Supplementary information

Innovative preparation of cellulose-mediated silver nanoparticles for multipurpose applications: experiment and molecular docking studies

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1. Materials preparation

Silver nitrate ($AgNO_3$), NH_4OH, N,N-dimethyalacetamide, urea, Rhodamine B, Sigma Aldrich supplied the AR grade of 2,2,6,6,6-tetramethylpiperidine-1-oxyl (TEMPO). Ethanol was purchased from Chem-O-Chem chemicals. All reagents were used without further purification.

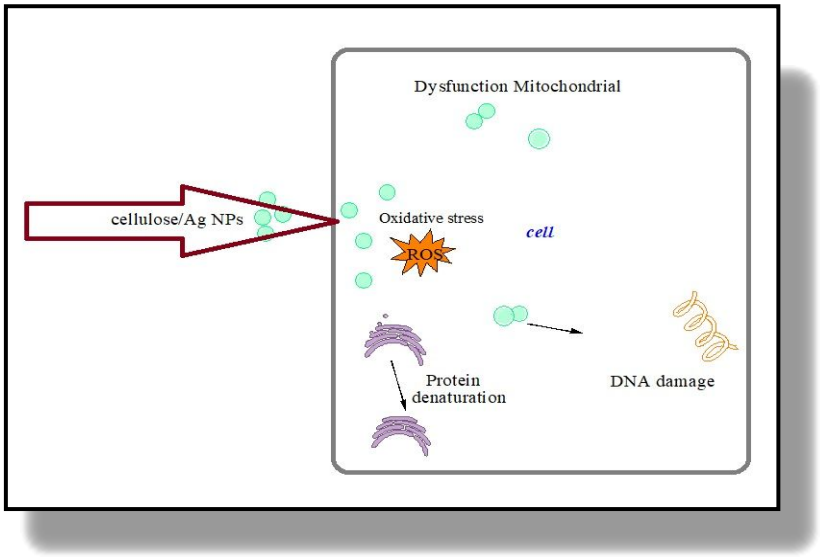

Figure S1. Antibacterial activity mechanism of preparation of cellulose-mediated silver nanoparticles.

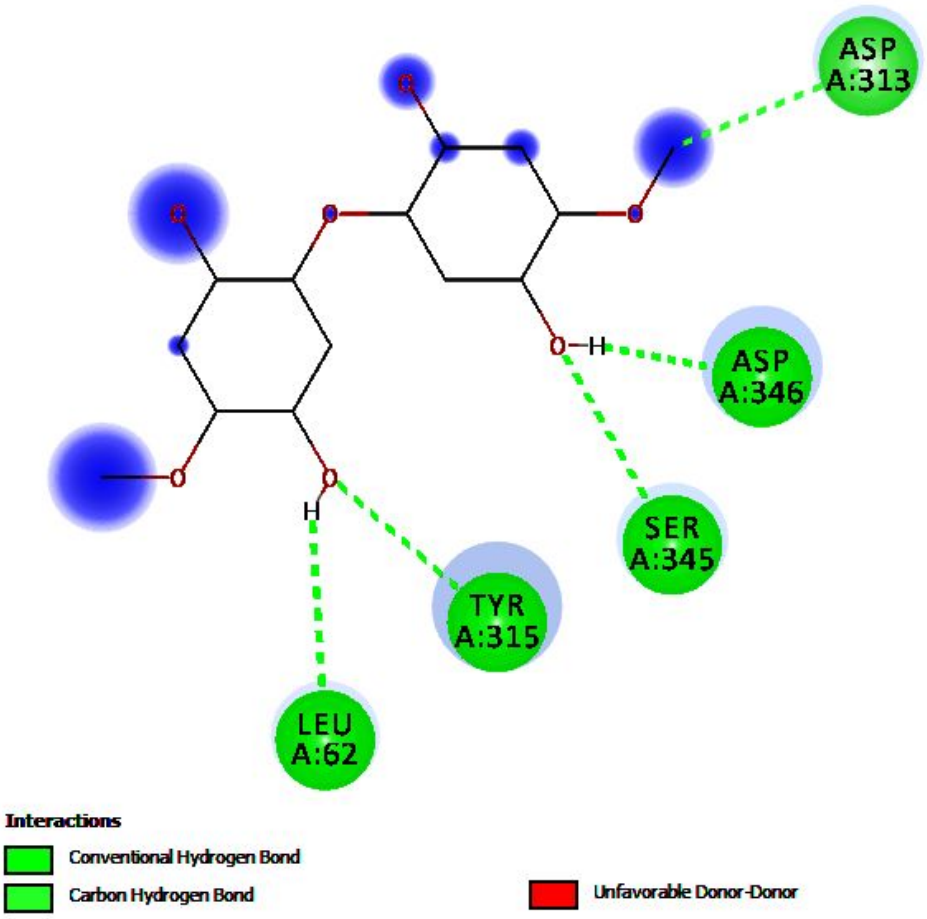

Figure S2. 2D-Hydrogen bond Interaction representation of cellulose/Ag ligand with 1TVF protein.

Table S1. AutoDock Vina results of the binding affinity and RMSD values of different poses in 1TVF inhibitor of cellulose/Ag NPs compounds.

Mode	Cellulose/Ag -1TVF		
	affinity (kcal/mol)	rmsd l.b.	rmsd u.b
1	-5.8	0.000	0.000
2	-5.5	19.892	21.648
3	-5.2	26.973	30.766
4	-5.1	20.203	21.343
5	-5.0	14.350	17.684
6	-4.9	21.263	23.617

7	-4.9	2.975	8.035
8	-4.9	3.783	7.551
9	-4.8	20.814	22.984
Inhibition Constant: 55.444 µM			

Table S2. The ligand- receptor residue interaction between Cellulose/Ag ligand with 1TVF protein.

S. NO	Pub chem. Id	Ligand Name	Residue Interaction	Type of bond	Distance(Å)
1	**1TVF**	**Cellulose/ Ag**	: UNKO: H – A: LEU62: O	Hydrogen	2.68
			A: TYR315: H-: UNKO: O	Hydrogen	2.47
			A: SER345: HN-: UNKO: O	Hydrogen	2.34
			: UNKO: H-A: ASP346: O	Hydrogen	2.20
			: UNKO: C-A: ASP313: O	Hydrogen	3.48

- In residue interaction column (UNK0) Symbol is described as ligand side functional groups such as O, S, N…..etc.
- X is taken Receptor protein chain.

Table S3. Percentage degradation of Rhodamine B on to cellulose/Ag

S. No	Sample	% Degradation Rhodamine B
1	Blank	7.37
2	Ag	37.68
3	Cellulose/Ag	97.38

Table S4. Rate constant k_{abs} value for the degradation of Rhodamine B on to Cellulose/Ag

Samples	k min^{-1}	
	Blank	Cellulose/Ag
Rhodamine B	0.0004	0.0181

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