ Hz, 2H), 8.48 (t, $J = 7.8$ Hz, 1H), 8.12 (t, $J = 7.1$ Hz, 2H), 5.00 (t, $J = 7.4$ Hz, 2H), 2.05 – 1.96 (m, 2H), 1.38 – 1.15 (m, 26H), 0.86 (t, $J = 6.9$ Hz, 3H). |
| <b><math>^{13}\text{C}</math> NMR</b> | $^{13}\text{C}$ NMR (101 MHz, $\text{CDCl}_3$ , 298K) $\delta$ 145.27, 145.16, 128.56, 62.08, 32.03, 31.94, 29.70, 29.57, 29.40, 29.15, 26.15, 22.71, 14.15.   |





**Figure S11.** <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>, 298 K) of pristine CPC used.



**Figure S12.** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (101 MHz, CDCl<sub>3</sub>, 298 K) of pristine CPC used.