Supporting information for

Copper(II)-based coordination polymer nanofibers as highly effective antibacterial material with synergistic mechanism

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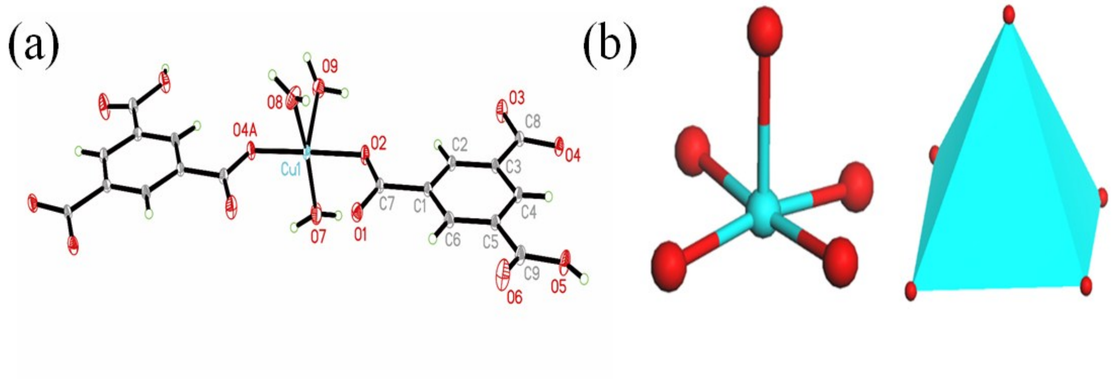

Fig. S1 (a), (b) View of coordination environment of Cu^{2+} centres in macro particle of $[Cu(HBTC)(H_2O)_3]$

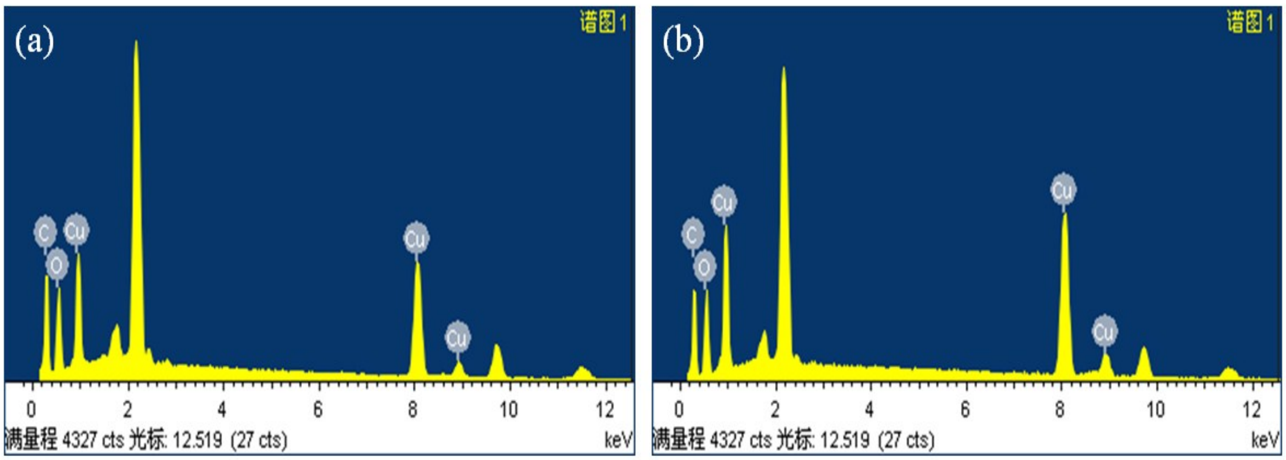

Fig. S2 EDS spectra of (a) macroparticle, (b) nanofiber of [Cu(HBTC)(H_2O)$_3$]

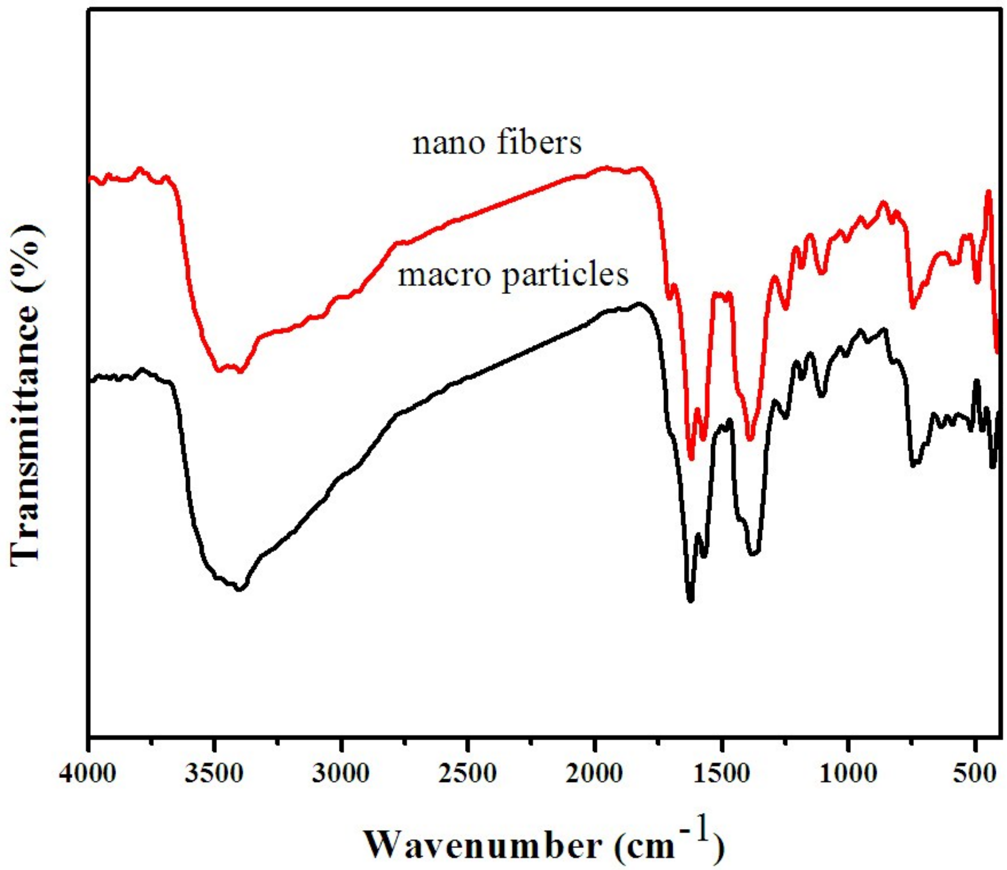

Fig. S3 IR-Spectra of macro particles and nanofibers of [Cu(HBTC)(H_2O)$_3$]

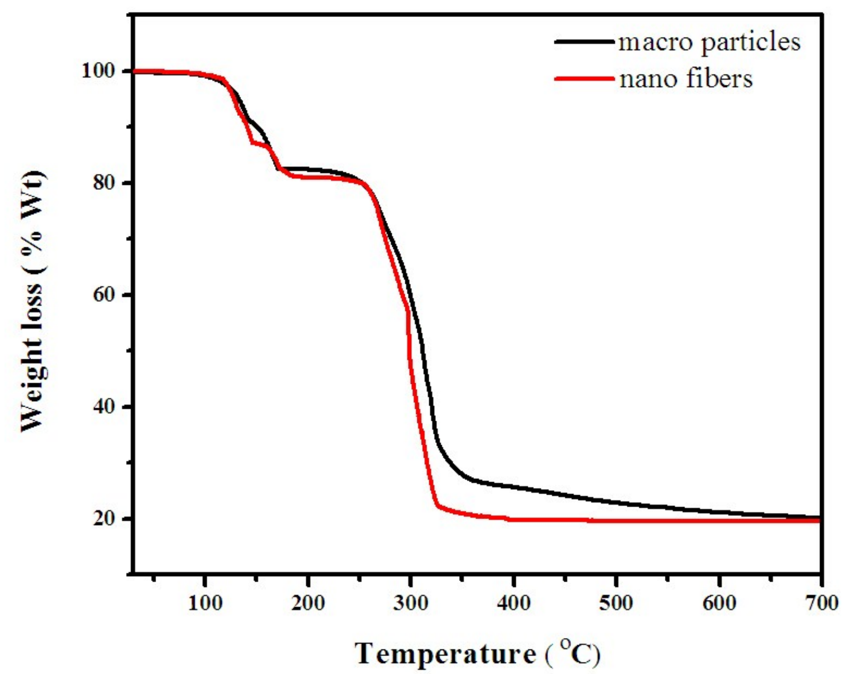

Fig. S4 Thermo-gravimetric curve of macroparticles and nanofibers of

$[Cu(HBTC)(H_2O)_3]$

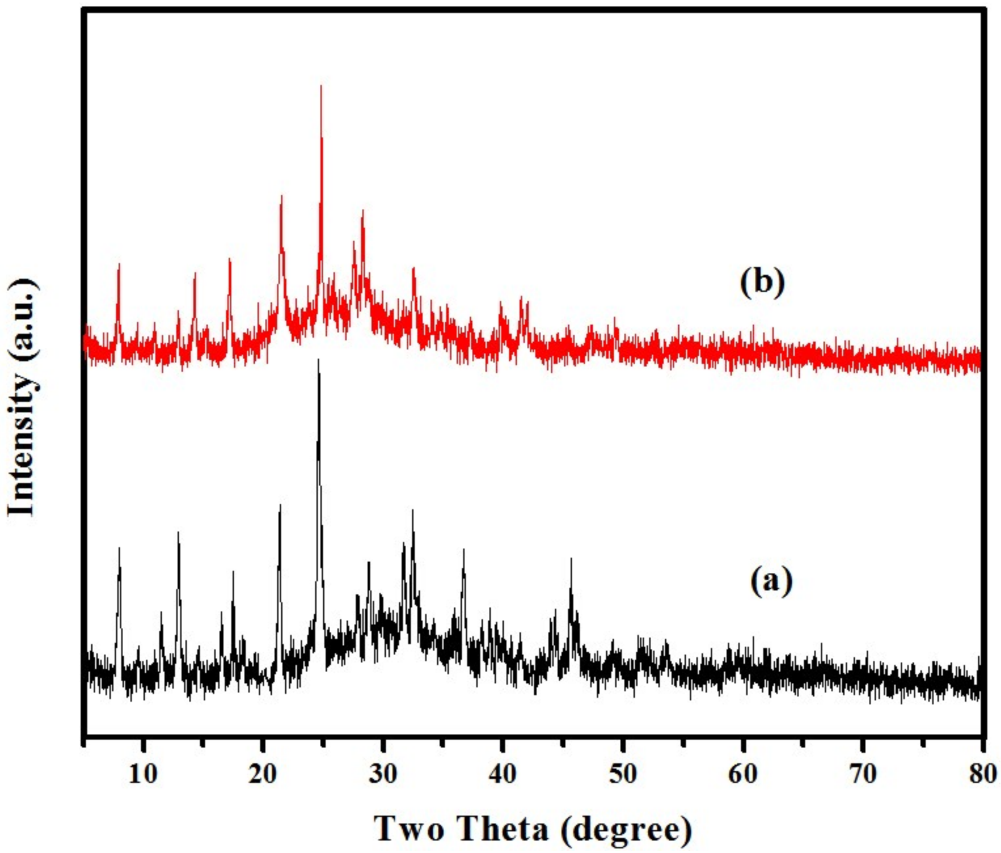

Fig. S5 The XRD patterns of nanofibers before (a) and after (b) immersing into distilled water for 24 h.

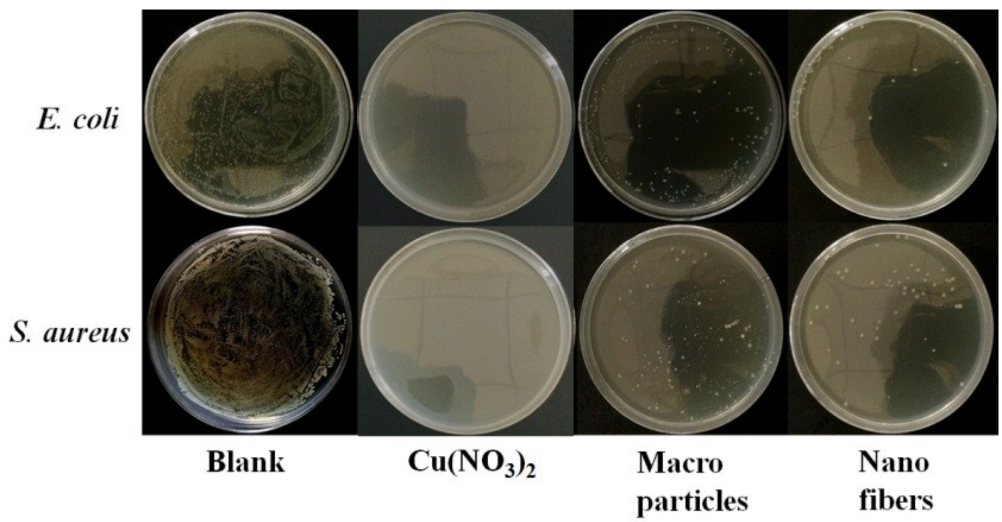

Fig. S6 Colony count Percentage of inhibition *E. coli* (a) and *S. aureus* (b) after being treated with the $Cu(NO_3)_2$, macroparticles and nanofibers with 250 µg/mL concentration.

Table S1 Crystal data and structure refinement for [Cu(HBTC)(H_2O)$_3$]

Empirical formula	$C_9H_{10}CuO_9$
Formula weight	325.72
Crystal system	Monoclinic, $P2_1/c$
T (K)	296(2)
a (Å)	6.8432(5)
b (Å)	18.8678(13)
c (Å)	10.6835(6)
β (º)	126.782(4)
Volume (Å^3)	1104.80(13)
Z	4
D_{Calc} (mg/m^{-3})	1.958
μ (mm^{-1})	2.021
$F_{(000)}$	660
R_{int}	0.0256
GOF on F^2	1.017
R_1 [I>2σ(I)]*	0.0372
wR_2 [I>2σ(I)]*	0.1020
R_1 (all data) *	0.0544
wR_2 (all data)*	0.1193

*$R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$; $wR_2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)]^2\}^{1/2}$

Table S2. Selected bond lengths [Å] and angles [°] for [Cu(HBTC)(H_2O)$_3$]

Cu(1)-O(2)	1.9176(16)	Cu(1)-O(8)	1.982(2)
Cu(1)-O(4)$^{\#1}$	1.9289(16)	Cu(1)-O(9)	2.2584(17)
Cu(1)-O(7)	1.988(2)	O(4)$^{\#1}$-Cu(1)-O(7)	88.42(8)
O(2)-Cu(1)-O(4)$^{\#1}$	174.43(7)	O(4)$^{\#1}$-Cu(1)-O(8)	91.08(8)
O(2)-Cu(1)-O(7)	87.30(8)	O(7)-Cu(1)-O(9)	95.25(9)
O(2)-Cu(1)-O(8)	93.79(8)	O(8)-Cu(1)-O(7)	169.26(9)
O(2)-Cu(1)-O(9)	90.28(7)	O(8)-Cu(1)-O(9)	95.43(8)

Symmetry transformations used to generate equivalent atoms: #1 -x, y-1/2, -z+1/2.

Table S3. Hydrogen bonds for [Cu(HBTC)(H_2O)$_3$] [Å and °]

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(5)-H(5)···O(3)$^{\#1}$	0.83	1.76	2.569(2)	164.0
O(7)-H(7A)···O(5)$^{\#2}$	0.88	2.01	2.867(3)	166.2
O(7)-H(7B)···O(1)$^{\#3}$	0.86	1.85	2.685(3)	161.6
O(8)-H(8A)···O(4)$^{\#4}$	0.87	2.29	3.123(3)	160.2
O(8)-H(8A)···O(9)$^{\#5}$	0.87	2.63	3.092(3)	114.4
O(8)-H(8B)···O(1)$^{\#6}$	0.87	1.86	2.707(3)	164.6
O(9)-H(9A)···O(3)$^{\#7}$	0.87	2.40	3.067(3)	133.5
O(9)-H(9B)···O(6)$^{\#8}$	0.89	1.91	2.795(3)	169.4

Symmetry transformations used to generate equivalent atoms: #1 x+1,y,z+1; #2 -x+1,-y,-z+1; #3 x,-y-1/2,z-1/2 #4 -x,-y,-z+1; #5 x,-y-1/2,z+1/2; #6 x-1,-y-1/2,z-1/2; #7 -x-1,-y,-z; #8 x-1,y,z-1

Table S4. Results of the percentage of inhibition of bacterial growth by colony count method (250 µg/mL)

Materials	Microorganism	Percentage of inhibition of bacterial growth $K = (N_{control} - N_{sample})/N_{control} \times 100\%$
Commercial Cu-NPs	*E. coli*	24.0 %
	S. aureus	24.3 %
Marcoparticles	*E. coli*	96.7 %
	S. aureus	96.2 %
Nanofibers	*E. coli*	99.9 %
	S. aureus	99.1 %

E. coli = Escherichia coli; *S. aureus* = Staphylococcus aureus