Electronic Supplementary Information

Chlorophenyl Pendant Decorated Graphene Sheet as a Potential Antimicrobial Agent: Synthesis and Characterization

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To estimate the percentage grafting of 4-chloro aniline (PCA) onto graphene sheet, a standard calibration curve was plotted. Various molar concentration of 4-chloro aniline was taken ranging from 0.017 mM to 0.142 mM with dried KBr. Typically, 2mg; 5 mg; 8mg and 16 mg of 4-chloro aniline were admixed with 75 mg of dried KBr powder. A pressure of 69-103 MPa was applied to generate fine disk of uniform thickness under hydraulic press. For background correction, a KBR disk was prepared under similar condition. After background correction, all the samples were analyzed between 450 cm^{-1} to 4000 cm^{-1} at a of resolution of 4cm^{-1}. The absorbance value corresponding to C-Cl bond was recorded and plotted against the molar concentration of PCA. To analyze the grafting level, 25 mg of CBG was admixed with 75 mg of dried KBr powder and uniform disk were prepared and analyzed as per the aforesaid conditions. The absorbance for C-Cl was recorded for CBG and compared with the standard calibration curve. From the curve, chlorine concentration was determined from which the grafting level was determined as shown in Figure S1.

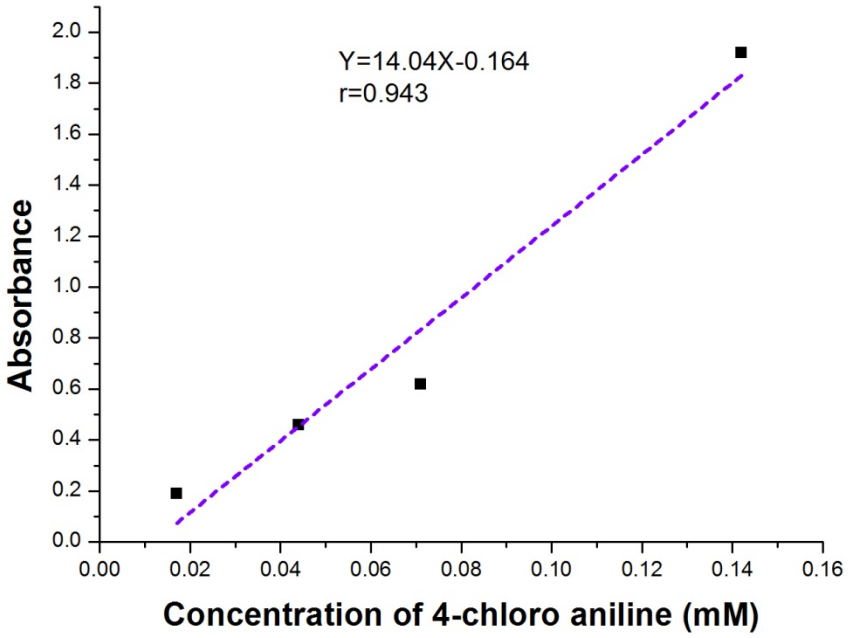

Figure S1: Standard calibration curve over known range of concentration of 4-chloro aniline considering C-Cl absorbance to estimate percentage grafting.

The thermal analysis was done in nitrogen atmosphere at between 25-800°C with a ramp rate of 10°/C. The degradation profile for CBG was marked by two step degradation with an onset at 250°C and the other around 450°C. The total weight loss was around 48%. This is not in line with the XPS and FTIR data. The higher degree of weight loss is attributed to 18 fold increase in the strain in the crystal structure of graphene due to modification, which upon heating preferred to break apart when high temperature was provided as shown in Figure S2.

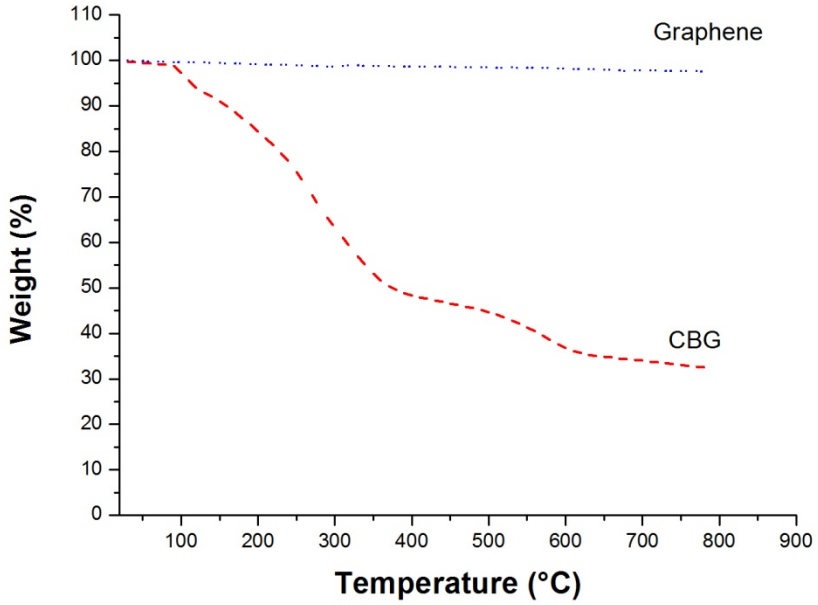

Figure S2: TGA thermogram of Graphene and CBG.

The zone forming ability of graphene oxide (GO) and CBG were compared under identical conditions using the Kirby Bauer test technique under identical condition of temperature and weight of material taken. In both the cases, 50 mg of GO and CBG were taken. It was kept on MAC plate containing E. coli and incubated at 37°C for 24 h. The antibacterial activity of the material was calculated by the zone of inhibition created measured using standard ruler scale and corrected with reference to area of the added graphene. Interestingly, zone formed by CBG was almost twice as that formed in case of GO as shown in Figure S3.

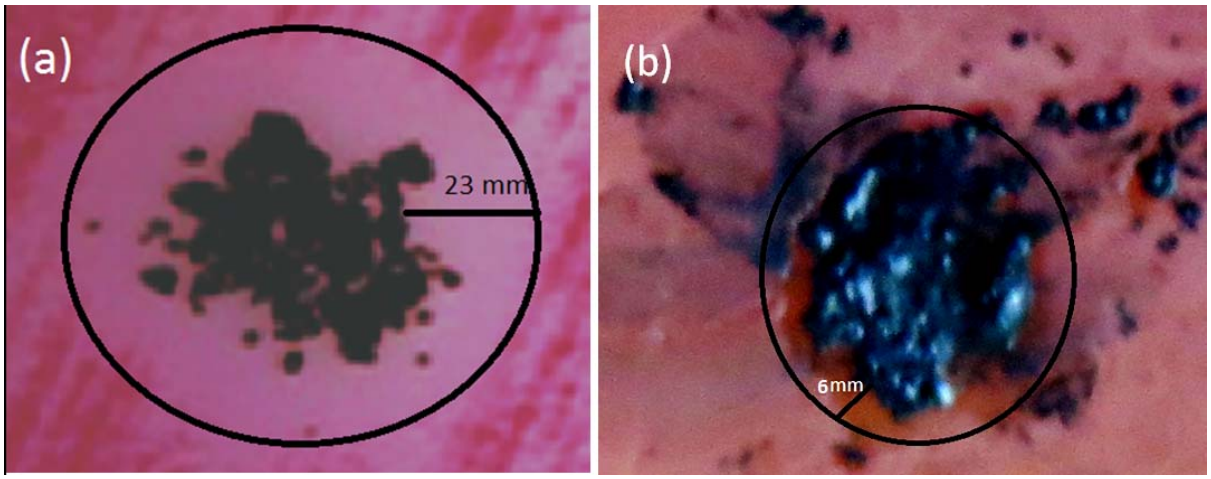

Figure S3: Optical image of MacConkey culture media plate with *E.coli* grown with (a) 50mg of CBG with 23 mm zone (Using 55 mm of zoom) and (b) 50 mg of GO with approx 6 mm of irregular zone (Using 55 mm of zoom). (Images captured by Canon Eos 1100 D).

The zone forming ability of CBG was modelled mathematically by standard curve fitting technique as well as Anova ® analysis technique using standard software package. The zone forming ability was predicted using several sets of fitting like linear, quadratic and cubic. Based on the smallest regression coefficient value, the quadratic model was the best choice which can predict the amount of zone which can be created by CBG. The fitting based on the equation is shown below as shown in Figure S4.

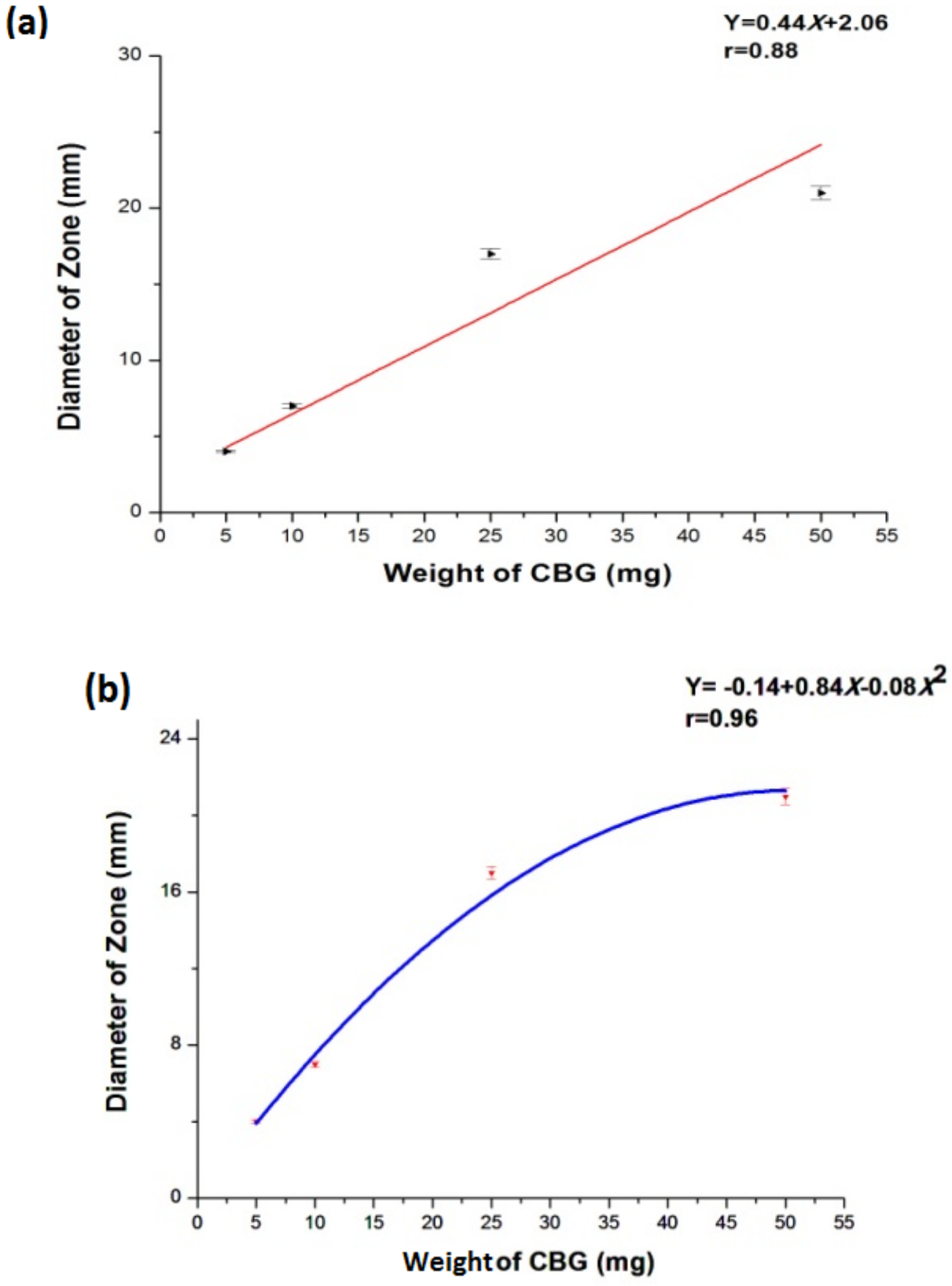

Figure S4: Mathematical modelling for the Kirby-Bauer test on *E.coli* based on (a) linear curve fitting and (b) quadratic curve fitting.