Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Calotropisprocera flower extract for the Synthesis of Double Edged Octahedral α-Fe_2O_3 Nanoparticles *via* Greener Approach: An Insight into its Structure Property Relationship for *Escherichia coli*

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Table S1. The docking analysis of non-covalent aminoacid residue interactions of **2mqe protease** and **6zhp protease** against **Fe_2O_3 NPs** (monomer), **Fe_4O_6 NPs** (dimer), **Fe_6O_9 NPs** (trimer) and **Fe_8O_{12} NPs** (tetramer) respectively.

S.No	Pub chem. Id	Lead molecule	Residue Interaction	Nature of bond				Distance (Å)
1	2mqe	Fe_2O_3 NPs	:UNK0:O - A:PHE202:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						:UNK0:O	A:PHE202:O	3.30
			A:SER198:HG - :UNK0:O			A:SER198:HG	:UNK0:O	2.29
			A:ARG256:HH21 - :UNK0:O			A:ARG256:HH21	:UNK0:O	2.53
			A:ARG256:HE - :UNK0:O			A:ARG256:HE	:UNK0:O	2.38
			:UNK0:O - A:LYS206:O			:UNK0:O	A:LYS206:O	3.29
			A:SER198:HB3 - :UNK0:O		Non-Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						A:SER198:HB3	:UNK0:O	2.74
			A:ARG256:HD2 - :UNK0:O			A:ARG256:HD2	:UNK0:O	2.89
2	2mqe	Fe_4O_6 NPs	:UNK0:O - A:ASN205:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						:UNK0:O	A:ASN205:O	3.37
			:UNK0:O - A:LYS206:O			:UNK0:O	A:LYS206:O	3.30
			:UNK0:O - A:ASN203:O			:UNK0:O	A:ASN203:O	3.27
			A:ARG307:HH11 - :UNK0:O			A:ARG307:HH11	:UNK0:O	3.05
			A:SER198:HG - :UNK0:O			A:SER198:HG	:UNK0:O	2.38
			A:ARG256:HH21 - :UNK0:O			A:ARG256:HH21	:UNK0:O	2.62
			A:ARG256:HE - :UNK0:O			A:ARG256:HE	:UNK0:O	2.39
			A:ARG256:HE - :UNK0:Fe			A:ARG256:HE	:UNK0:Fe	2.17
			A:ARG256:HE - :UNK0:O			A:ARG256:HE	:UNK0:O	2.60
			A:ARG256:HD2 - :UNK0:O		Non-Classical	***H-Donor***	***H-Acceptor***	
						A:ARG256:HD2	:UNK0:O	2.48
			A:THR240:HA - :UNK0:O			A:THR240:HA	:UNK0:O	2.86

			A:SER198:HB3 - :UNK0:O		**Interactions**	A:SER198:HB3	:UNK0:O	2.75
			A:ARG307:HD3 - :UNK0:Fe			A:ARG307:HD3	:UNK0:Fe	2.37
			A:ARG307:HD3 - :UNK0:O			A:ARG307:HD3	:UNK0:O	2.00
						Positive	***Negative***	
			A:ARG307:NH1 - :UNK0:Fe	**Electrostatic Interactions**	**Attractive Charge**	A:ARG307:NH1	:UNK0:Fe	4.65
			A:ARG307:NH1 - :UNK0:Fe			A:ARG307:NH1	:UNK0:Fe	4.65
			A:ARG256:NH2 - :UNK0:Fe			A:ARG256:NH2	:UNK0:Fe	4.90
			A:ARG256:NH2 - :UNK0:Fe			A:ARG256:NH2	:UNK0:Fe	4.08
						H-Donor	***H-Acceptor***	
			:UNK0:O - A:ASP241:OD1		**Classical H-Bonding Interactions**	:UNK0:O	A:ASP241:OD1	3.17
			A:ASP241:HN - :UNK0:O			A:ASP241:HN	:UNK0:O	2.37
			A:ARG307:HH11 - :UNK0:O			A:ARG307:HH11	:UNK0:O	2.83
			:UNK0:O - A:ASN203:O			:UNK0:O	A:ASN203:O	3.18
			:UNK0:O - A:ASN203:O			:UNK0:O	A:ASN203:O	3.18
			:UNK0:O - A:ASN205:O			:UNK0:O	A:ASN205:O	3.26
			:UNK0:O - A:LYS206:O	**H-Bonding Interactions**		:UNK0:O	A:LYS206:O	3.12
			:UNK0:O - A:PHE202:O			:UNK0:O	A:PHE202:O	2.91
			:UNK0:O - A:LYS206:O			:UNK0:O	A:LYS206:O	2.83
			A:ARG256:HE - :UNK0:O			A:ARG256:HE	:UNK0:O	2.68
			A:ARG256:HE - :UNK0:Fe			A:ARG256:HE	:UNK0:Fe	2.32
			A:ARG256:HE - :UNK0:O			A:ARG256:HE	:UNK0:O	2.24
			A:ARG256:HH21 - :UNK0:O			A:ARG256:HH21	:UNK0:O	2.86
			A:SER198:HG - :UNK0:O			A:SER198:HG	:UNK0:O	2.76
						H-Donor	***H-Acceptor***	
			A:ARG307:HD3 - :UNK0:O		**Non Classical H-Bonding Interactions**	A:ARG307:HD3	:UNK0:O	1.65
			A:ARG307:HD3 - :UNK0:Fe			A:ARG307:HD3	:UNK0:Fe	2.19
			A:THR240:HB - :UNK0:O			A:THR240:HB	:UNK0:O	3.08
			A:THR240:HA - :UNK0:O			A:THR240:HA	:UNK0:O	2.56
			A:ARG256:HD2 - :UNK0:O			A:ARG256:HD2	:UNK0:O	3.05
						Positive	***Negative***	
			A:ARG307:NH1 - :UNK0:Fe	**Electrostatic Interactions**	**Attractive Charge**	A:ARG307:NH1	:UNK0:Fe	4.30
			A:ARG307:NH1 - :UNK0:Fe			A:ARG307:NH1	:UNK0:Fe	5.51
			A:ARG307:NH1 - :UNK0:Fe			A:ARG307:NH1	:UNK0:Fe	4.55
			A:ARG307:NH1 - :UNK0:Fe			A:ARG307:NH1	:UNK0:Fe	4.99
			A:ARG256:NH2 - :UNK0:Fe			A:ARG256:NH2	:UNK0:Fe	4.24
			A:ARG256:NH2 - :UNK0:Fe			A:ARG256:NH2	:UNK0:Fe	4.93
3	**2mqe**	**Fe_6O_9 NPs**				***H-Donor***	***H-Acceptor***	
			:UNK0:O - A:PHE204:O			:UNK0:O	A:PHE204:O	2.65
			:UNK0:O - A:ASN205:O			:UNK0:O	A:ASN205:O	3.23
			:UNK0:O - A:ASN203:O			:UNK0:O	A:ASN203:O	3.20
			A:ARG307:HH12-:UNK0:O		**Classical H-Bonding Interactions**	A:ARG307:HH12	:UNK0:O	3.05
			:UNK0:O - A:ASN205:O			:UNK0:O	A:ASN205:O	3.19
			:UNK0:O - A:ASN203:O	**H-Bonding Interactions**		:UNK0:O	A:ASN203:O	3.37
			:UNK0:O - A:ASP241:OD1			:UNK0:O	A:ASP241:OD1	2.92

4	**2mqe**	**Fe_8O_{12} NPs**	:UNK0:O - A:TYR248:OH			:UNK0:O	A:TYR248:OH	2.91
					Non Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
			A:PHE204:HA - :UNK0:O			A:PHE204:HA	:UNK0:O	2.17
			A:PHE204:HA - :UNK0:Fe			A:PHE204:HA	:UNK0:Fe	2.94
						Positive	***Negative***	
			A:ARG307:NH1 - :UNK0:Fe	**Electrostatic Interactions**	**Attractive Charge**	A:ARG307:NH1	:UNK0:Fe	5.51
			A:ARG307:NH1 - :UNK0:Fe			A:ARG307:NH1	:UNK0:Fe	5.20
			A:ARG307:NH1 - :UNK0:Fe			A:ARG307:NH1	:UNK0:Fe	4.87
			A:ARG307:NH1 - :UNK0:Fe			A:ARG307:NH1	:UNK0:Fe	3.08
			A:ARG307:NH2 - :UNK0:Fe			A:ARG307:NH2	:UNK0:Fe	5.11
			A:ARG307:NH2 - :UNK0:Fe			A:ARG307:NH2	:UNK0:Fe	4.99
			A:ARG307:NH2 - :UNK0:Fe			A:ARG307:NH2	:UNK0:Fe	4.64
5	**6zhp**	**Fe_2O_3 NPs**				***H-Donor***	***H-Acceptor***	
			:UNK0:O - B:TYR124:O	**H-Bonding Interactions**	**Classical H-Bonding Interactions**	:UNK0:O	B:TYR124:O	2.93
			B:GLN178:HE21 - :UNK0:O			B:GLN178:HE21	:UNK0:O	2.67
			B:THR160:HG1 - :UNK0:O			B:THR160:HG1	:UNK0:O	1.81
			B:THR160:HG1 - :UNK0:Fe			B:THR160:HG1	:UNK0:Fe	2.19
			B:ARG162:HH22 - :UNK0:O			B:ARG162:HH22	:UNK0:O	3.02
			B:ARG162:HE - :UNK0:Fe			B:ARG162:HE	:UNK0:Fe	2.60
			B:ARG162:HE - :UNK0:O			B:ARG162:HE	:UNK0:O	1.87
			B:ASN123:HD21 - :UNK0:Fe			B:ASN123:HD21	:UNK0:Fe	2.50
			B:ASN123:HD22 - :UNK0:O			B:ASN123:HD22	:UNK0:O	2.84
			:UNK0:O - B:ASP119:OD1			:UNK0:O	B:ASP119:OD1	3.13
				Electrostatic Interactions	**Attractive Charge**	***Positive***	***Negative***	
			B:ARG162:NH2 - :UNK0:Fe			B:ARG162:NH2	:UNK0:Fe	4.52
6	**6zhp**	**Fe_4O_6 NPs**				***H-Donor***	***H-Acceptor***	
			:UNK0:O - B:TYR62:OH	**H-Bonding Interactions**	**Classical H-Bonding Interactions**	:UNK0:O	B:TYR62:OH	3.12
			B:TYR62:HH - :UNK0:O			B:TYR62:HH	:UNK0:O	2.06
			B:ARG64:HH22 - :UNK0:O			B:ARG64:HH22	:UNK0:O	2.11
			B:ARG64:HH22 - :UNK0:O			B:ARG64:HH22	:UNK0:O	2.68
			B:LYS38:HZ1 - :UNK0:O			B:LYS38:HZ1	:UNK0:O	1.93
			B:ARG64:HH12 - :UNK0:O			B:ARG64:HH12	:UNK0:O	2.23
			B:ARG64:HH22 - :UNK0:O			B:ARG64:HH22	:UNK0:O	2.14
			B:ARG64:HH12 - :UNK0:O			B:ARG64:HH12	:UNK0:O	2.56
			B:ARG104:HH11 - :UNK0:O			B:ARG104:HH11	:UNK0:O	2.43
			B:ARG104:HH21 - :UNK0:O			B:ARG104:HH21	:UNK0:O	2.51
					Salt Bridge	***H-Donor***	***H-Acceptor***	
			B:ARG64:HH22 - :UNK0:Fe			B:ARG64:HH22	:UNK0:Fe	2.27
			B:ARG64:HH22 - :UNK0:Fe			B:ARG64:HH22	:UNK0:Fe	2.75
			B:ARG64:HH12 - :UNK0:Fe			B:ARG64:HH12	:UNK0:Fe	2.23
			:UNK0:O - B:ASP135:OD2			***H-Donor***	***H-Acceptor***	3.21
						:UNK0:O	B:ASP135:OD2	
			:UNK0:O - B:ASP135:OD2			:UNK0:O	B:ASP135:OD2	3.35

7	**6zhp**	**Fe_6O_9 NPs**	:UNK0:O - B:ALA145:O	**H-Bonding Interactions**	**Classical H-Bonding Interactions**	:UNK0:O	B:ALA145:O	3.23
			:UNK0:O - B:ALA145:O			:UNK0:O	B:ALA145:O	3.24
			B:ARG154:HN - :UNK0:O			B:ARG154:HN	:UNK0:O	2.41
			B:SER147:HN - :UNK0:O			B:SER147:HN	:UNK0:O	2.79
			:UNK0:O - B:SER147:OG			:UNK0:O	B:SER147:OG	2.70
			B:ARG154:HH21 - :UNK0:O			B:ARG154:HH21	:UNK0:O	2.92
			B:ARG154:HH11 - :UNK0:O			B:ARG154:HH11	:UNK0:O	2.31
			B:ARG154:HH11 - :UNK0:O			B:ARG154:HH11	:UNK0:O	2.16
			B:ARG154:HH11 - :UNK0:O			B:ARG154:HH11	:UNK0:O	2.12
			B:TYR124:HH - :UNK0:O			B:TYR124:HH	:UNK0:O	2.08
			B:ARG154:HH21 - :UNK0:O			B:ARG154:HH21	:UNK0:O	2.86
			B:ARG104:HH21 - :UNK0:O			B:ARG104:HH21	:UNK0:O	2.36
			B:ARG104:HH11 - :UNK0:O			B:ARG104:HH11	:UNK0:O	1.86
			B:GLY153:CA - :UNK0:O		**Non-Classical H-Bonding Interactions**	***H-Donor***	***H-Acceptor***	
						B:GLY153:CA	:UNK0:O	3.65
						Positive	***Negative***	
			B:ARG104:NH2 - :UNK0:Fe	**Electrostatic Interactions**	**Attractive Charge**	B:ARG104:NH2	:UNK0:Fe	4.02
			B:ARG104:NH1 - :UNK0:Fe			B:ARG104:NH1	:UNK0:Fe	3.86
			B:ARG154:HH11 - :UNK0:Fe			B:ARG154:HH11	:UNK0:Fe	2.50
			B:ARG154:HH11 - :UNK0:Fe			B:ARG154:HH11	:UNK0:Fe	2.39
			B:ARG154:HH11 - :UNK0:Fe			B:ARG154:HH11	:UNK0:Fe	2.60
			B:ARG154:NH1 - :UNK0:Fe			B:ARG154:NH1	:UNK0:Fe	4.79
			B:ARG154:HH11 - :UNK0:Fe			B:ARG154:HH11	:UNK0:Fe	2.98
			B:ARG154:HH21 - :UNK0:Fe			B:ARG154:HH21	:UNK0:Fe	2.80
			B:ARG154:NH2 - :UNK0:Fe			B:ARG154:NH2	:UNK0:Fe	4.35
8	**6zhp**	**Fe_8O_{12} NPs**				***H-Donor***	***H-Acceptor***	
			:UNK0:O - B:LEU137:O	**H-Bonding Interactions**	**Classical H-Bonding Interactions**	:UNK0:O	B:LEU137:O	3.33
			:UNK0:O - B:GLU139:O			:UNK0:O	B:GLU139:O	3.30
			:UNK0:O - B:PRO138:O			:UNK0:O	B:PRO138:O	3.26
			:UNK0:O - B:PRO138:O			:UNK0:O	B:PRO138:O	3.36
			:UNK0:O - B:PRO138:O			:UNK0:O	B:PRO138:O	2.88
			:UNK0:O - B:GLU139:OE1			:UNK0:O	B:GLU139:OE1	3.28
			:UNK0:O - B:GLU139:OE1			:UNK0:O	B:GLU139:OE1	3.10
			:UNK0:O - B:TYR332:OH			:UNK0:O	B:TYR332:OH	3.08
			:UNK0:O - B:TYR62:OH			:UNK0:O	B:TYR62:OH	2.70
			B:LYS38:HZ3 - :UNK0:O			B:LYS38:HZ3	:UNK0:O	2.15
			B:TYR62:HH - :UNK0:O			B:TYR62:HH	:UNK0:O	2.23
			B:LYS38:HZ1 - :UNK0:O			B:LYS38:HZ1	:UNK0:O	2.65
			B:ARG64:HH12 - :UNK0:O			B:ARG64:HH12	:UNK0:O	2.22
			B:ARG64:HH22 - :UNK0:O			B:ARG64:HH22	:UNK0:O	2.66
						Positive	***Negative***	
			B:ARG104:NH2 - :UNK0:Fe			B:ARG104:NH2	:UNK0:Fe	5.52
			B:ARG64:NH2 - :UNK0:Fe			B:ARG64:NH2	:UNK0:Fe	5.59

			B:ARG64:NH1 - :UNK0:Fe	**Electrostatic Interactions**	**Attractive Charge**	B:ARG64:NH1	:UNK0:Fe	4.45
			B:ARG64:HH22 - :UNK0:Fe			*B:ARG64:HH22*	*:UNK0:Fe*	2.85
			B:LYS38:HZ1 - :UNK0:Fe			B:LYS38:HZ1	:UNK0:Fe	1.80
			B:LYS38:NZ - :UNK0:Fe			B:LYS38:NZ	:UNK0:Fe	4.23
			B:LYS38:NZ - :UNK0:Fe			B:LYS38:NZ	:UNK0:Fe	5.59
			B:LYS38:NZ - :UNK0:Fe			B:LYS38:NZ	:UNK0:Fe	4.63
			B:LYS38:NZ - :UNK0:Fe			B:LYS38:NZ	:UNK0:Fe	3.78
			B:LYS38:HZ3 - :UNK0:Fe			B:LYS38:HZ3	:UNK0:Fe	2.67
			B:LYS38:NZ - :UNK0:Fe			B:LYS38:NZ	:UNK0:Fe	5.09

Table S2. Cartesian co-ordinates for the ground state geometry of **Fe_2O_3 NPs (monomer)** at DFT B3LYP//6-31G (d,p) level

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	26	0	1.310600	-0.285042	2.923989
2	8	0	0.739889	-1.781391	2.905221
3	8	0	0.382449	1 .412865	2.980110
4	8	0	3.130696	*0.366640*	*2.823675*
5	26	0	*2.103576*	*1.818845*	*2.784337*

Table S3. Cartesian co-ordinates for the ground state geometry of **Fe_4O_6 NPs (dimer)** at DFT B3LYP//6-31G (d,p) level

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	26	0	-1.688336	-0.223512	-1.419555
2	8	0	-1.689933	1.570840	-1.115089
3	8	0	-0.204279	-0.978265	-2.154620
4	8	0	-2.796392	-1.273462	-0.428486
5	26	0	0.489425	-0.843257	-0.477435
6	26	0	-0.675276	1.155152	0.337520
7	26	0	-1.542700	-1.074681	0.875792
8	8	0	1.087948	0.780313	0.086648
9	8	0	-0.018510	-2.063989	0.773250
10	8	0	-1.504165	0.485116	1.812781

Table S4. Cartesian co-ordinates for the ground state geometry of **Fe_6O_9 NPs (trimer)** at DFT B3LYP//6-31G (d,p) level

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	26	0	-1.226114	0.227329	1.124618
2	26	0	0.798771	-0.247073	0.009260
3	26	0	-1.782168	-1.627646	-1.167552
4	26	0	-2.425192	-1.762455	1.186240
5	26	0	0.563521	-2.569900	0.643878
6	26	0	0.479077	-1.768790	-1.976331
7	8	0	0.159035	1.370493	0.726370
8	8	0	-0.714511	-1.114325	0.192001
9	8	0	-2.674213	-0.150663	2.072719
10	8	0	1.474853	-0.273612	-1.676293
11	8	0	0.881068	-3.271989	-1.021963
12	8	0	-0.998788	-2.905053	1.670708
13	8	0	-3.327527	-2.079753	-0.391022
14	8	0	-1.100763	-1.726156	-2.831464
15	8	0	1.802701	-1.269131	1.060408

Table S5. Cartesian co-ordinates for the ground state geometry of **Fe_8O_{12} NPs (tetramer)** at DFT B3LYP//6-31G (d,p) level

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	26	0	-0.604592	-1.647038	0.157579
2	26	0	-2.131473	0.331080	-0.945405
3	26	0	-1.658209	-3.666223	-0.198481
4	26	0	1.356107	-1.582025	-1.591859
5	26	0	0.295263	0.920280	-1.069178
6	26	0	-3.163493	-1.827978	-0.403992
7	26	0	-1.712763	-2.091086	-2.160351
8	26	0	0.986303	-3.694794	-0.417137
9	8	0	-1.207387	2.035774	-0.942475
10	8	0	-0.565105	-0.384765	-0.964562
11	8	0	-3.500967	-0.128848	0.302598
12	8	0	1.944343	0.284149	-1.557887
13	8	0	2.174733	-3.276328	-1.784668
14	8	0	-0.353918	-4.972113	-0.021982
15	8	0	-2.804385	-3.491255	-1.498669
16	8	0	-2.951582	-0.859146	-2.019774
17	8	0	-0.043528	-1.740799	-3.007642
18	8	0	-1.982692	-2.564236	1.102812
19	8	0	0.999374	-2.028955	0.174334
20	8	0	-1.610633	-2.142570	-0.660488

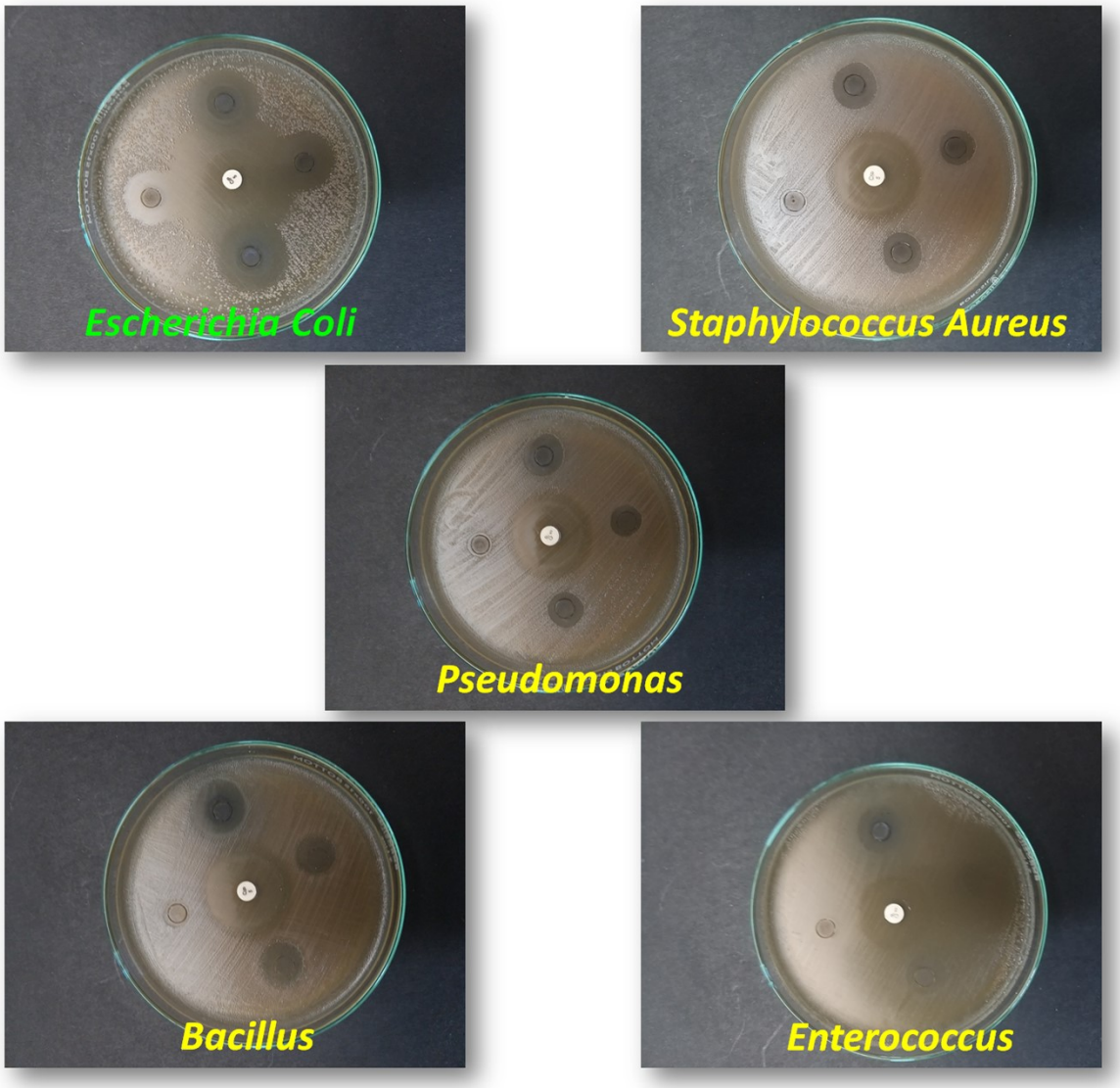

Figure S1. Pictorial illustration of zone of inhibition of antimicrobial activity of iron oxide nanoparticles against the bacterial strains *Staphylococcus aureus*, *Escherichia coli*, *Pseudomonas sp*., *Bacillus sp*., and *Enterococcus sp.*