## Catalytic performance and antibacterial behaviour with molecular docking analysis of Silver and Polyacrylic acid doped Graphene quantum dots

Tahreem Aziz<sup>a</sup>, Muhammad Imran<sup>a</sup>, Ali Haider<sup>b</sup>, Anum Shahzadi<sup>c</sup>, Muhammad Zain Ul Abidin<sup>d</sup>, Anwar Ul-Hamid<sup>e\*</sup>, Walid Nabgan<sup>f\*</sup>, Mohammed M Algaradah<sup>g</sup>, Ahmed M. Fouda<sup>h</sup>

Muhammad Ikram<sup>d\*</sup>

<sup>a</sup>Department of Chemistry, Government College University, Faisalabad, Pakpattan Road, Sahiwal, Punjab, 57000, Pakistan

<sup>b</sup>Department of Clinical Sciences, Faculty of Veterinary and Animal Sciences, Muhammad Nawaz Shareef, University of Agriculture, Multan 66000, Punjab, Pakistan

<sup>c</sup>Faculty of Pharmacy, The university of Lahore, Lahore, 54000, Pakistan

<sup>d</sup>Solar Cell Applications Research Lab, Department of Physics, Government College University Lahore, Lahore 54000, Punjab, Pakistan

<sup>e</sup>Core Research Facilities, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia

<sup>f</sup>Departament d'Enginyeria Química, Universitat Rovira i Virgili, Av Països Catalans 26, 43007 Tarragona, Spain

<sup>g</sup>Chemistry Department, Faculty of Science, King Khalid University, Abha 61413, Saudi Arabia 
<sup>h</sup>Chemistry Department, Faculty of Science, King Khalid University, Abha 61413, Saudi Arabia 
Corresponding author email: <sup>d</sup>dr.muhammadikram@gcu.edu.pk

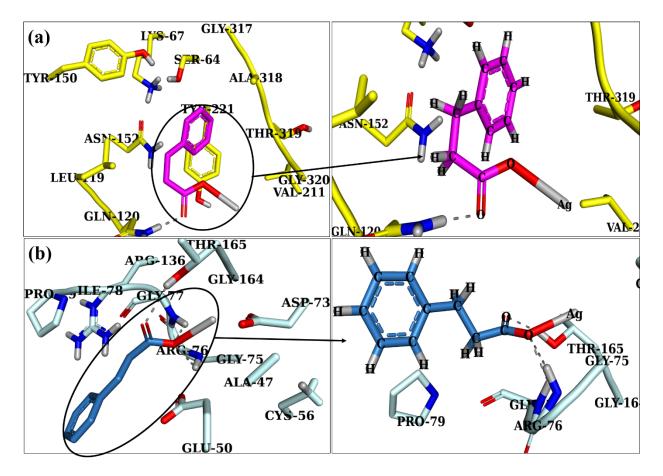


Fig S1. Binding interaction pattern of ligand with active site residues of  $\beta$ -lactamase (a) and DNA gyrase (b) enzyme from *E. coli*.

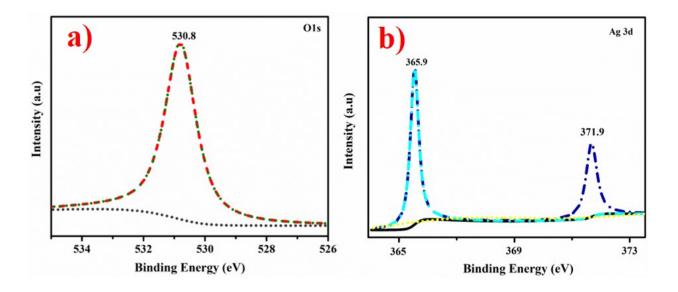
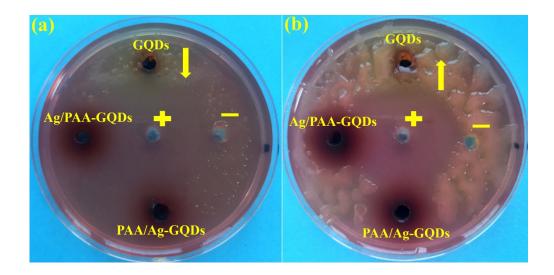


Fig S2. XPS spectra of as PAA/Ag-GQDs (a) O1s (b) Ag 3d



**Fig S3**. In vitro antimicrobial activity of the prepared sample against (a) *S. Aureus* at low dose (b) *S. Aureus* at high dose.

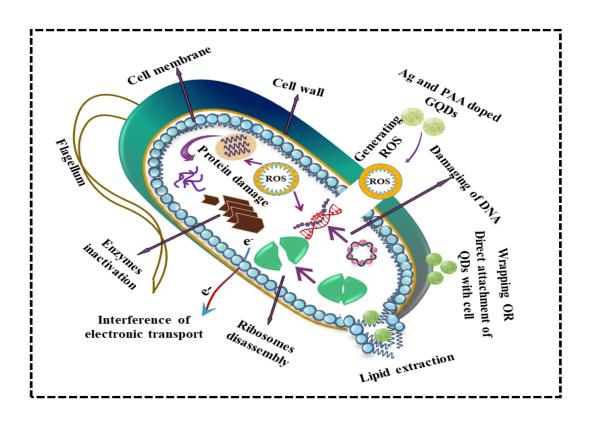


Fig S4. Antibacterial mechanism of GQDs, Ag: PAA GQDs, and PAA: Ag GQDs