

## **Sustainable $\gamma$ -cyclodextrin frameworks containing ultra-fine silver nanoparticles with enhanced antimicrobial efficacy**

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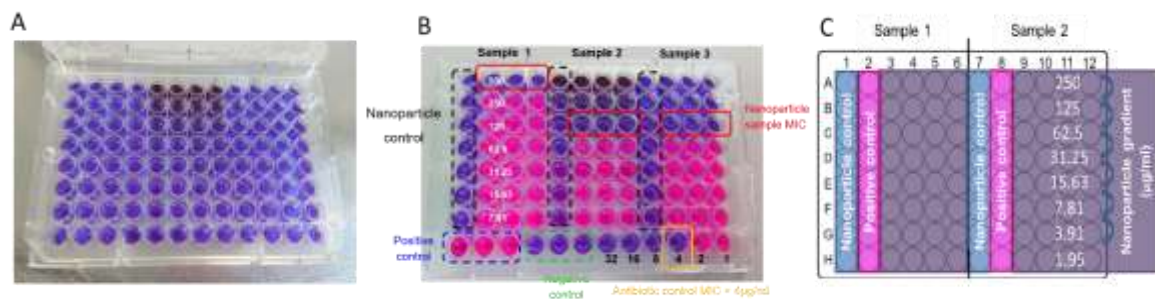
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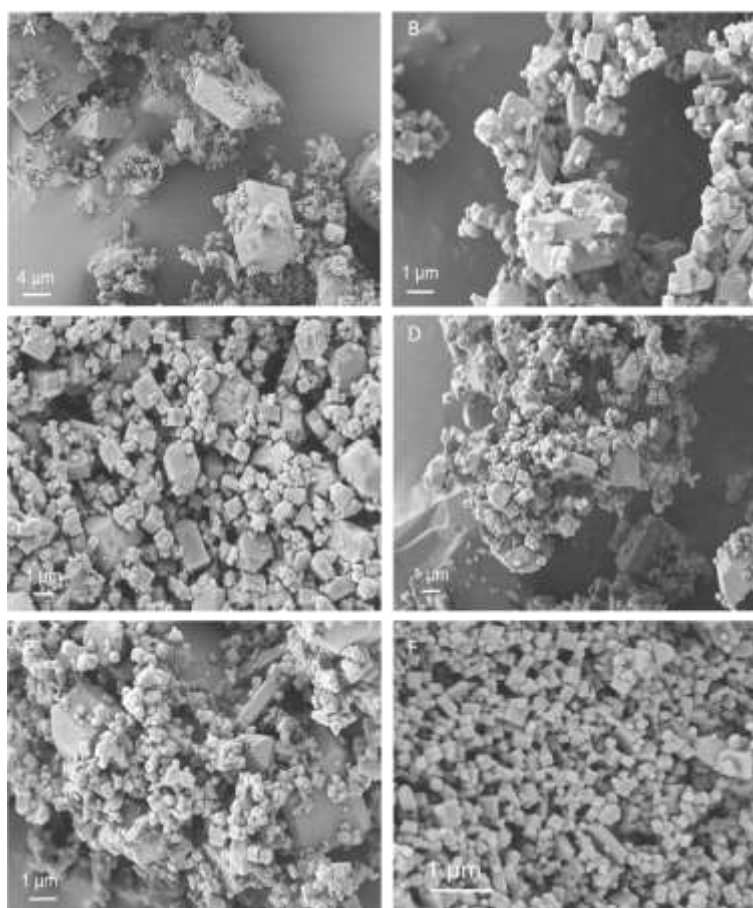
### ***Synthesis of CD-MOF, CD-MOF-CTAB & CD-MOF-PEG***

10 mL aqueous solution of  $\gamma$ -CD (324 mg, 25 mM) and KOH (112 mg, 200 mM) was prepared in a 20 mL clean glass vial. MeOH (50 mL) was allowed to vapour diffuse slowly into the vial at 50 °C for 3-4 days. CD-MOF crystals were collected and washed with EtOH for three times and dried at 50 °C under vacuum and stored until further use. In order to synthesise the nanosized CD-MOF particles, 1 mL MeOH solution was directly added to the vial and heated for 30 minutes at 70 °C. Then, CTAB (8 mg/mL) or PEG 20,000 (256 mg) were added. After that 10 mL of MeOH was added to trigger the rapid precipitation of particles. The suspension was incubated at room temperature for overnight. Finally, the precipitate was harvested and repeatedly washed for three

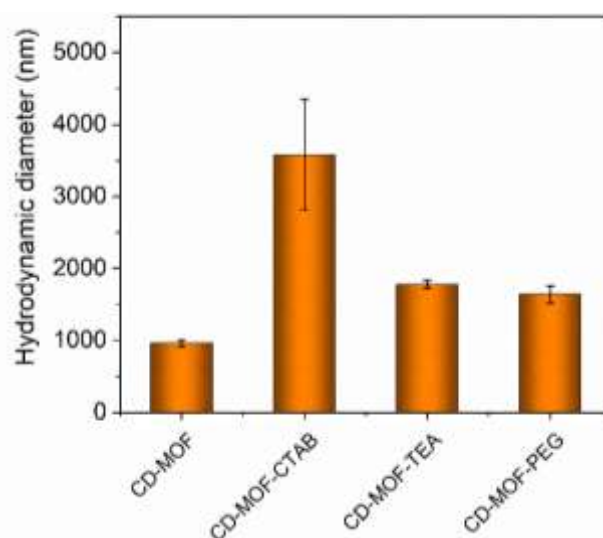
times with EtOH and dried at 50 °C overnight under vacuum (Liu et al., 2017; Liu et al., 2016; Smaldone et al., 2010).



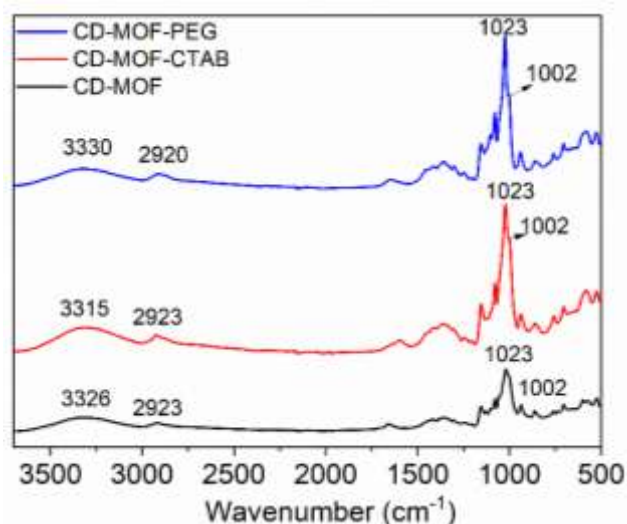
**Supplementary Figure S1** Example of MIC plate with resazurin indicator dye. (A) Immediately after resazurin dye was added to the samples, 24 hours after the addition of resazurin with colour change in wells indicate live viable cells through the reduction of resazurin to resorufin (B), and 96 well plate template for kinetic growth assay. 2 samples were tested on a plate, with 6 columns per sample; one column was used as a nanoparticle control (as highlighted in blue), one column was used as a positive control (as highlighted in pink) and four columns were used to test the nanoparticles in quadruplets (as highlighted in purple) in a 2-fold reducing concentration gradient, as indicated on the right (C).



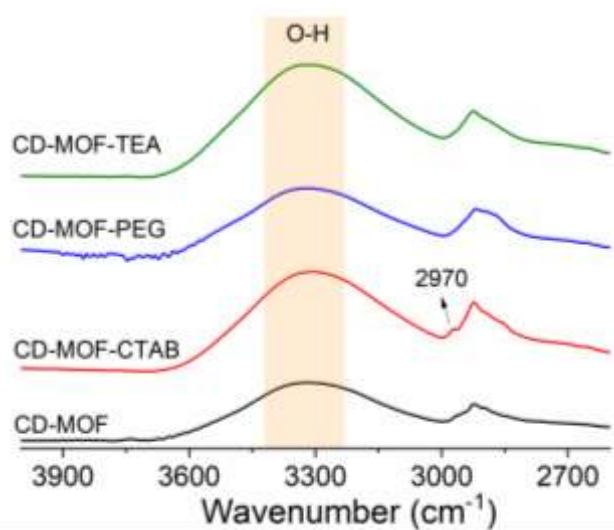
**Supplementary Figure S2** SEM images of CD-MOF crystals showing effect of TEA concentration varying from (A) 0 mL, (B) 1 mL, (C) 1.5 mL, (D) 2.0 mL, (E) 2.5 mL and (F) 3.0 mL in 10 mL solution of  $\gamma$ -CD and KOH.



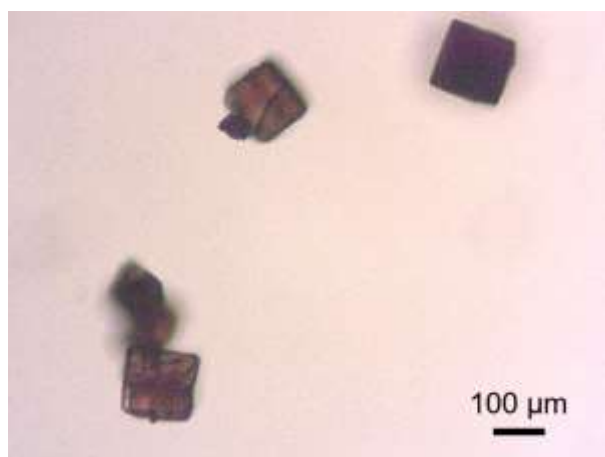
**Supplementary Figure S3.** Hydrodynamic size of different CD-MOF samples measured using dynamic light scattering method.



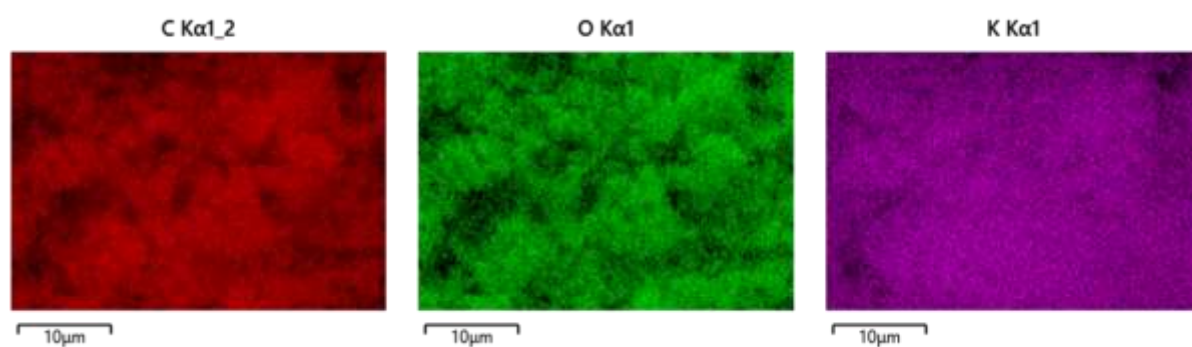
**Supplementary Figure S4.** FTIR spectrum of CD-MOF, CD-MOF-CTAB and CD-MOF-PEG.



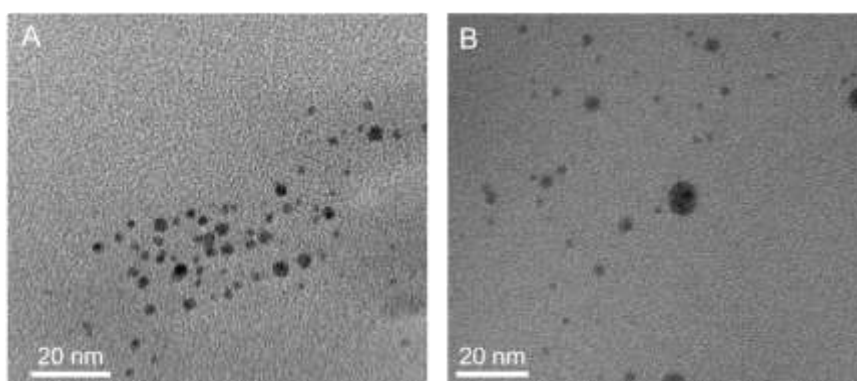
**Supplementary Figure S5.** Short range FTIR spectra showing extra peak at 2970  $\text{cm}^{-1}$  recorded from CD-MOF-CTAB samples. This confirmed that it is difficult to remove bulky modulators from the framework network of MOF.



**Supplementary Figure S6.** Optical image of CD-MOF microcrystals recorded after silver nanoparticle synthesis.



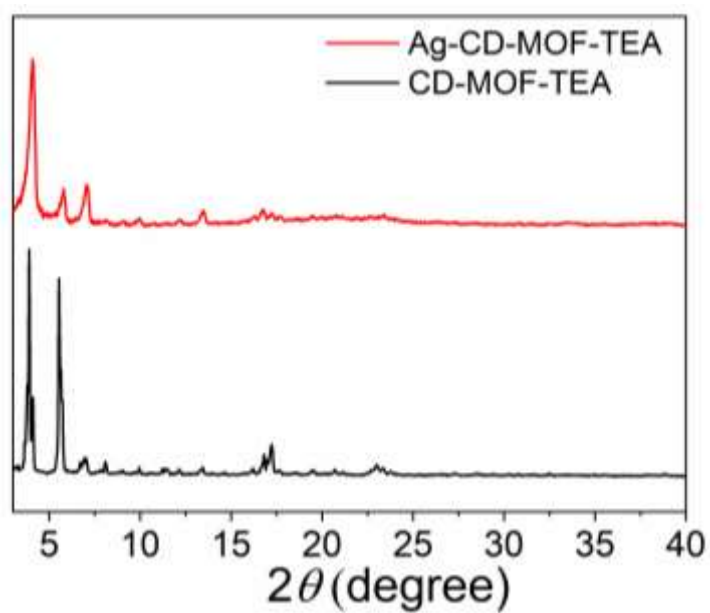
**Supplementary Figure S7.** EDS elemental mapping of Ag-CD-MOF-TEA sample showing distribution of C, O and K distribution in crystals.



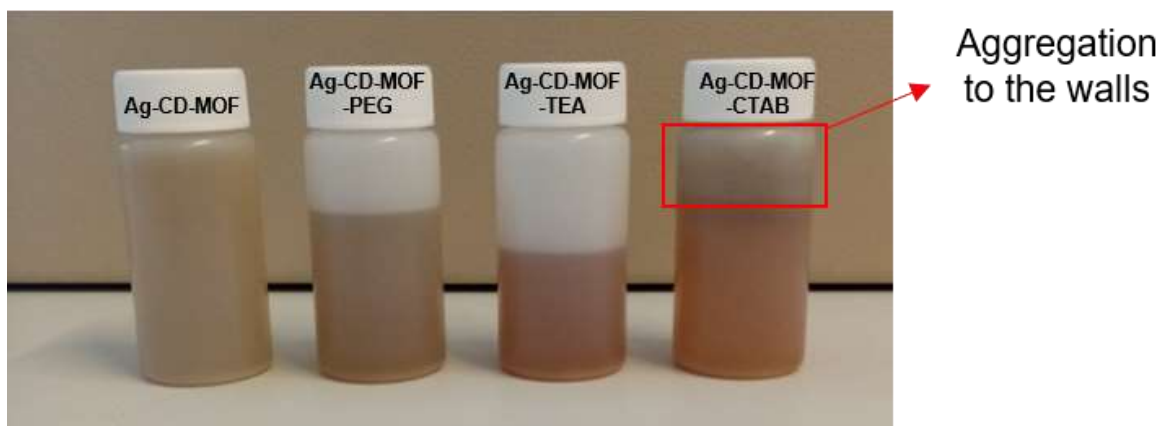
**Supplementary Figure S8.** TEM image of AgNPs from (A) Ag-CD-MOF-CTAB and (B) Ag-CD-MOF-PEG samples.

**Supplementary Table S1.** the percentage of the average Ag in the Ag-CD-MOF synthesised by CTAB, PEG & TEAS as modulators which were acquired by EDS analysis.

Modulators	Ag%
CTAB	10.7 ± 2.5
PEG	12.6 ± 0.7
TEA	13.1 ± 3.6

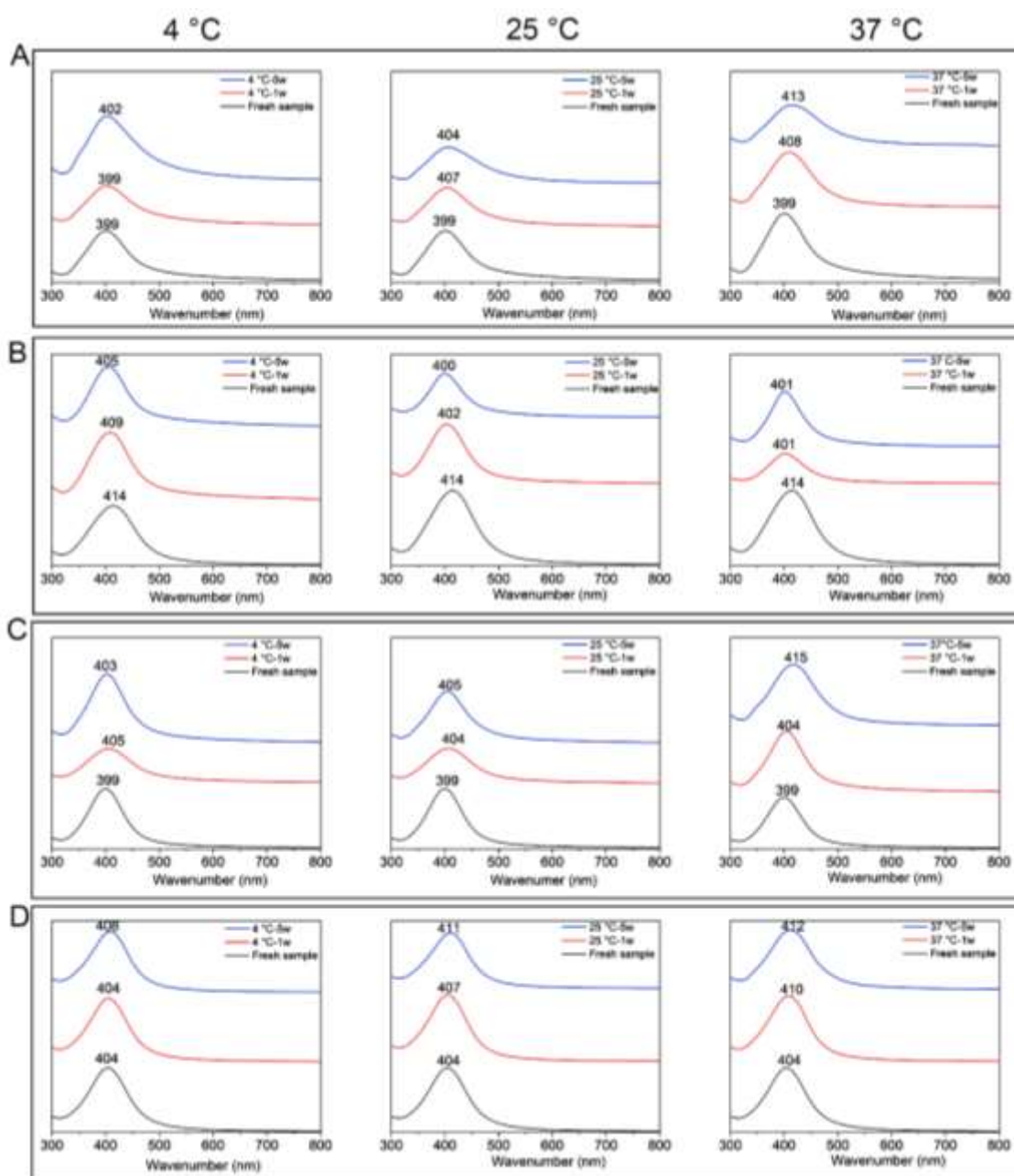


**Supplementary Figure S9.** FTIR spectrum of CD-MOF-TEA and Ag-CD-MOF-TEA.



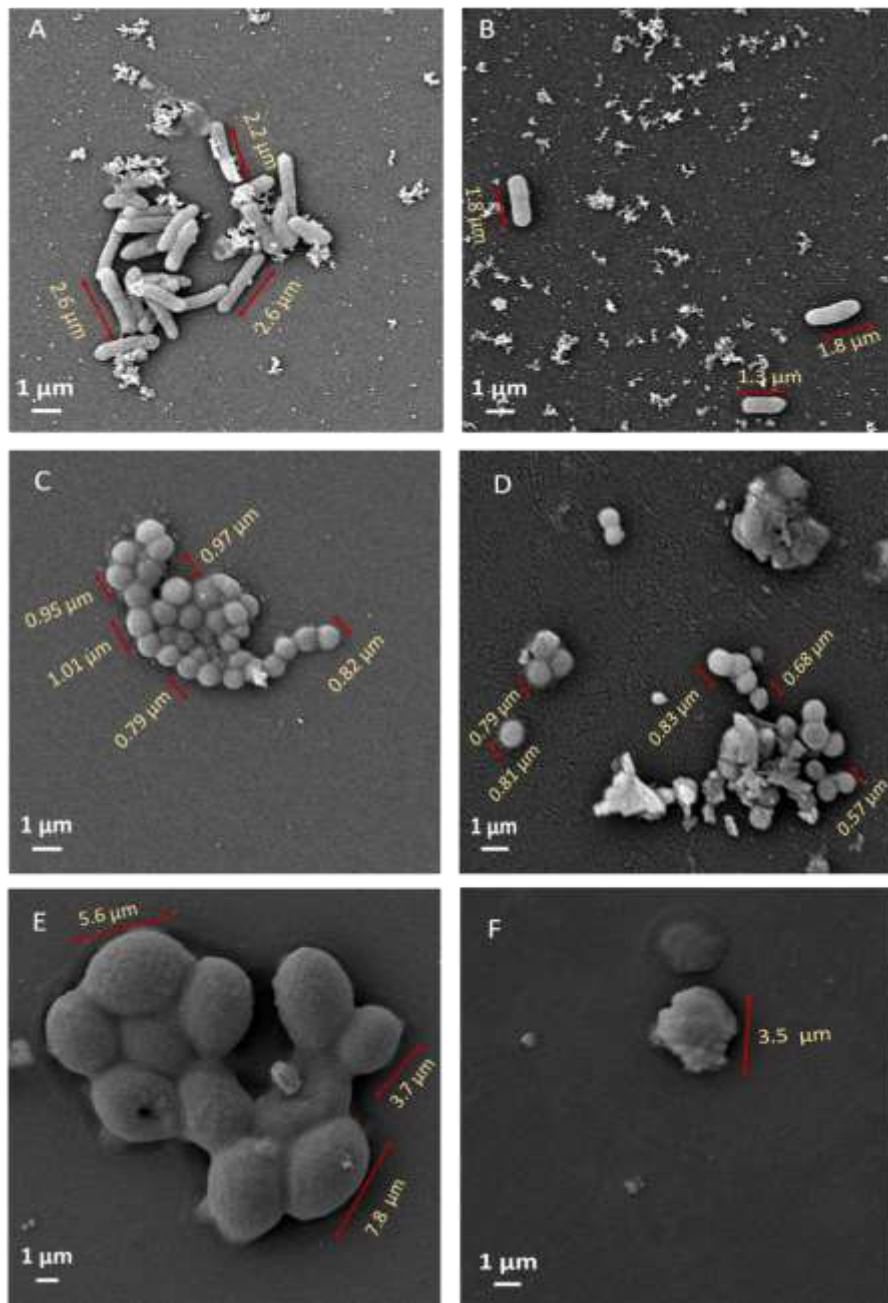
**Supplementary Figure S10.** From left to right, suspension of Ag-CD-MOF, Ag-CD-MOF-PEG, Ag-CD-MOF-TEA & Ag-CD-MOF-CTAB in water at concentration of 0.5 mg/mL.





**Supplementary Figure S11.** Stability testing using UV-Vis spectroscopy. (A) Spectrum of Ag-CD-MOF, (B) Ag-CD-MOF-CTAB, (C) Ag-CD-MOF-PEG and (D) Ag-CD-MOF-TEA suspensions stored at 4 °C, 25 °C and 37 °C, respectively.





**Supplementary Figure S12.** SEM images of control and treated samples processed using ImageJ for size reduction quantification (A) *E. coli* control, (B) *E. coli* treated with Ag-CD-MOF-TEA samples. (C) *S. aureus* control and (D) *S. aureus* treated with Ag-CD-MOF-TEA samples. (E) *C. albicans* control and (F) *C. albicans* treated with Ag-CD-MOF-TEA.

## References

Liu, B., He, Y., Han, L., Singh, V., Xu, X., Guo, T., Meng, F., Xu, X., York, P., Liu, Z., *et al.* (2017). Microwave-assisted rapid synthesis of  $\gamma$ -cyclodextrin metal–organic frameworks for size control and efficient drug loading. *Crystal Growth & Design* *17*, 1654-1660.

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