Supporting Information

Theoretical and experimental study of folic acid conjugated silver nanoparticles through electrostatic interaction for enhance antibacterial activity

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TGA Analysis

The TGA thermogram of Ag@TEA@FA was shown in Figure S1. It showed that thermo gram of Ag@TEA@FA had two stages of weight loss. The first one started at about 95 °C due to the loss of adsorbed water and bound TEA with Ag nanoparticles .In contrast with TEA represents more weight loss at this stage. The second stage registered at nearly above 240 °C for organic molecule, FA. TGA result was confirmed here the silver incorporated within the TEA and FA both.

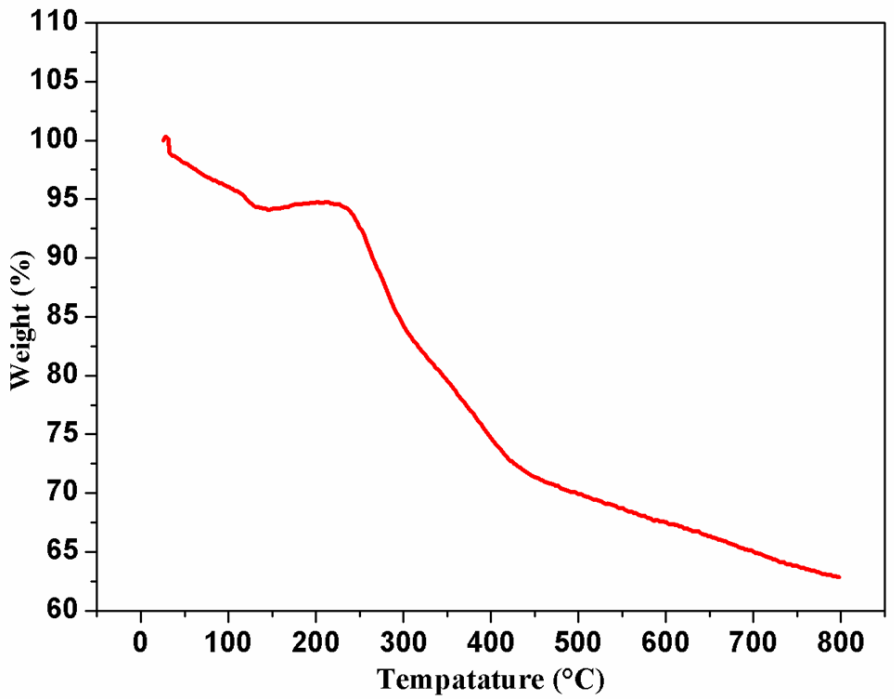

Figure S1 TGA weight loss profile of Ag@TEA@FA, heated in N2 atmosphere at 10 ° C/min ramping rate from 30 °C to 800 °C.

Minimum Inhibitory Concentration

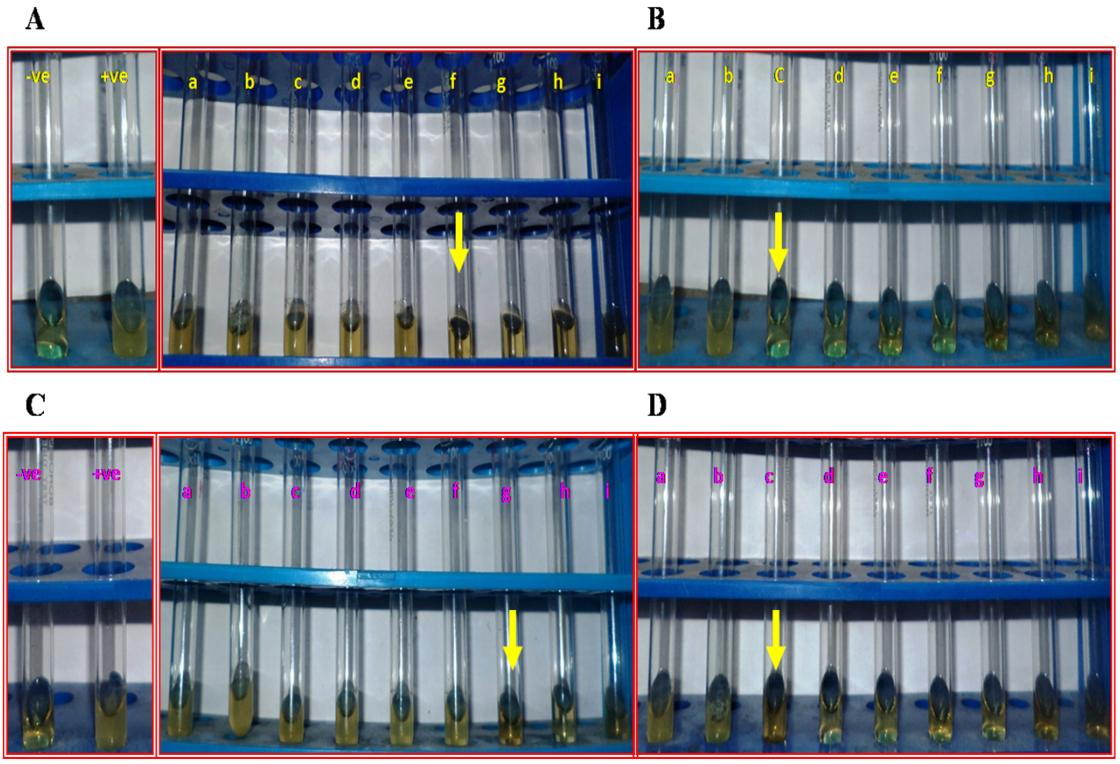

Figure S2 Determination of the minimum inhibitory concentration of (A) Ag@TEA against *S. aureus*, (B) Ag@TEA@FA against *S. aureus*, (C) Ag@TEA against *E. coli*, (D) Ag@TEA@FA against *E. coli*, (a = 1 μg ml^{-1}, b = 5 μg ml^{-1}, c = 10 μg ml^{-1}, d = 25 μg ml^{-1}, e = 50 μg ml^{-1}, f = 100 μg ml^{-1}, g = 250 μg ml^{-1}, h = 500 μg ml^{-1}, i = 1000 μg ml^{-1}).

MTT assay of Ag@TEA@FA nanoparticles

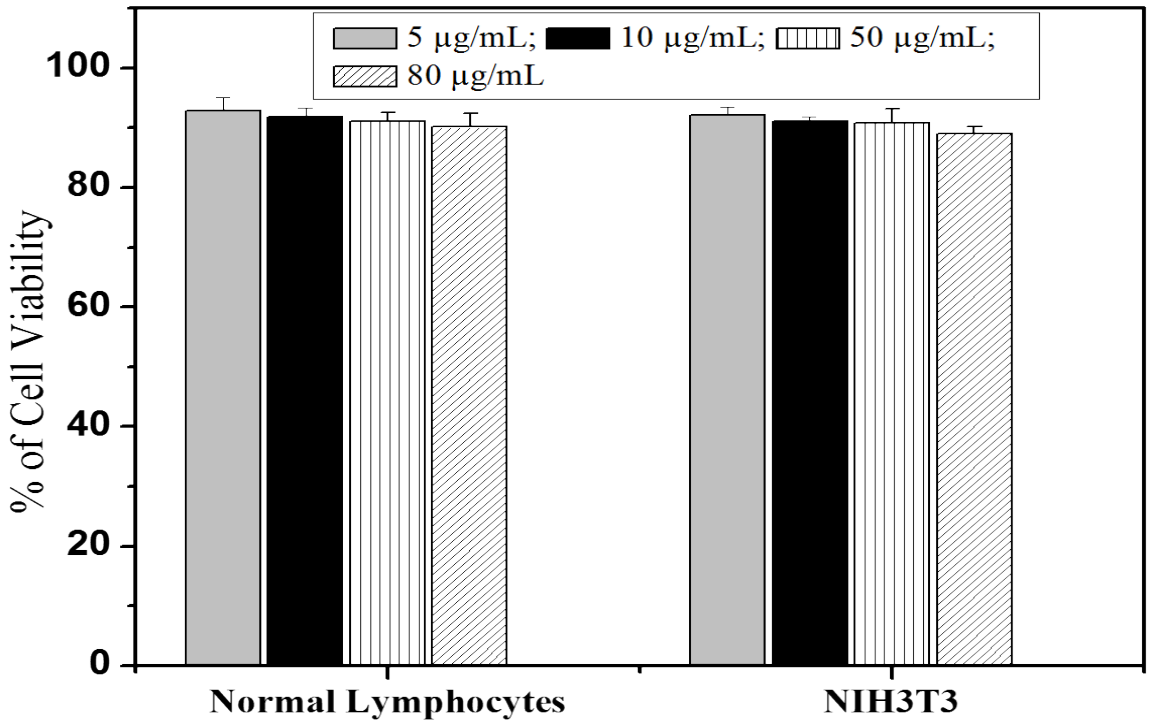

Figure S3 Cytotoxicity of nanoparticles against primary human blood lymphocytes and mouse fibroblast NIH 3T3 cells after 24 h incubation.

Table S1 TEA@Ag@FA interaction, electrostatic interaction distance, dipole moment and binding energies for the studied TEA@Ag@FA and Di-TEA@Ag@FA cluster. [a]

Sl No.	Bond distance / Interaction distance (Å)	Literature value (Å)	Calculated value (HF/LAN2MB) (Å)
1	Ag-N	2.12-2.40[a]	2.58-2.85
2	Ag-N	2.12-2.13[b]	
3	Ag-N	2.14-2.32[c]	
2	Ag-O	2.26-2.34[c]	2.58-2.92
3	Ag…O (interaction)	2.53-2.99[c]	2.58-2.92

[a] Values in the parentheses are those for TEA…Ag…FA with same binding mode calculate at the same level of theory.

Table S2 Comparison between calculated and literature value of Bond Distance and interaction distance between Ag...N and Ag…O:

Complexes	μ	Distance (Å)	ΔE (Kcal/mol)
TEA@Ag@FA Clusters			
Molecular cluster 1	3.0514	$r_{52N-74Ag} = 2.586$ $r_{74Ag-23O} = 2.585$	14.57
Molecular Cluster 2	9.883	$r_{52N-74Ag} = 2.598$ $r_{74Ag-31O} = 2.601$ $r_{74Ag-73H} = 2.852$ $r_{74Ag-69H} = 2.875$ $r_{74Ag-65H} = 2.992$ $r_{31O-73H} = 2.869$ $r_{31O-68H} = 2.945$	65.54

Molecular Cluster 3	11.605	$r_{52N-74Ag}$= 2.688 $r_{74Ag-6O}$ = 2.928 $r_{74Ag-7O}$= 2.583 $r_{74Ag-69H}$ = 2.990 $r_{74Ag-73H}$ = 2.869 r_{6O-69H} = 2.706 r_{7O-73H} = 2.930	71.13
Molecular Cluster 4	7.976	$r_{52N-74Ag}$= 2.648 $r_{74Ag-6O}$ = 2.805 $r_{74Ag-7O}$= 2.678 $r_{74Ag-65H}$ = 2.874 $r_{74Ag-69H}$ = 2.973 r_{7O-73H} = 2.533	71.99
Di-TEA@Ag@FA Clusters			
Di-Molecular Cluster 1	9.723	$r_{23Ag-1N}$ = 2.856 $r_{23Ag-24N}$ = 2.759 $r_{23Ag-43H}$ = 2.998 $r_{23Ag-35H}$ = 2.896 $r_{76O-36H}$ = 2.339	10.87
Di-Molecular Cluster 2	12.331	$r_{23Ag-1N}$ = 2.709 $r_{23Ag-77O}$ = 2.624 $r_{23Ag-14H}$=2.996 $r_{23Ag-18H}$ = 2.906 $r_{24N-96H}$ = 1.647 $r_{76O-33H}$ = 2.586 $r_{76O-43H}$ = 2.998 r_{51O-9H} = 2.329	21.772
Di-Molecular Cluster 3	10.150	$r_{23Ag-1N}$ = 2.798 $r_{23Ag-72N}$ = 2.807 $r_{23Ag-74N}$ = 2.582 $r_{23Ag-14H}$ = 2.969 $r_{24N-93H}$ =1.771	26.429

		$r_{72N\text{-}18H}$ =2.664	