

Supplementary Material

Photocatalytic and Antibacterial activity of graphene oxide/cellulose-doped TiO₂ quantum dots: In silico molecular docking studies

Muhammad Ikram^{a*}, Fahad Rasheed^b, Ali Haider^c, Sadia Naz^d, Anwar Ul-Hamid^{e*}, Anum Shahzadi^e, Junaid Haider^f, Iram Shahzadi^g; Shaukat Hayat^b, Salamat Ali^b

^aSolar Cell Application Research Lab, Department of Physics, Government College University Lahore, Lahore, 54000, Punjab, Pakistan

^bDepartment of Physics, Riphah Institute of Computing and Applied Sciences (RICAS), Riphah International University, 14 Ali Road, Lahore, Pakistan

^cDepartment of Clinical Sciences, Faculty of Veterinary and Animal Sciences, Muhammad Nawaz Shareef University of Agriculture, Multan, 66000, Pakistan

^dTianjin Institute of Industrial Biotechnology, Chinese Academy of Sciences, Tianjin 300308, China.

^eCore Research Facilities, King Fahd University of Petroleum & Minerals, Dhahran, 31261, Saudi Arabia

^fFaculty of Pharmacy, The University of Lahore, Lahore, Pakistan

^gPunjab University College of Pharmacy, University of the Punjab, 54000, Pakistan

*Corresponding authors emails: ^adr.muhammadikram@gcu.edu.pk, ^eanwar@kfupm.edu.sa

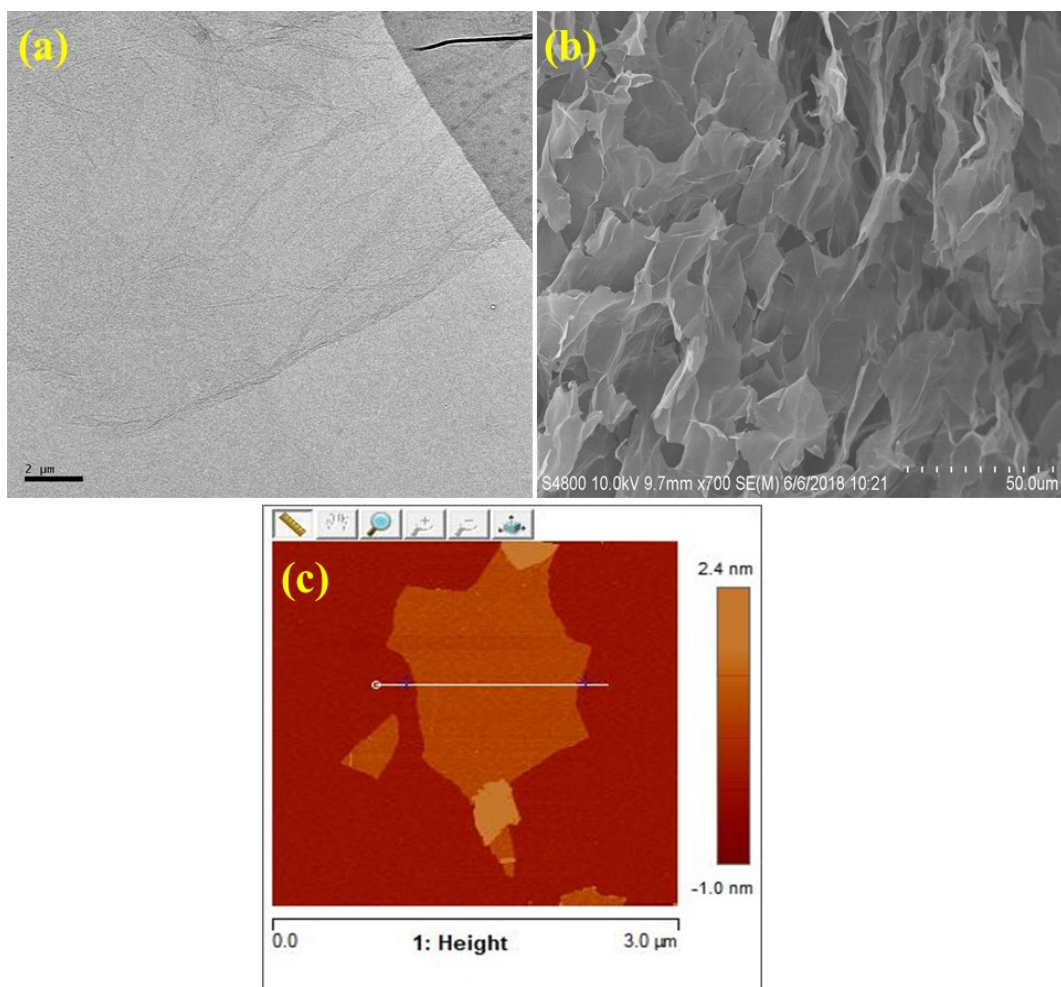


Fig. S1: (a) HR-TEM, (b) SEM, and (c) Atomic Force Microscopy images of GO

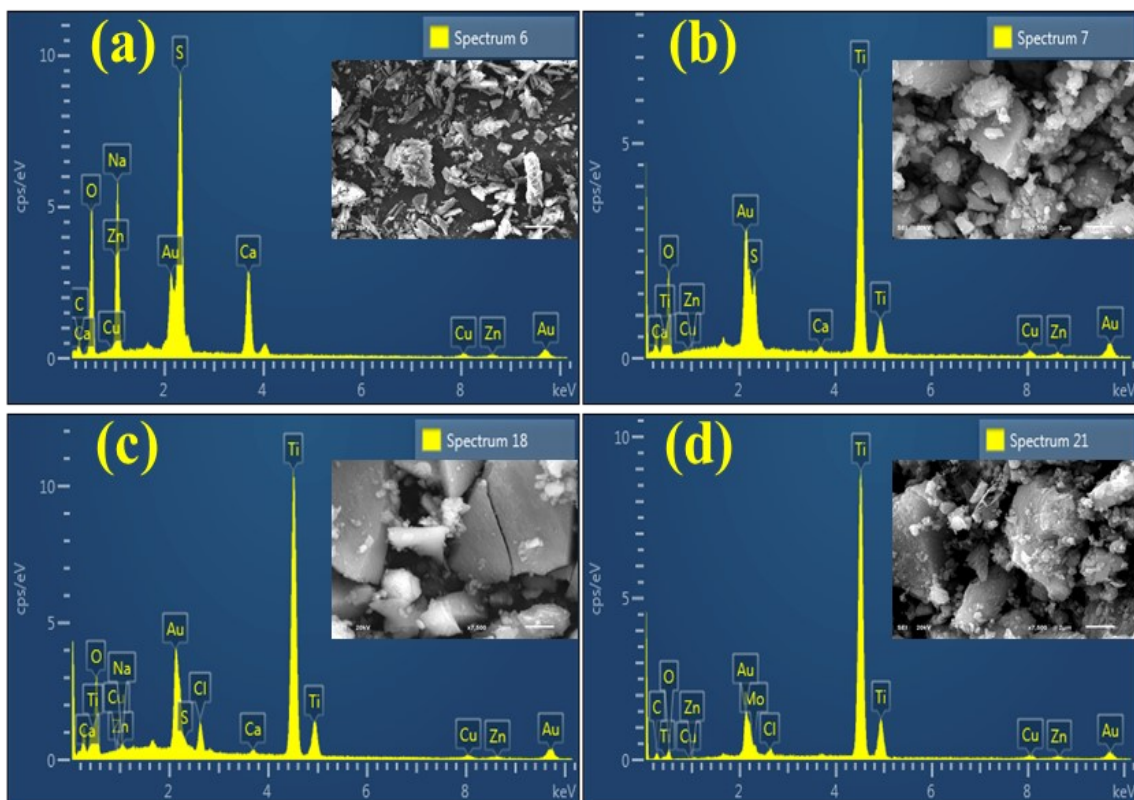


Fig. S2: Energy dispersive x-ray spectroscopy (EDS) results obtained from (a) CNC, (b) TiO_2 , (c) $\text{CNC}:\text{TiO}_2$ and (d) $\text{GO}:\text{CNC}:\text{TiO}_2$

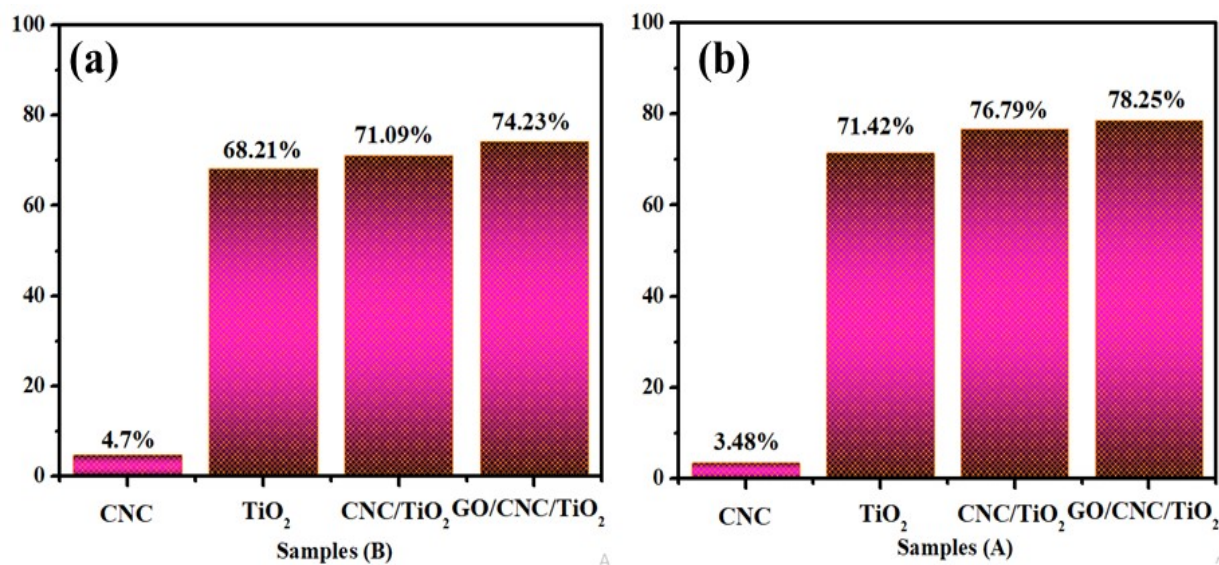


Figure S3. Photocatalysis of CNC, TiO_2 , CNC/TiO_2 , $\text{GO}/\text{CNC}/\text{TiO}_2$ in (a) basic and (b) acidic medium, respectively

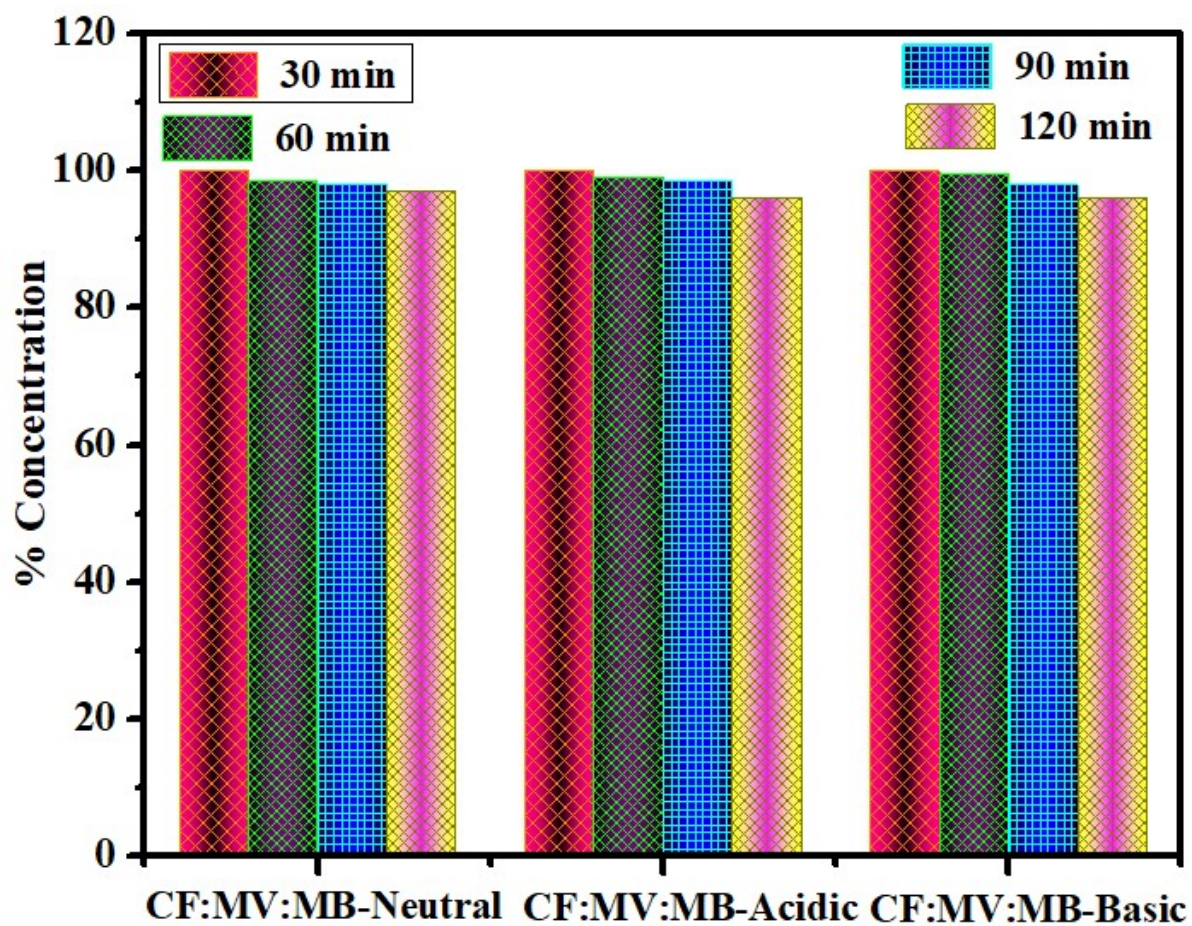


Figure S4. Dye degradation in the dark for comparison.

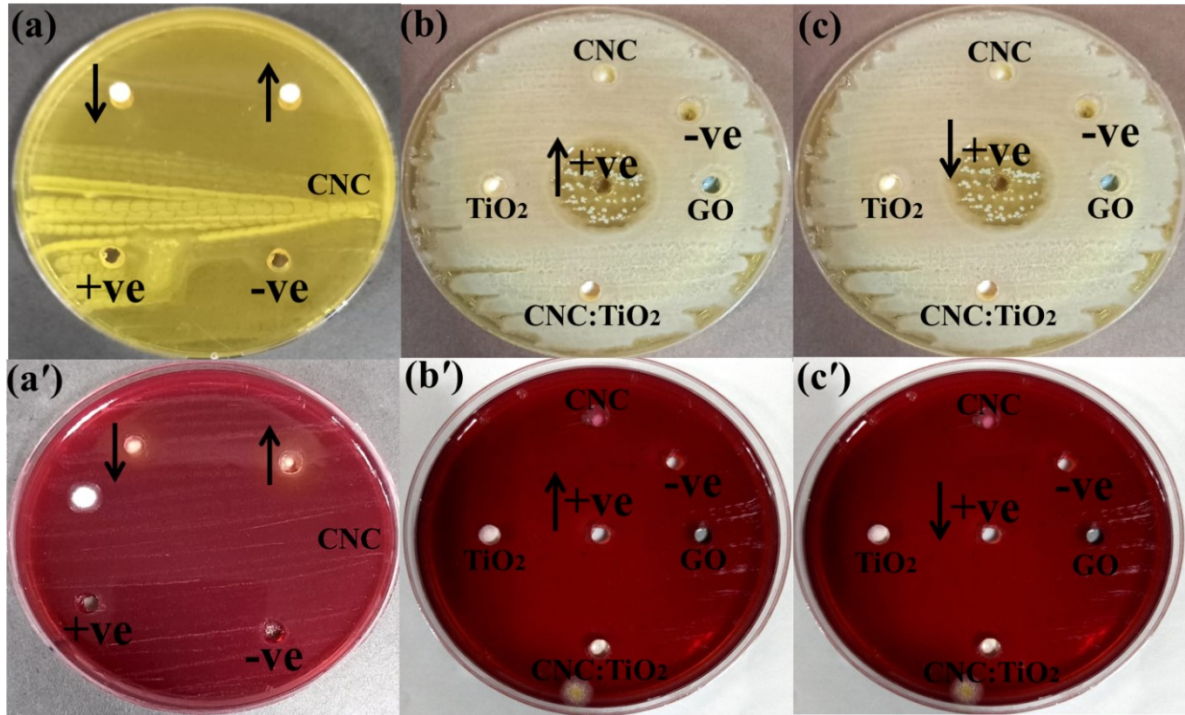


Fig. S5: In vitro antibacterial activity of (a, a') CNC and (b, b'-c, c') bare and doped TiO₂ for low and high concentration against SA and EC, respectively.

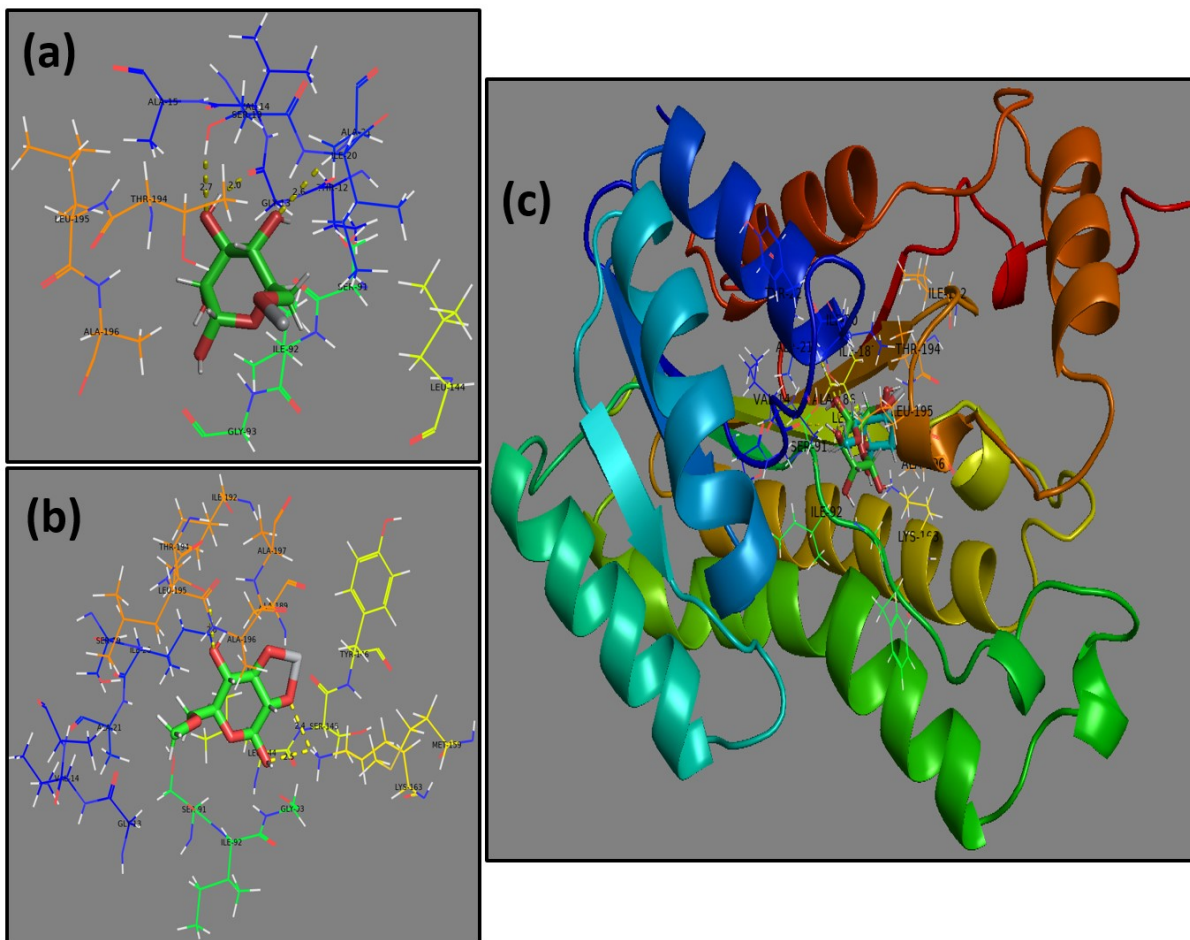


Figure S6: Binding interaction pattern inside active pocket of FabI from *E. coli* (a). TiO₂-CNC, (b). GO/CNC-doped TiO₂, (c). Superimposed docked complexes of TiO₂-CNC and GO/CNC-doped TiO₂ with FabI

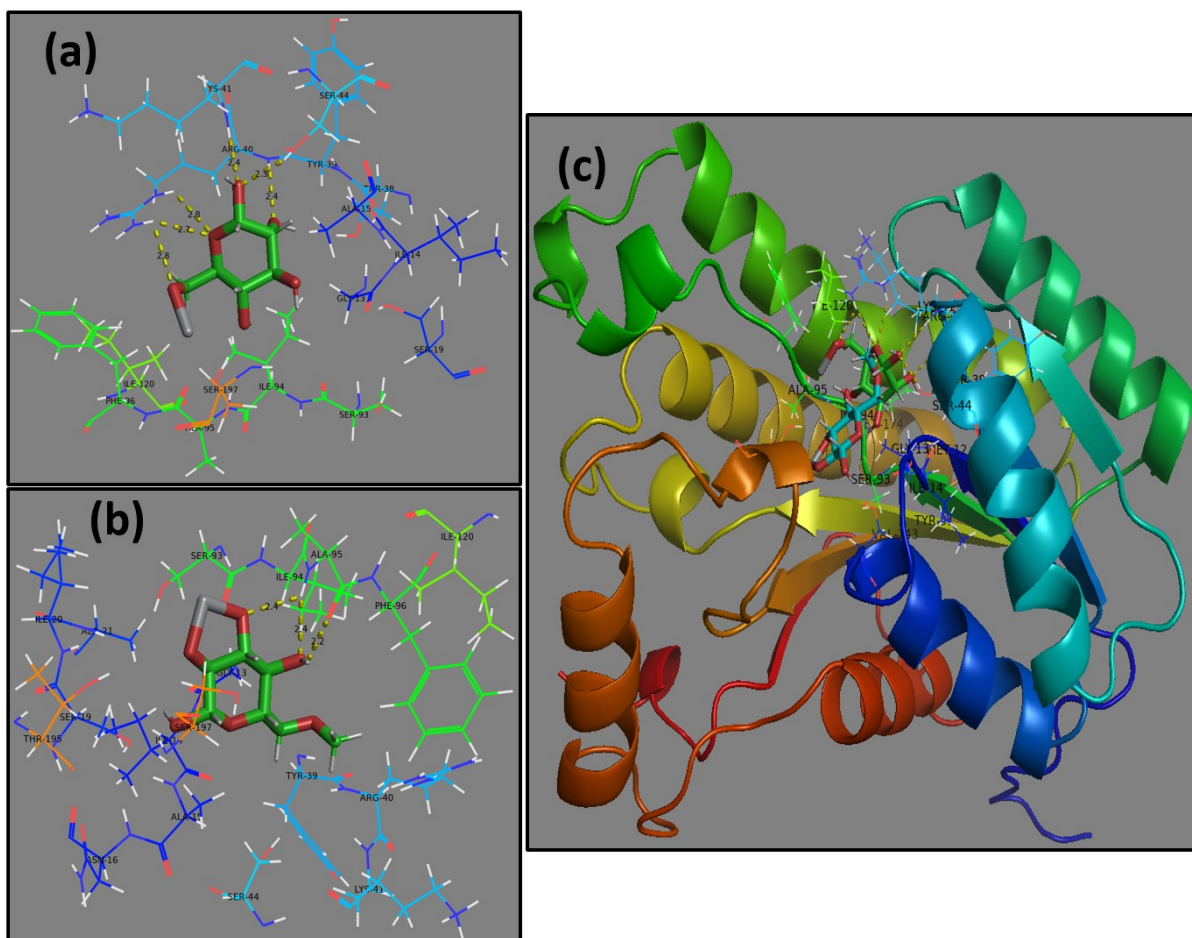


Figure S7: Binding interaction pattern inside active pocket of FabI from *S. aureus* (a). TiO₂-CNC, (b). GO/CNC-doped TiO₂, (c). Superimposed docked complexes of TiO₂-CNC and GO/CNC-doped TiO₂ with FabI

Figure S8 demonstrated that the MB degradation occurs around λ of 665 nm for MV = 605 and CF = 290 nm, respectively. Dyes degrade gradually under illumination upon doping GO/CNC doped TiO₂, while observed UV-Vis spectra are given below.

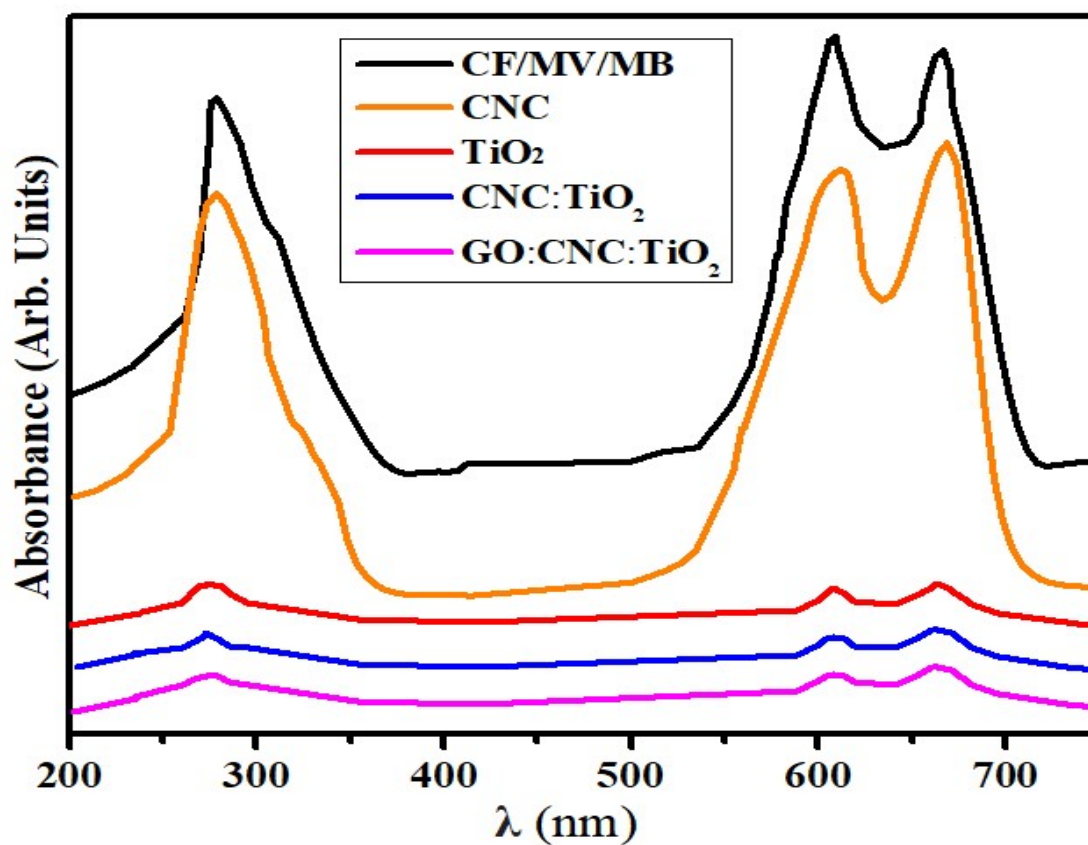


Figure S8. Represents the CF, MV, and MB absorption peaks for the neutral medium of the prepared sample

Table S1 Bactericidal action of GO/CNC:TiO₂

Samples	<i>S. aureus</i>		<i>E. coli</i>	
	Inhibition zone ^a (mm)		Inhibition zone ^b (mm)	
	1 %	2 %	1 %	2 %
CNC	0.95±0.05	1.67±0.06	3.36±0.07	4.49±0.05
TiO ₂	0±0.00	1.26±0.03	0±0.00	0±0.00
CNC:TiO ₂	0±0.00	1.73±0.07	3.17±0.02	4.52±0.02
GO/CNC:TiO ₂	1.03±0.12	2.10±0.05	3.49±0.05	5.21±0.02
Ciprofloxacin	7.75±0.00	7.75±0.00	7.15±0.00	7.15±0.00
DIW	0±0.00	0±0.00	0±0.00	0±0.00

^a Inhibition zone (mm) of GO/CNC-doped TiO₂ for *S. aureus*

^b Inhibition zone measurements for *E. coli*.