Supplementary information

Molecular nanoinformatics approach assessing the biocompatibility of biogenic silver nanoparticles with channelized intrinsic steatosis and apoptosis

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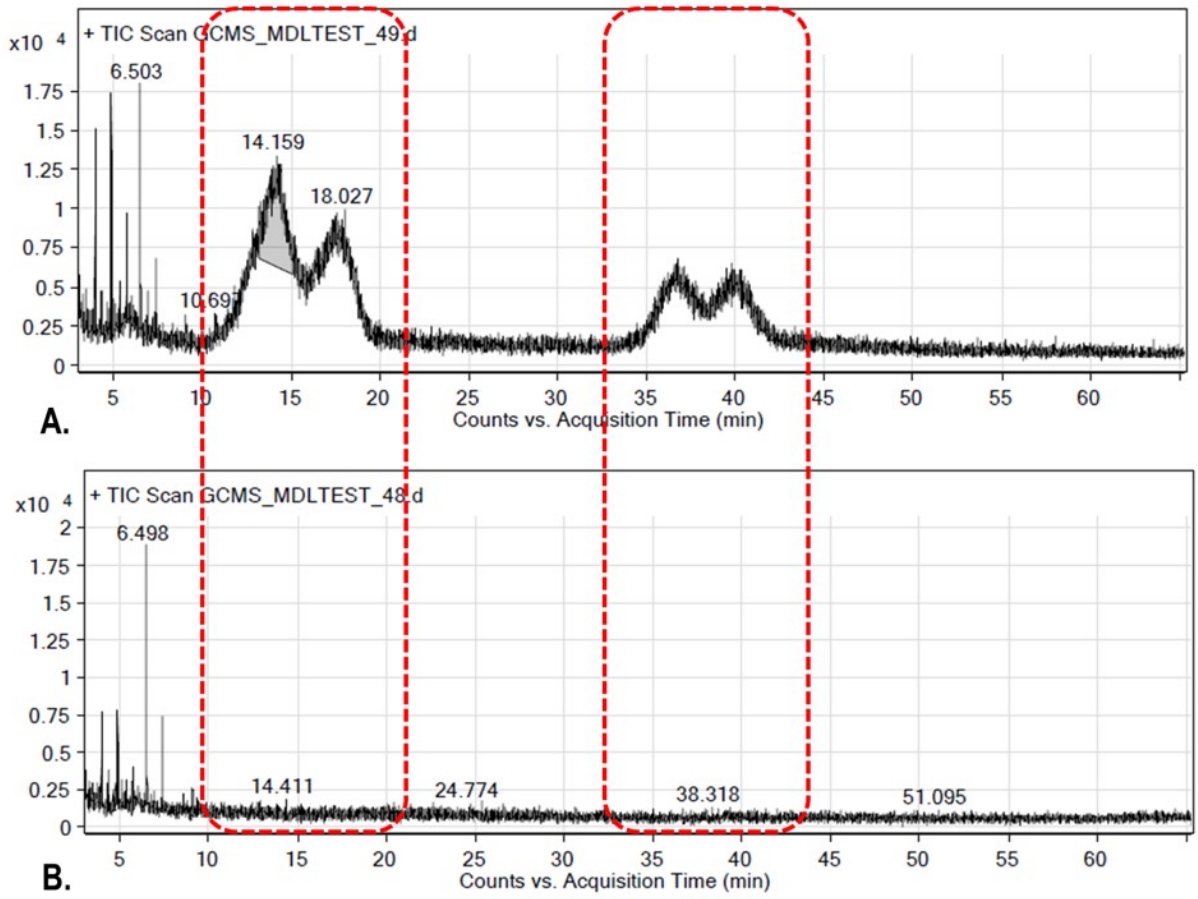

Figure S1: GCMS analyses of the leaf extract of silver grass (*Miscanthus sinesis*). (A) Chromatogram of the leaf extract before G-AgNPs synthesis. (B) Chromatogram of the floral extract after G-AgNPs synthesis. The peak areas at different retention times were compared to determine the probable biomolecules used for green synthesis of G-AgNPs.

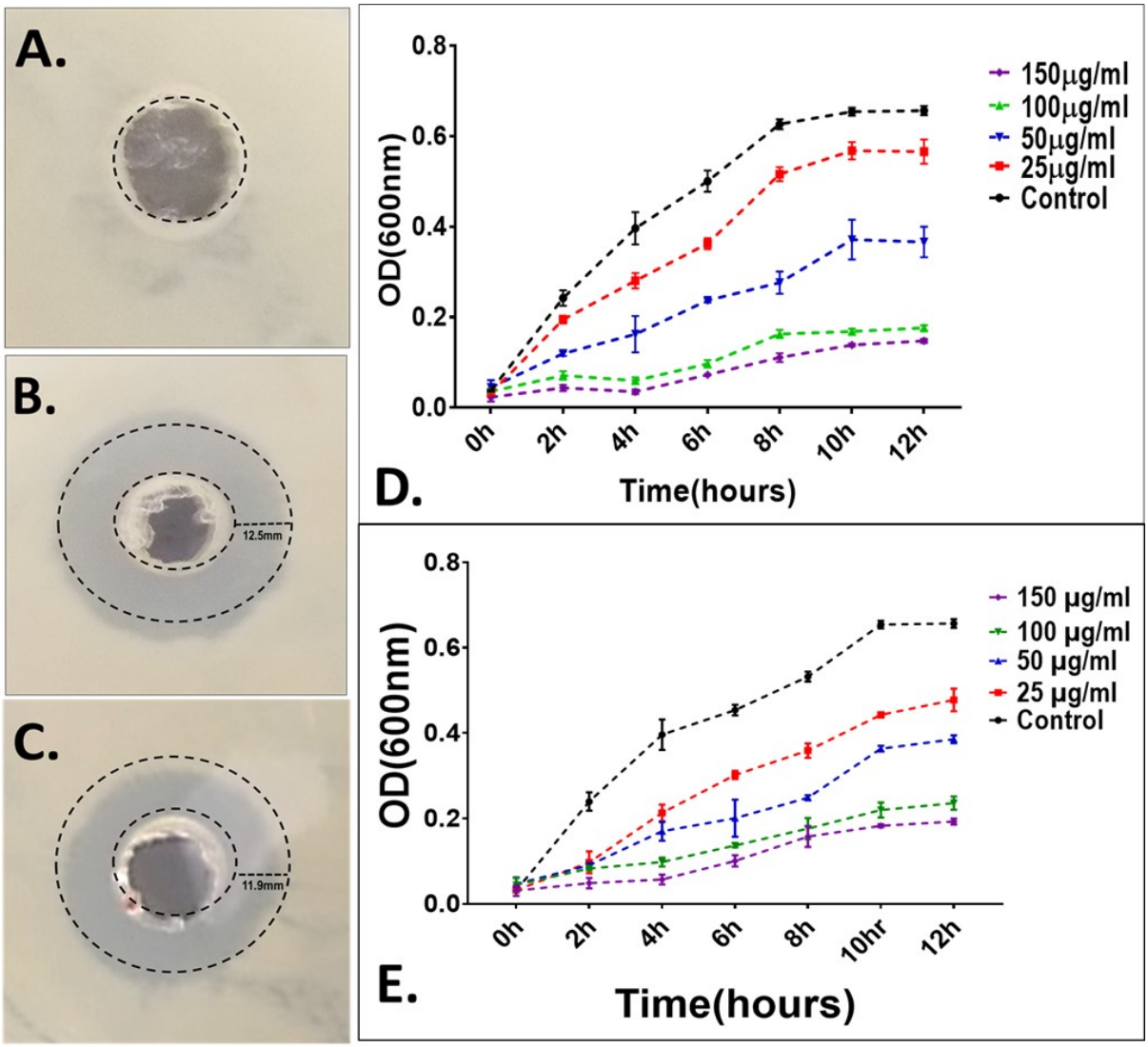

Figure S2: Antibacterial activity of G-AgNPs and C-AgNPs. Zone of inhibition determined by the well diffusion assay with *E. coli*. (A) Untreated control (B) 50µg/ml of G-AgNPs (C) 50µg/ml of C-AgNPs. Growth kinetics of *E. coli* in the presence of different concentrations of (D) G-AgNPs (E) C-AgNPs. The bacterial culture taken were 4 h sub-culture of overnight grown culture in LB medium.

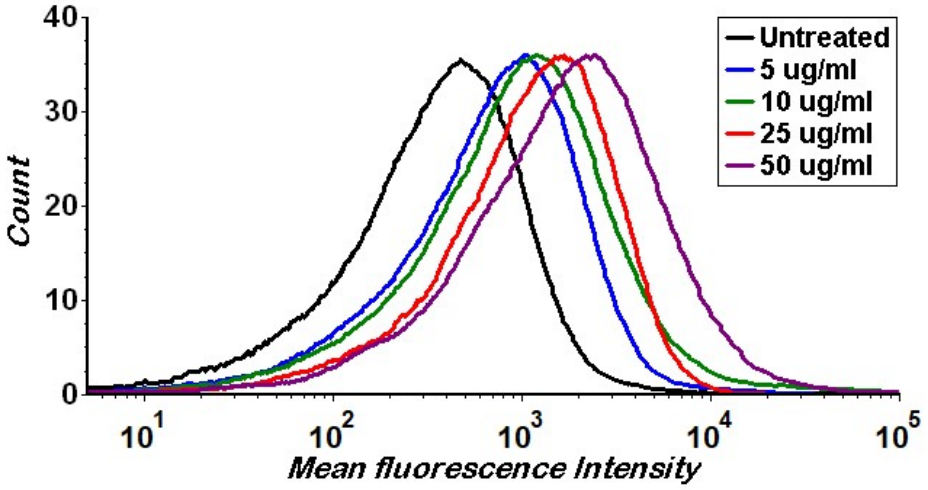

Figure S3: Histogram presentation of induced neutral lipid accumulation presented by LipidTox^{tm} fluorescence intensity in zebrafish embryos exposed to C-AgNPs for 72 h. All experiments were performed in triplicate and thrice independently. The analysis of flow cytometry results was done using FACS Xpress7.

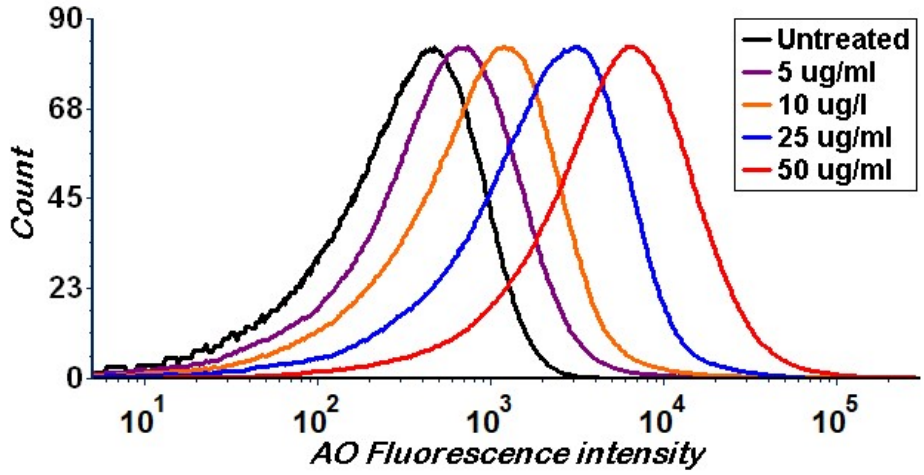

Figure S4: Histogram presentation of apoptosis presented by acridine orange (AO) fluorescence intensity in zebrafish embryos exposed to C-AgNPs for 72 h. All experiments were performed in triplicate and thrice independently. The analysis of flow cytometry results was done using FACS Xpress7.

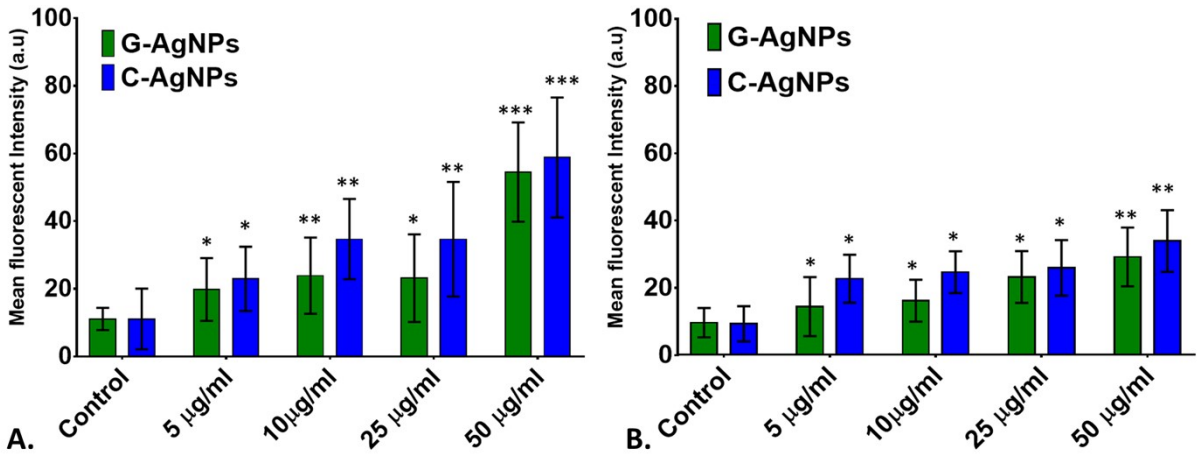

Figure S5: Histogram presentation of apoptosis presented by acridine orange (AO) fluorescence intensity in zebrafish embryos exposed to C-AgNPs and G-AgNPs for 72 h. The embryos were stained by AO. All experiments were performed in triplicate and thrice independently. The analysis of the images was done by Image J. The values represent the mean ± SD of three independent experiments. *P > 0.5, and ***P > 0.001 denote the compared significant change at each exposed concentration as obtained from post hoc analysis after one-way ANOVA

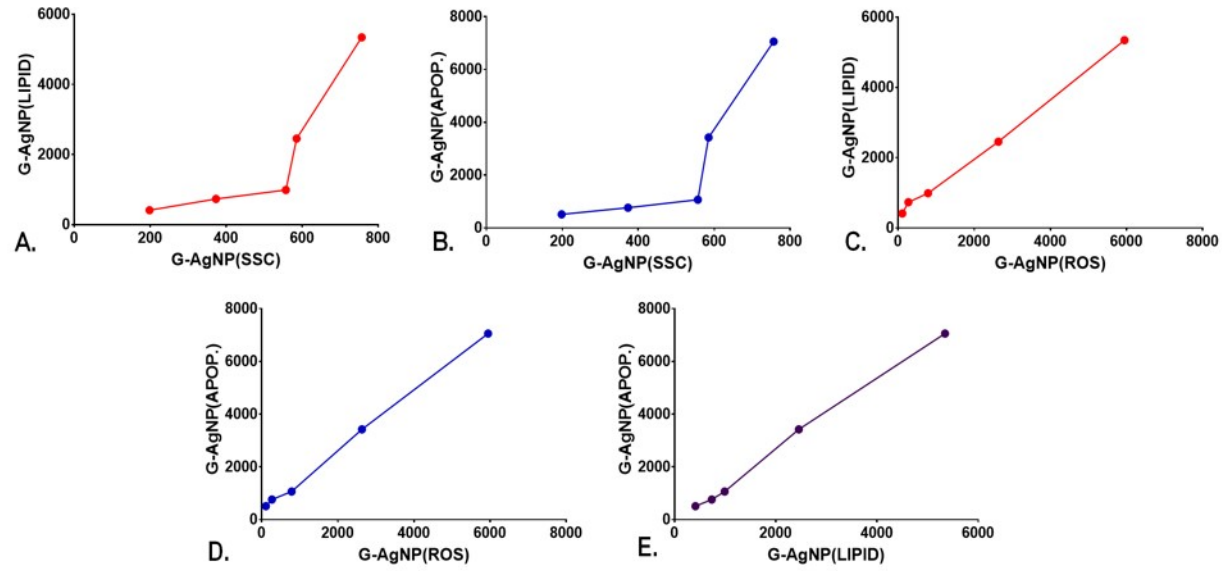

Figure S6: Correlation analysis of different experimental results determined by flow cytometry in zebrafish embryo cells for 72 h. (A) SSC (uptake of G-AgNPs) with neutral Lipid accumulation (B) SSC (uptake of G-AgNPs) with Apoptosis (C) ROS with neutral Lipid accumulation (D) ROS with Apoptosis (E)Apoptosis with neutral Lipid accumulation.

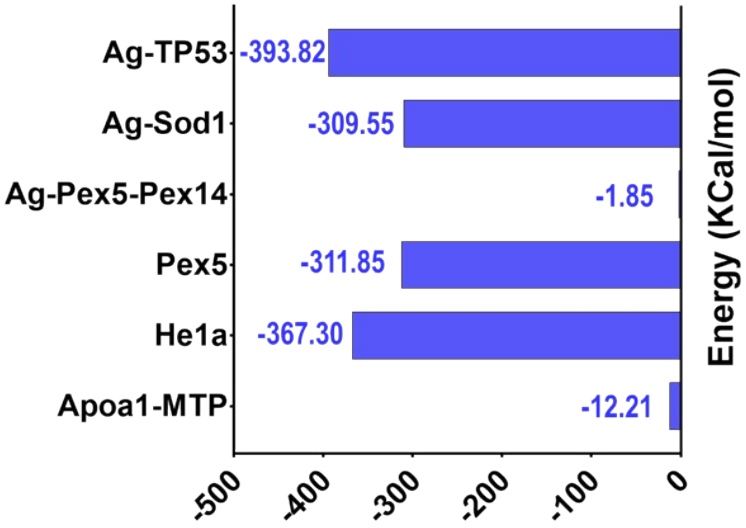

Figure S7: Energy of different AgNPs-Protein's interaction complex determined by the docking analysis. The docking was performed by using HEX docking program. The energy presents the average energy during the interaction of proteins with AgNPs.