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Facile and Simultaneous Synthesis of Graphene Quantum Dots and Reduced Graphene Oxide for Bio-imaging and Supercapacitor Applications

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S1. Quantum yield (QY) calculations

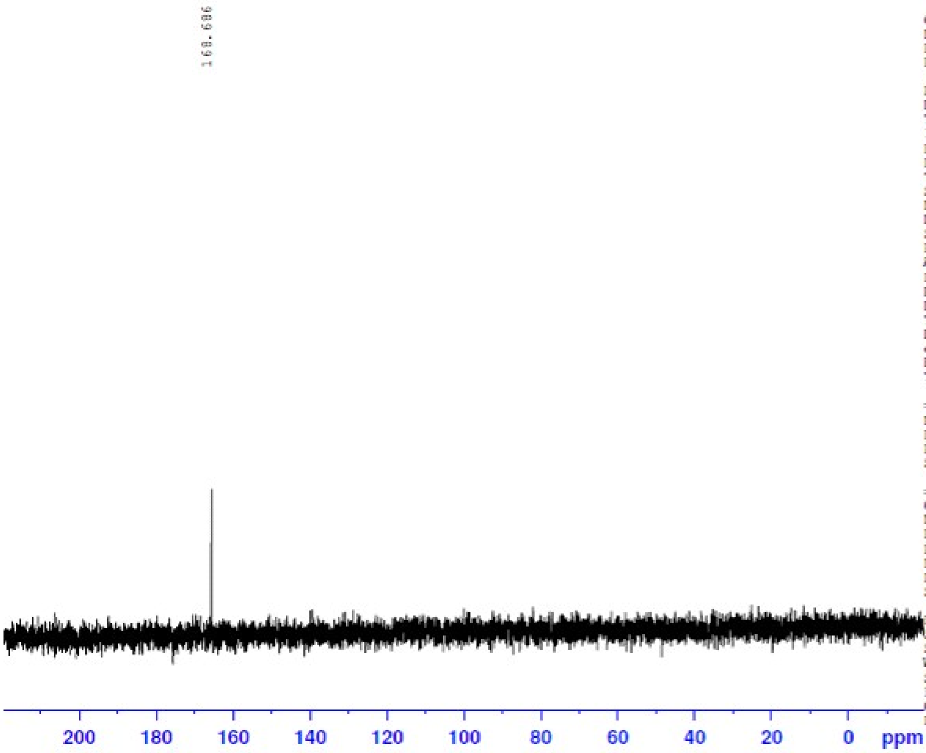
Quantum Yield (QY) measurements were carried out using quinine sulphate in aqueous medium and Rhodamine B in water (quantum yield is 0.31) and in ethanol (quantum yield is 0.49) were chosen as a standard sample. The quantum yield of graphene quantum dots (GQDs) in water was calculated using the following equation:

$$\Phi = \Phi_{st} (I_x/I_{st}) (\eta^2/\eta^2_{st}) (A_{st}/A_x)$$

Where Φ is the quantum yield, I is the measured integrated emission intensity, η is the refractive index (1.33 for water), and A is the optical density values respectively. The subscript "st" refers to the reference fluorophore possessing a known quantum yield value and further the subscript "x" denotes the value corresponding to GQDs.

S2. ^{13}C NMR

^{13}C NMR (100 MHz, D_2O_2)	δ–values	Functional groups
y–GQDs	169.68–170	C=O functionalities, namely hydrazine and carboxylic groups
g–GQDs	182.60 181.43 168.34 23, 20 68	C=O –COOMe C=C 2° –CH –C–OH



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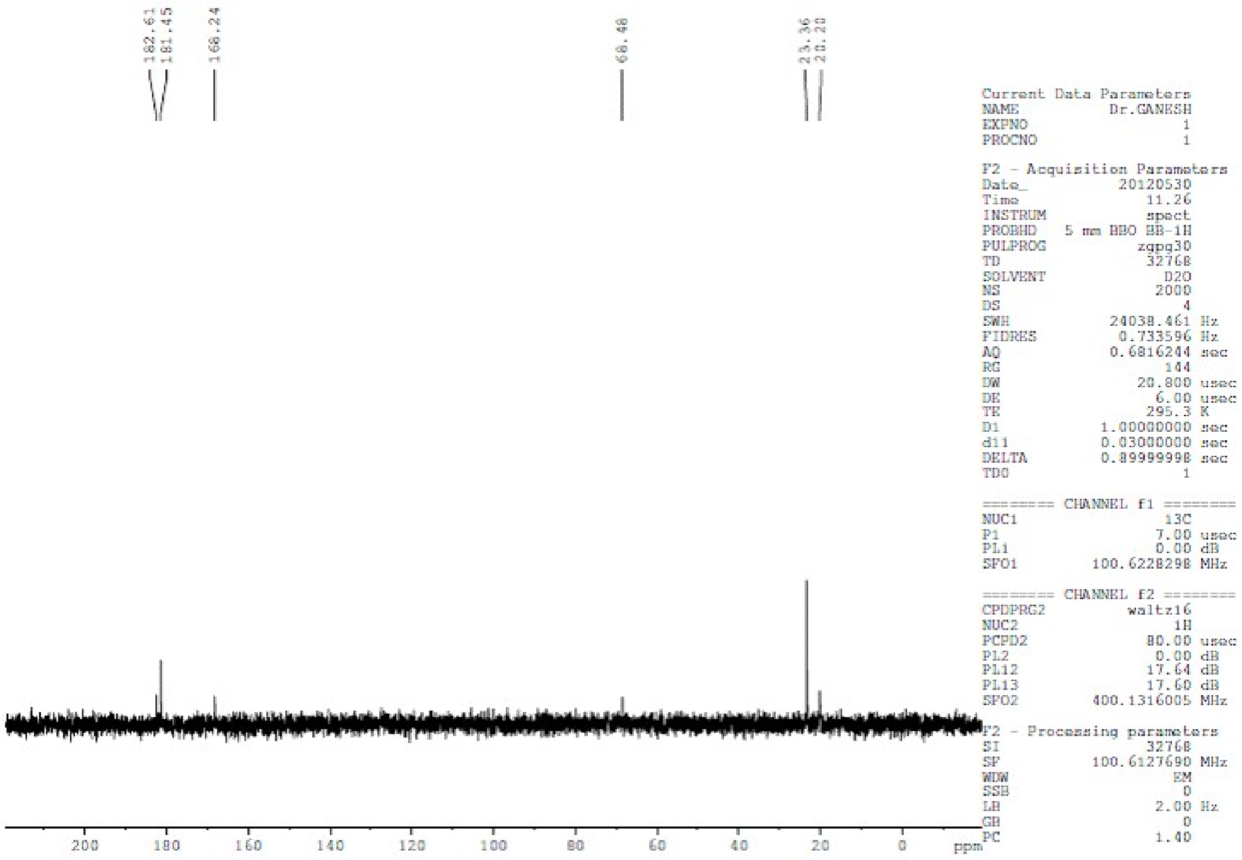
<u>Figure: S1</u> NMR spectrum of y–GQDs obtained by using hydrazine monohydrate as a reducing agent in aqueous medium.



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PL13                17.60 dB
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F2 - Processing parameters
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GB                      0
PC                   1.40
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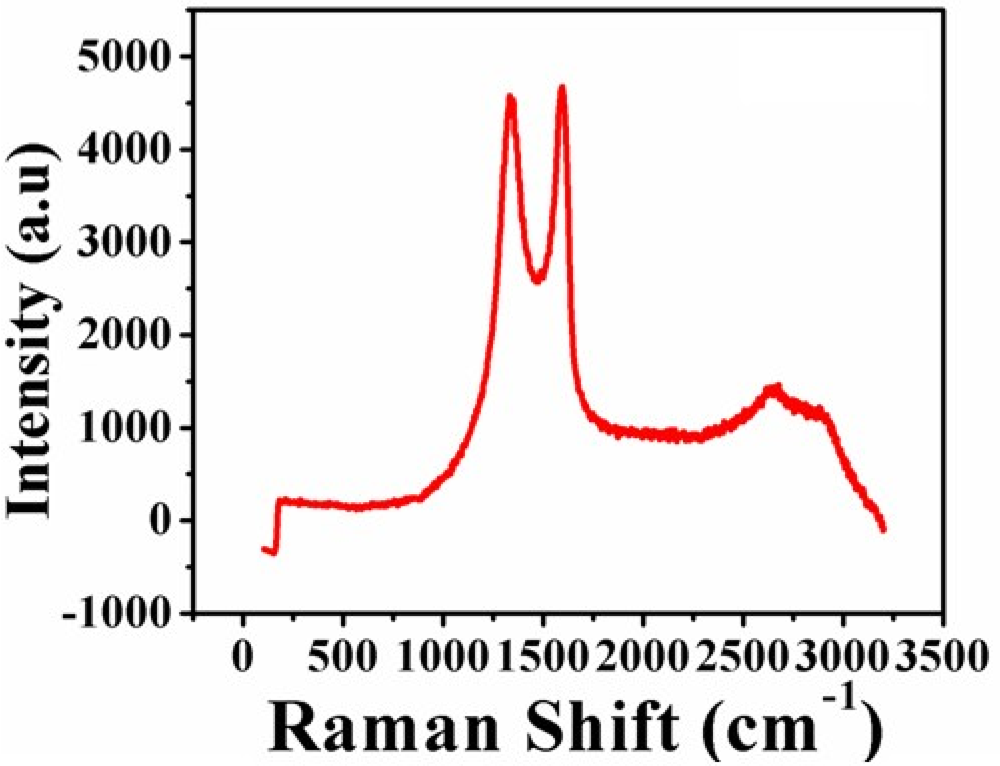
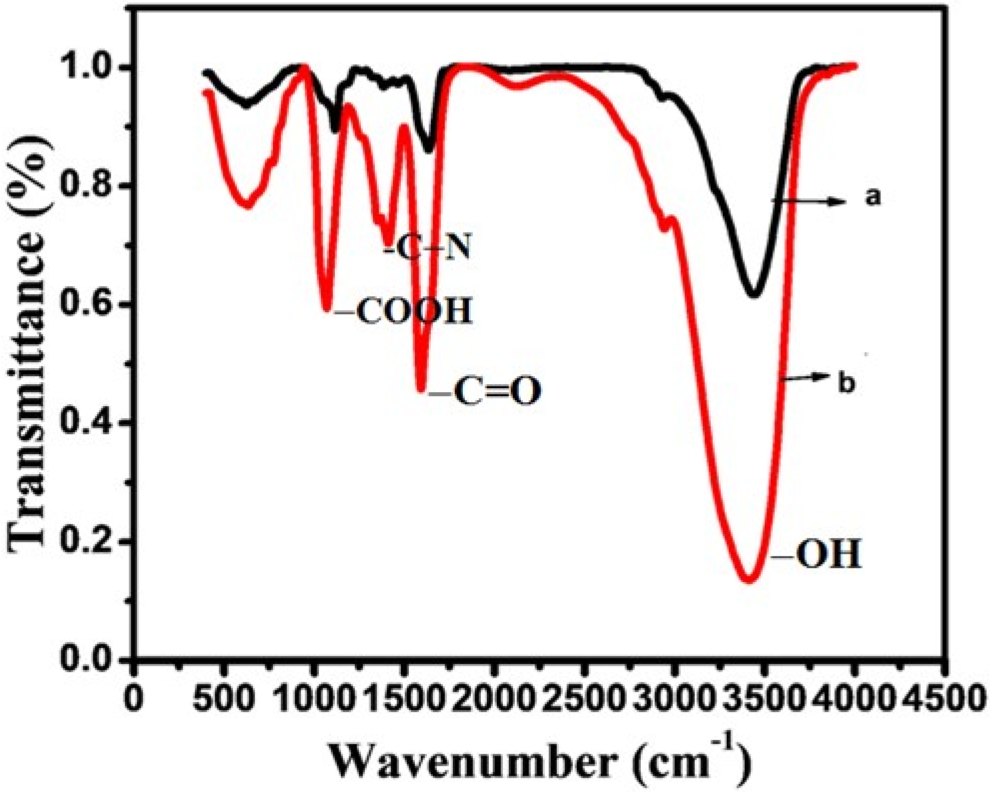
<u>Figure: S2</u> NMR spectrum of g–GQDs prepared by employing glucose as a reducing agent in the aqueous medium.



<u>Figure: S3</u> Raman spectra of pristine graphene obtained from chemical exfoliation of graphite.

S3. FTIR spectroscopic studies

FTIR studies reveal the presence of various functional group moieties such as aromatic, carboxylic and carbonyl groups in RGO as shown in Figure S3. Appearance of a broad peak centered at 3441 cm^{-1} and 3412 cm^{-1} is attributed to –OH vibrational stretching arising out of the carboxylic moiety of RGO. Similarly the formation of a shoulder peak at 1635 cm^{-1} corresponding to –C=O vibration, and the peak at 1412 cm^{-1} is due to the C–N stretching vibration. Finally the other peak appeared at 1045 cm^{-1} may be ascribed to the bending stretch of the carboxylic acid moieties.



<u>Figure: S4</u> FTIR spectra of reduced graphene oxides (RGO) obtained during the synthesis of (a) g−GQDs and (b) y−GQDs.

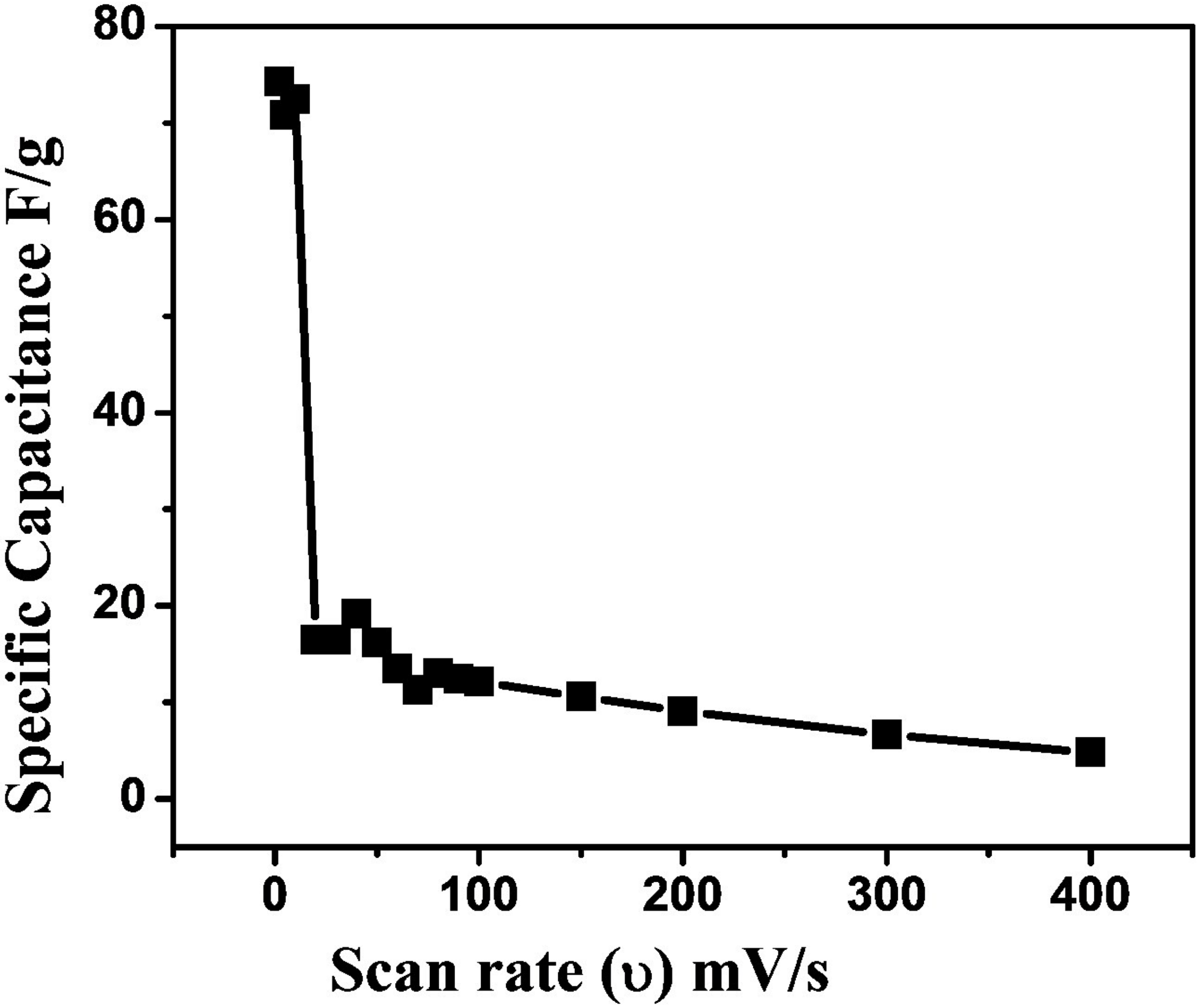


Figure: S5 A plot of specific capacitance vs. scan rate obtained using RGO modified electrode. These data points are collected by analyzing over a wide range of scan rate varying from 2 mV/s to 400 mV/s.

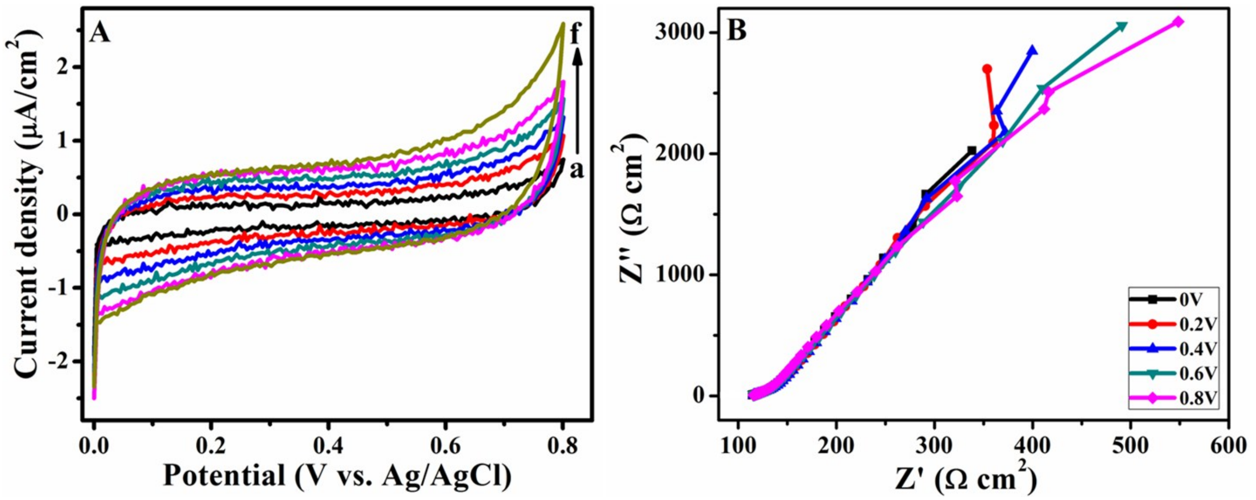


Figure: S6 (A) Comparative CVs recorded at various scan rates ranging from 10 mV/s to 100 mV/s (a to f) using bare GC electrode. (B) Nyquist plots recorded at different potentials starting from 0V to 0.8V with 200 mV interval using bare GC electrode. Electrolyte used is 0.1M NaCl aqueous solution.

S4. Complex capacitance and complex power analysis

Following equations can be used to understand the stepwise and detailed calculations of both the complex power and complex capacitance analyzed. Complex capacitance C(ω) value essentially consists of both real part of the complex capacitance C'(ω) and imaginary part of complex capacitance C''(ω). These values can be calculated by the following expression as shown below.

$$C(\omega) = C'(\omega) - jC''(\omega) \qquad (1)$$

where

$$C'(\omega) = -Z''(\omega)/\,\omega\,|Z(\omega)|^2 \qquad (2)$$

$$C''(\omega) = -Z'(\omega)/\,\omega\,|Z(\omega)|^2 \qquad (3)$$

In these equations Z'(ω) and Z''(ω) are the real and imaginary parts of complex impedance Z(ω) and it should be noted that low frequency part of C'(ω) corresponds to the capacitance of cell and C''(ω) represents the energy dissipation by an irreversible process which can lead to hysteresis of the electrochemical process[1–3] and the angular frequency ω is given by ω = 2πf.

Similarly, the complex power can be expressed as the following equation.

$$S(\omega) = P(\omega) + jQ(\omega) \qquad (4)$$

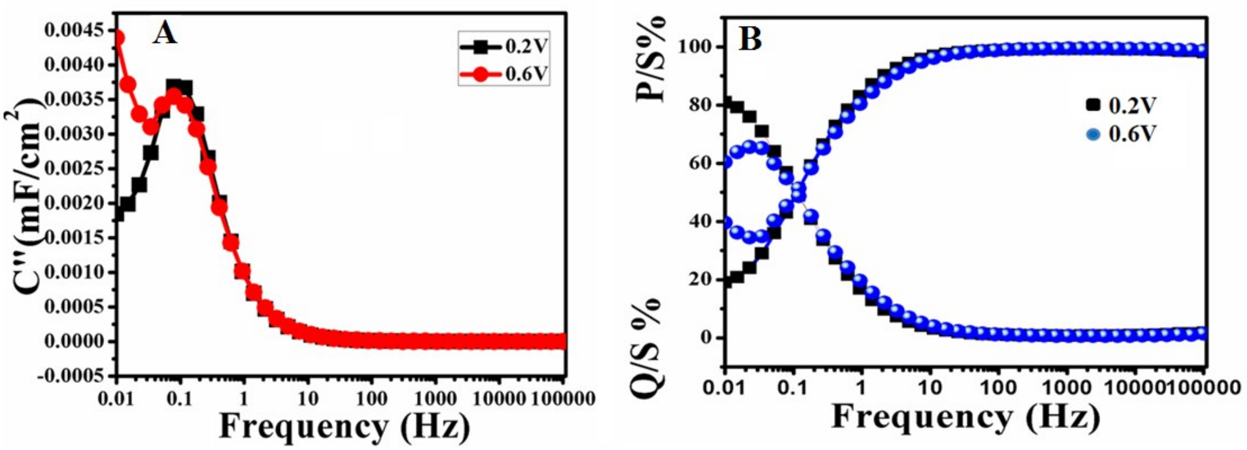
Where the P (ω) is the real part of complex power which is called as active power and that can be expressed as the following equation.

$$P(\omega) = \omega C''(\omega)\,|\Delta V_{rms}|^2 \qquad (5)$$

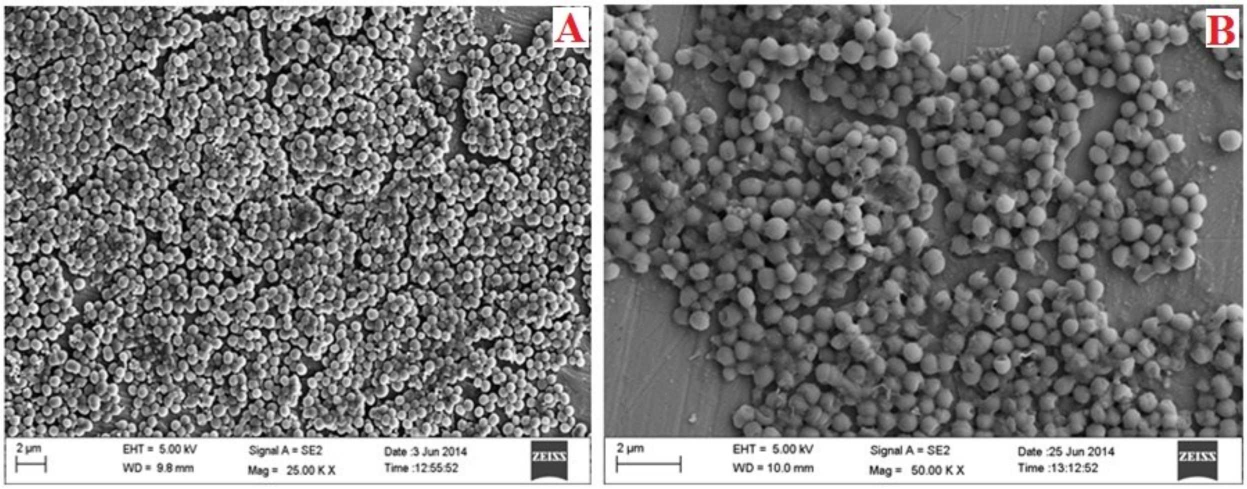
Likewise Q (ω) is the imaginary part of complex power which is called as reactive power and that can be given by the following expression.

$$Q(\omega) = -\omega C'(\omega)\,|\Delta V_{rms}|^2 \qquad (6)$$

Where = $|\Delta V_{rms}|^2 = \Delta V_{max} / \sqrt{2}$ (V_{max} is being the maximum amplitude of ac voltage)



<u>Figure: S7</u> Plots of imaginary part of the complex capacitance vs. frequency (in logarithmic scale) [A] and the plots of normalized active power and reactive power vs. frequency (in logarithmic scale) [B] obtained at two different potentials namely 0.2V and 0.6V using complex power analysis for RGO. Electrolyte used: An aqueous solution of 0.1M NaCl.



<u>Figure: S8</u> FESEM images of *S. aureus* bacteria obtained for (A) control without GQDs and (B) with y–GQDs obtained by using hydrazine monohydrate as a reducing agent in aqueous medium.

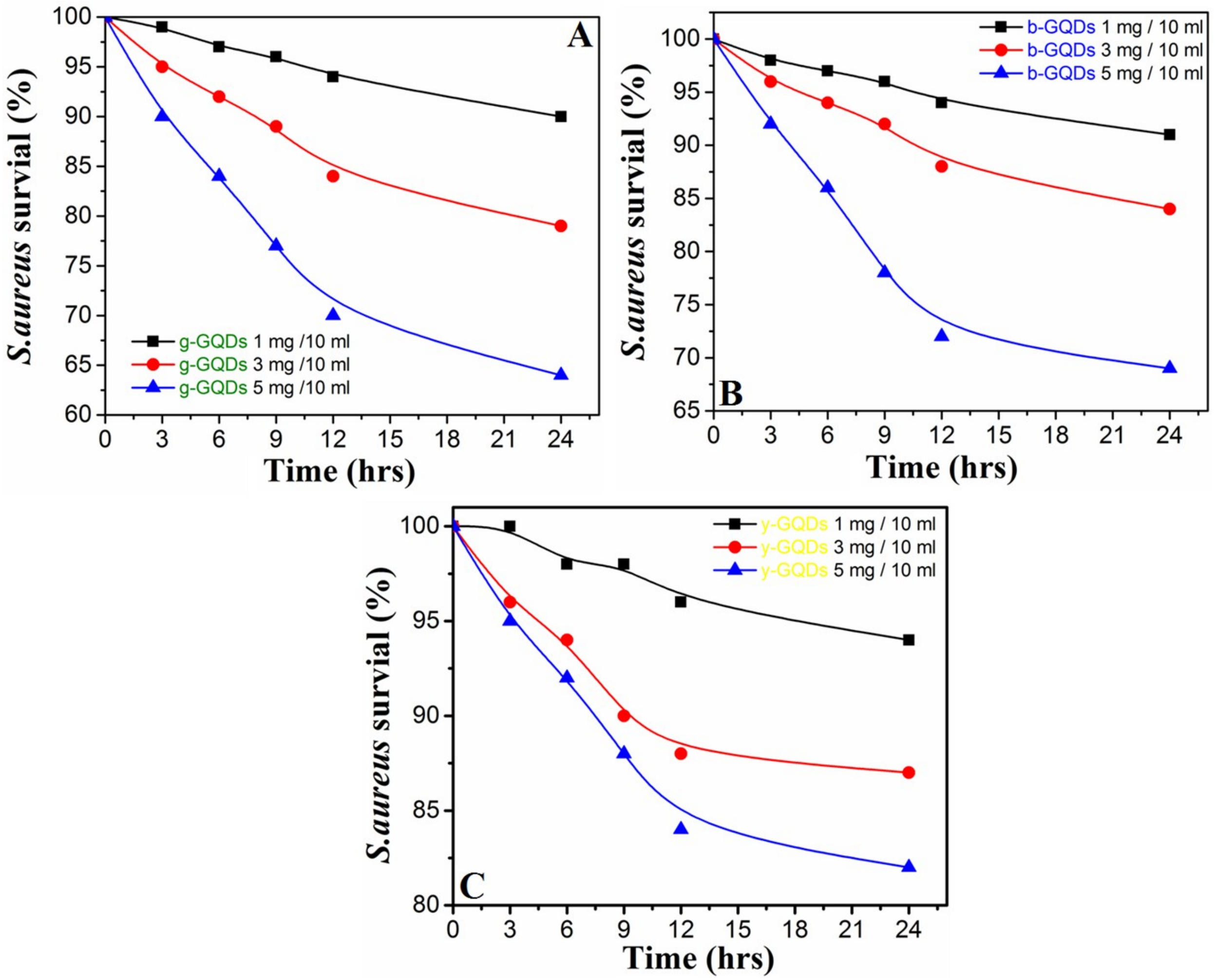


Figure: S9 Dose – survival curves recorded using *S. aureus* bacterial culture for different GQDs namely (A) g–GQDs, (B) b–GQDs and (C) y–GQDs for various time intervals.

References:

1. V. Ganesh, S. Pitchumani and V. Lakshminarayanan, *J. Power Sources*, 2006, **158**, 1523–1532.
2. K. S. Cole and R. H. Cole, *J. Chem. Phys.*, 1941, **9**, 341–352.
3. B. E. Conway, *J. Electrochem. Soc.*, 1991, **138**, 1539–1548.