

Supporting Information

Synthesis, Antimicrobial Potential and Computational Studies of Crystalline 4-Bromo-2-(1,4,5-triphenyl-1-H-imidazole-2-yl)phenol and its Metal Complexes

Abu Bakar Siddique,^a Saeed Ahmad,^b Muhammad Ashraf Shaheen,^a Akbar Ali,^{*c} Muhammad Nawaz Tahir,^d Lucas Campos Curcino Vieira,^e Shabbir Muhammad,^f Saifeldin M. Siddeeg,^f

^aDepartment of Chemistry, University of Sargodha, Sargodha 40100, Pakistan

^bGovt. Postgraduate College Toba Tek Singh, Pakistan

^cDepartment of Chemistry, Government College University Faisalabad, Faisalabad-38000 Pakistan

^dDepartment of Physics, University of Sargodha, Sargodha-40100, Pakistan

^eEngineering Faculty, Federal University of Mato Grosso, V_arzea Grande, Brazil

^fDepartment of Chemistry, College of Science, King Khalid University, P.O. Box 9004, Abha 61413, Saudi Arabia

*Corresponding Author

Akbar Ali – Department of Chemistry, Government College University Faisalabad, Faisalabad 38000, Pakistan;
orcid.org/0000-0002-2914-0934; Email: akbarchm@gmail.com, akbar.ali@gcuf.edu.pk

Table S1: Optimized coordinates of Ligand (1a)

Br	7.38041200	0.63503400	10.82123800
O	3.64216200	2.35369500	6.42745000
H	2.69939100	2.27974800	6.71293600
N	1.93394800	2.27426900	10.24626700
N	1.60566500	1.97871000	8.08306700
C	-0.91603800	1.51392700	6.68921300
H	-0.07004400	0.89444700	6.40828700
C	-2.05885800	1.55350700	5.89824000
H	-2.10619200	0.95822300	4.99149700
C	-3.13941900	2.35098300	6.26773600
H	-4.03199800	2.38110900	5.65053500
C	-3.06528300	3.11663400	7.42916800
H	-3.89702600	3.75288800	7.71584300
C	-1.92214000	3.08310900	8.22022200
H	-1.86205800	3.69986200	9.11166900
C	-0.83869100	2.27181400	7.86292600
C	0.39091600	2.21817200	8.67139100
C	0.56457400	2.39307600	10.02838600
C	-0.40814100	2.61688100	11.11161500
C	-1.51974500	1.77236800	11.21977500
H	-1.63855500	0.96185800	10.50649500
C	-2.46293200	1.97511800	12.22106900
H	-3.32151200	1.31482500	12.29272300
C	-2.30254200	3.01652600	13.13271400

H	-3.03697800	3.17180000	13.91684000
C	-1.19783300	3.85885400	13.03406100
H	-1.06989900	4.67474000	13.73848400
C	-0.25730800	3.66464600	12.02777600
H	0.59789800	4.32936800	11.94747700
C	2.58489300	2.45657000	11.50560800
C	2.31540700	1.57986100	12.55234900
H	1.60448900	0.77316200	12.40340400
C	2.96394300	1.75709100	13.77093300
H	2.75960300	1.07664200	14.59097800
C	3.87737400	2.79597000	13.93369200
H	4.38894900	2.92412500	14.88202300
C	4.13540900	3.67105800	12.88033000
H	4.84681600	4.48070600	13.00491100
C	3.48187300	3.51046600	11.66309400
H	3.67281900	4.17744800	10.82792000
C	2.52008000	2.00809200	9.03502600
C	3.94866700	1.78941900	8.76965900
C	4.42877400	2.00474600	7.45524200
C	5.79577200	1.85730900	7.19027700
H	6.13542500	2.04777000	6.17815900
C	6.67869000	1.46746300	8.18192200
H	7.73540800	1.35147200	7.96819200
C	6.19113000	1.20427200	9.45988700
C	4.84840000	1.35479600	9.75402600

H 4.50259000 1.12162900 10.75312900

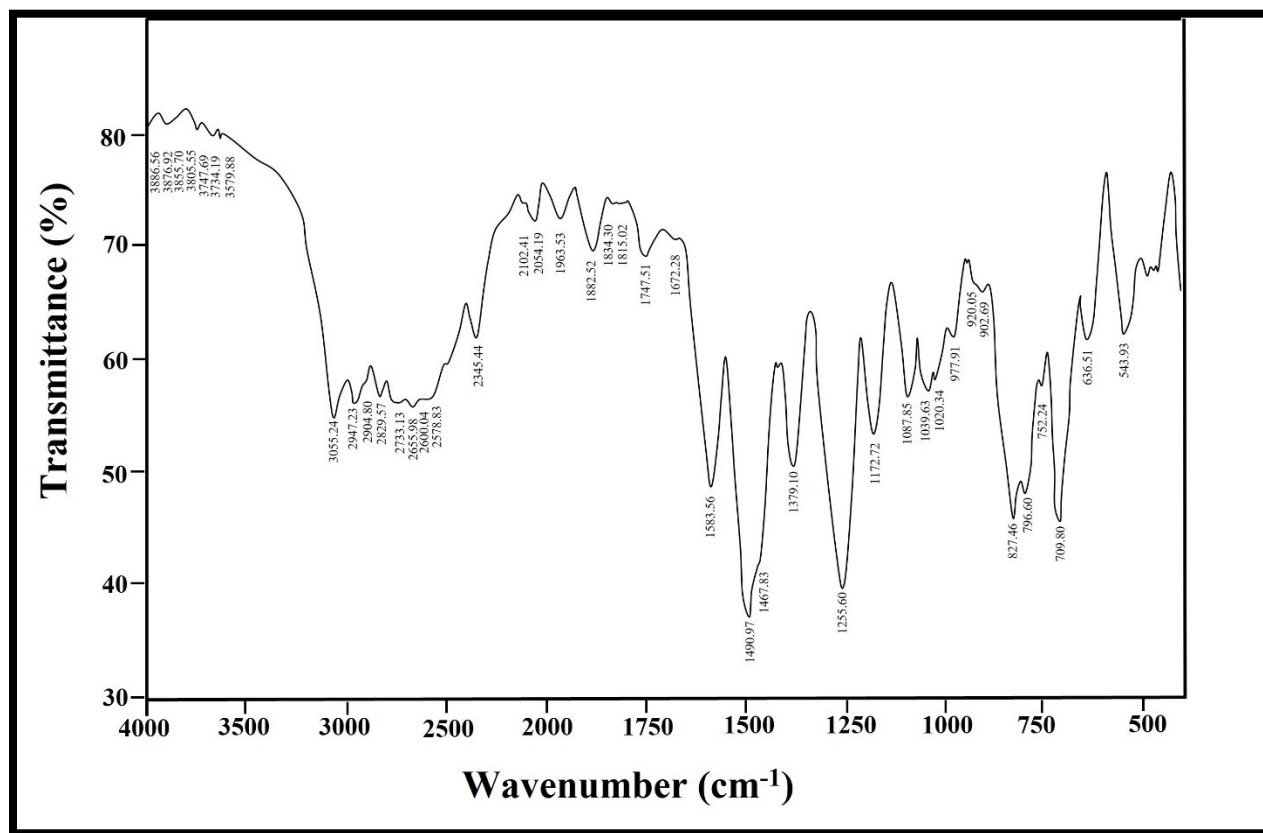


Fig. S1: FT-IR (KBr) % Transmittance Spectrum of Ligand (1a)

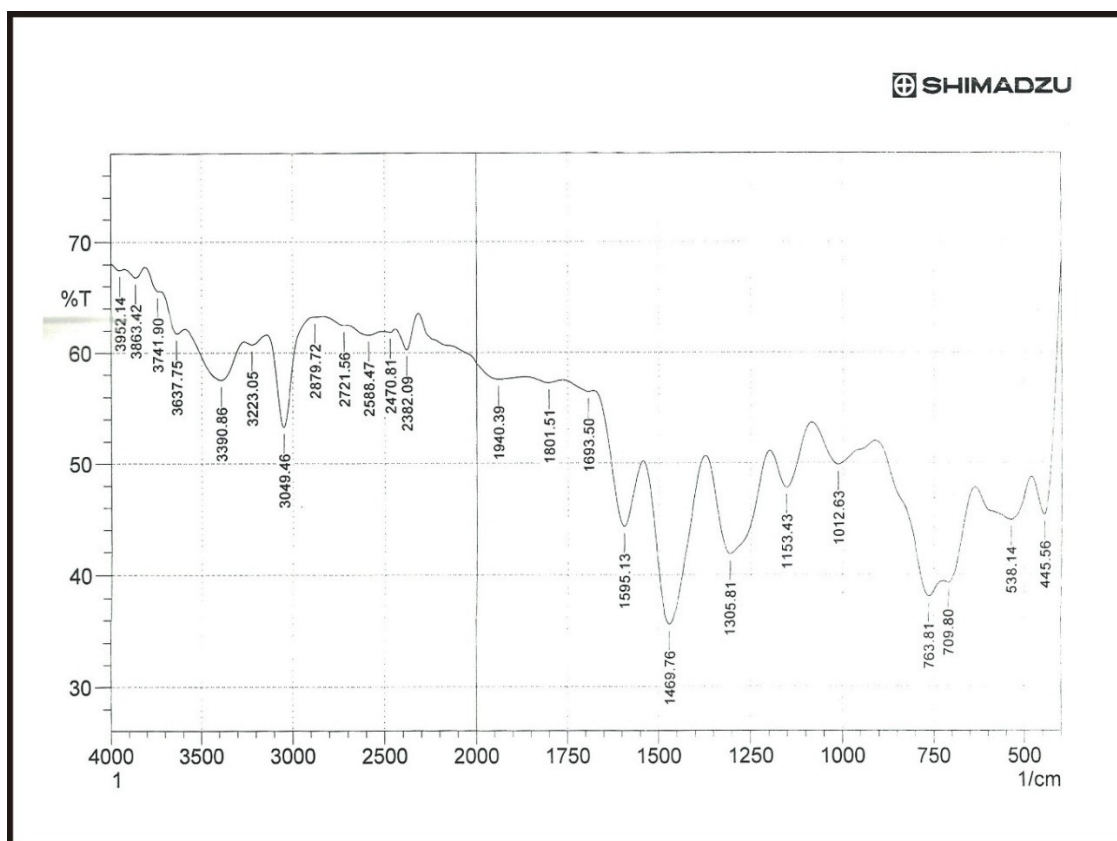


Fig. S2: FT-IR (KBr) % Transmittance Spectrum of Zn²⁺ Complex (2a)

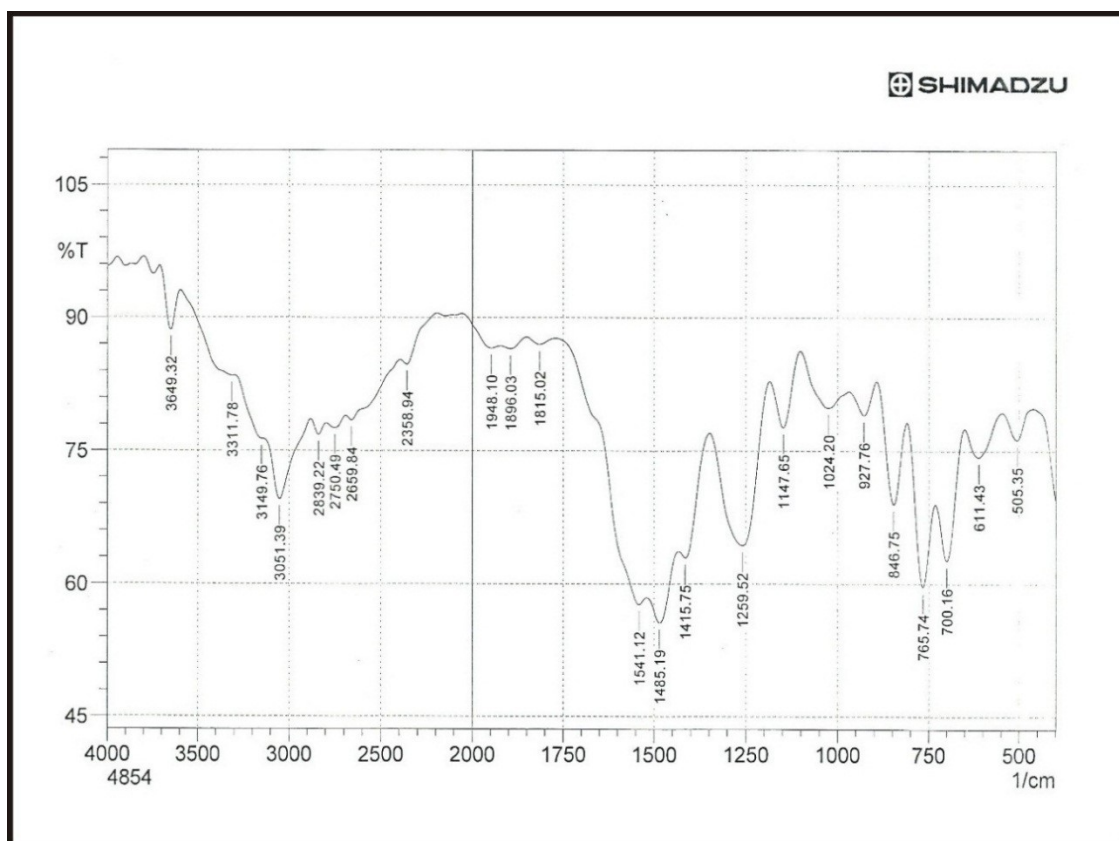


Fig. S3: FT-IR (KBr) % Transmittance Spectrum of Co²⁺ Complex (3a)

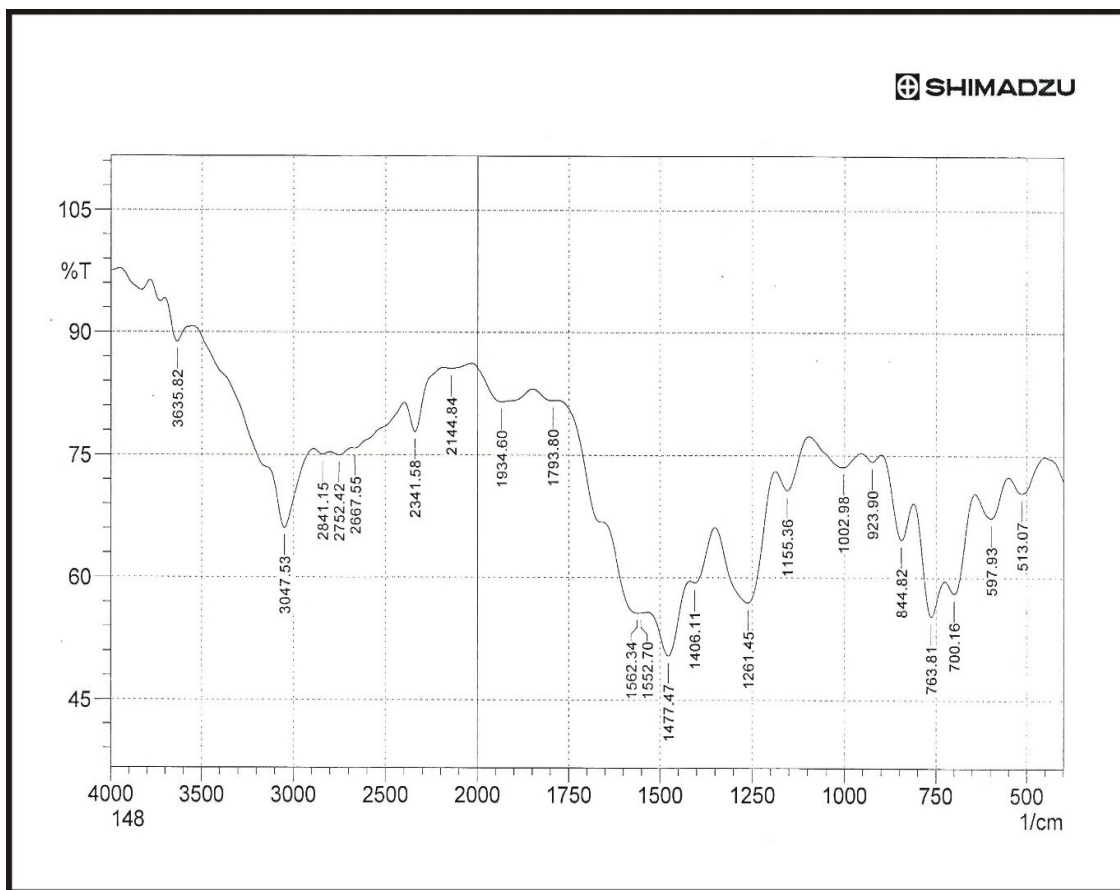


Fig. S4: FT-IR (KBr) % Transmittance Spectrum of Ni²⁺ Complex (4a)

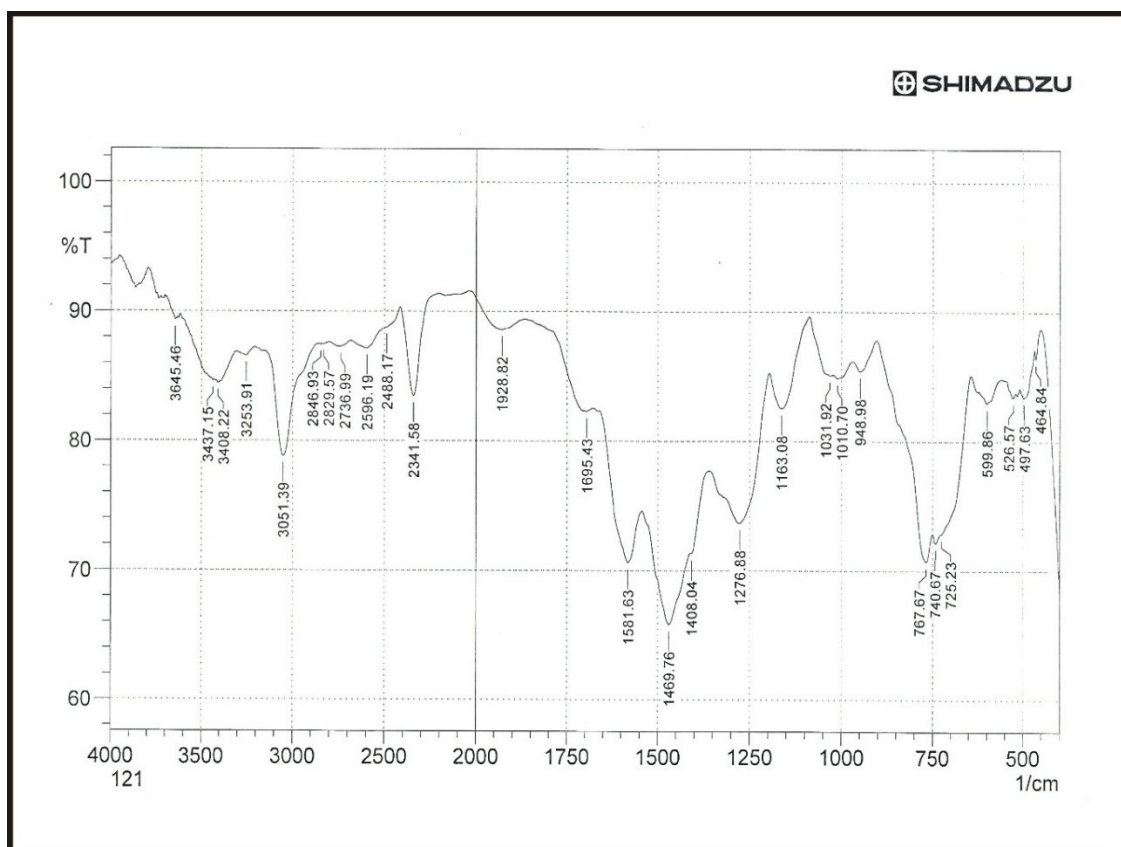


Fig. S5: FT-IR (KBr) % Transmittance Spectrum of Cu²⁺ Complex (5a)

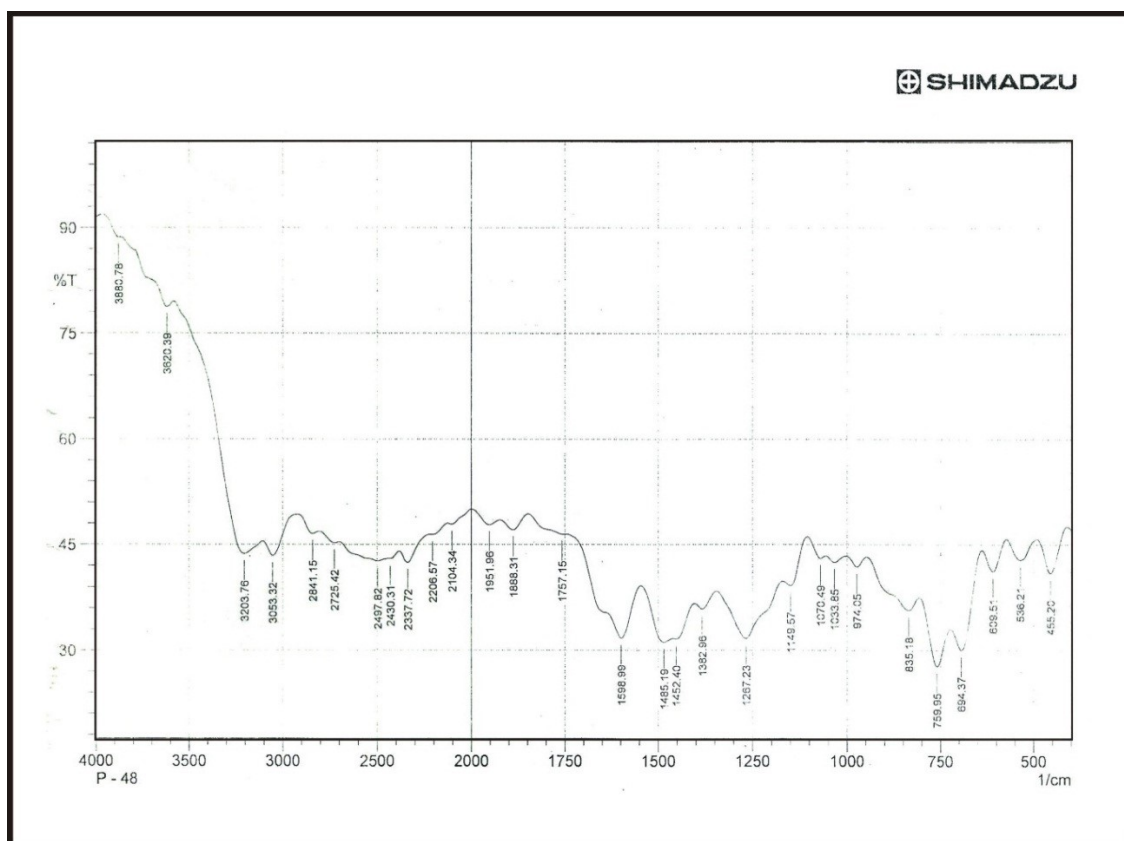
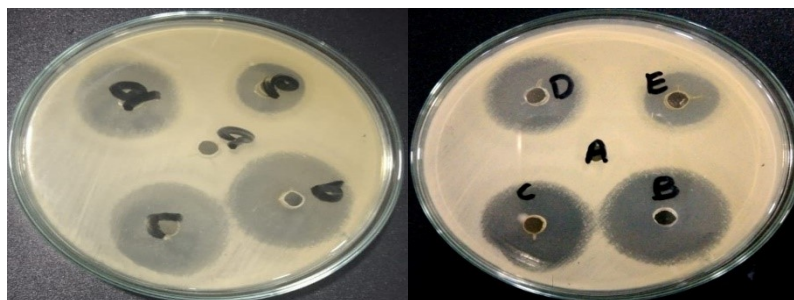


Fig. S6: FT-IR (KBr) % Transmittance Spectrum of Mn^{2+} Complex (6a)

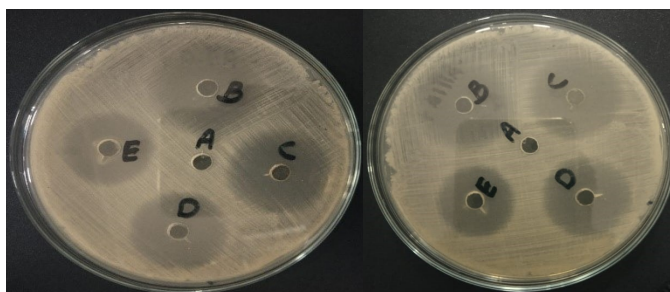
Fig. S7: Antibacterial Activity against *E. Coli*:



A) b= Standard, C= 5a, e= 1a, d= 3a

B) b= standard, E= 6a, C= 2a, d= 4a

Fig. S8: Antibacterial Activity against *P. multocida*:



C) b= Standard, C= 5a, e= 1a, d= 3a

D) b= standard, E= 6a, C= 2a, d= 4a

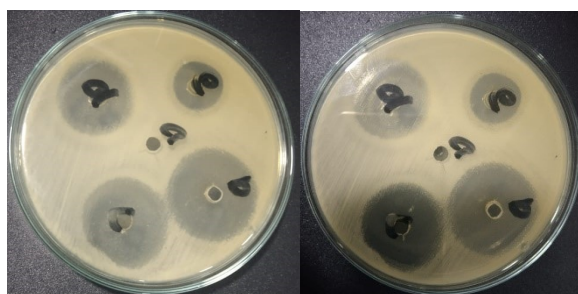
Fig. S9: Antibacterial Activity against *S. aureus*:



E) b= Standard, C= 5a, e= 1a, d= 3a

F) b= standard, E= 6a, C= 2a, d= 4a

Fig. S10: Antibacterial Activity against *B. subtilis*:



G) b= Standard, C= 5a, e= 1a, d= 3a

H) b= standard, E= 6a, C= 2a, d= 4a