Supporting Information

Synthesis, Crystal structure, Lipophilicity, Antioxidant, Binding interaction and Antibacterial investigation against Methicillin-Resistant *Staphylococcus aureus* of Ni(II) Schiff base complex: Combined Theoretical and Experimental Approaches

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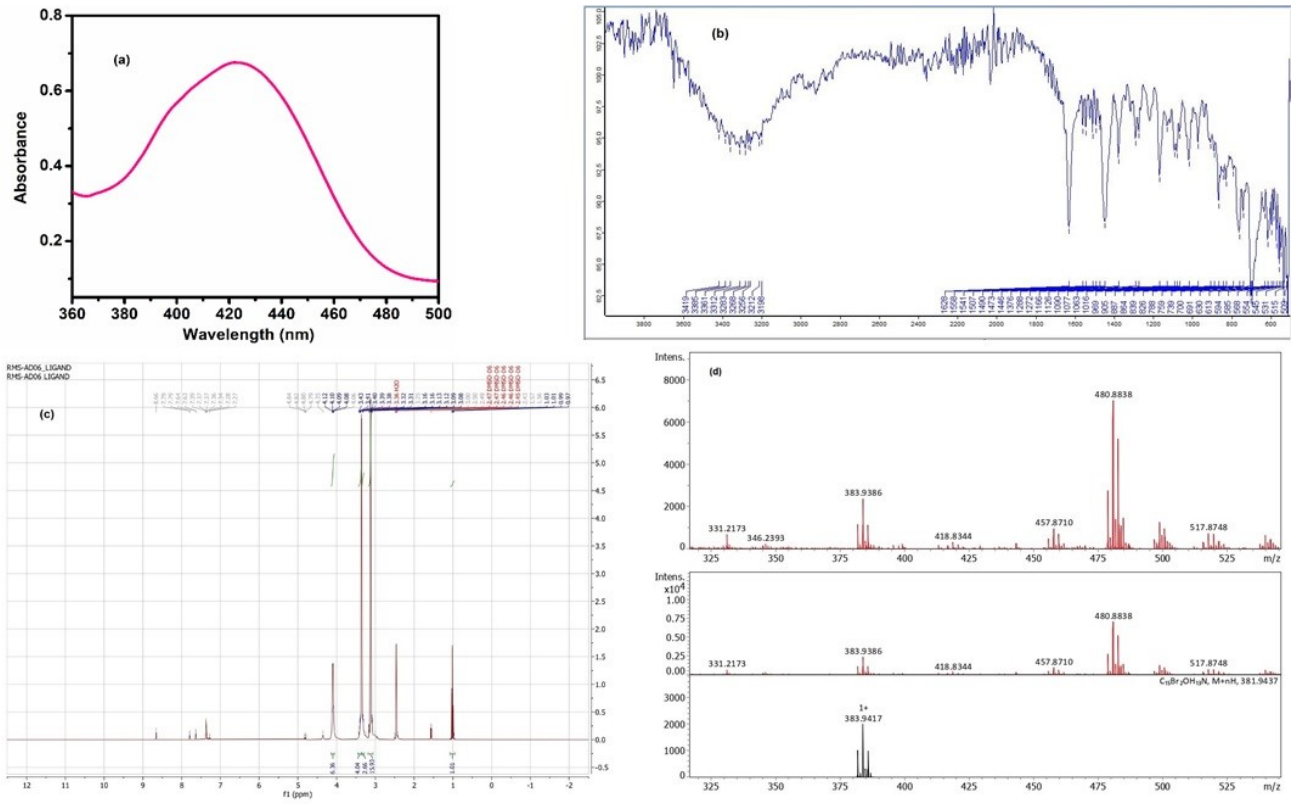

Figure S1 (a) UV-Vis, (b) FTIR and (c) 1H NMR (d) Mass spectra of the ligand

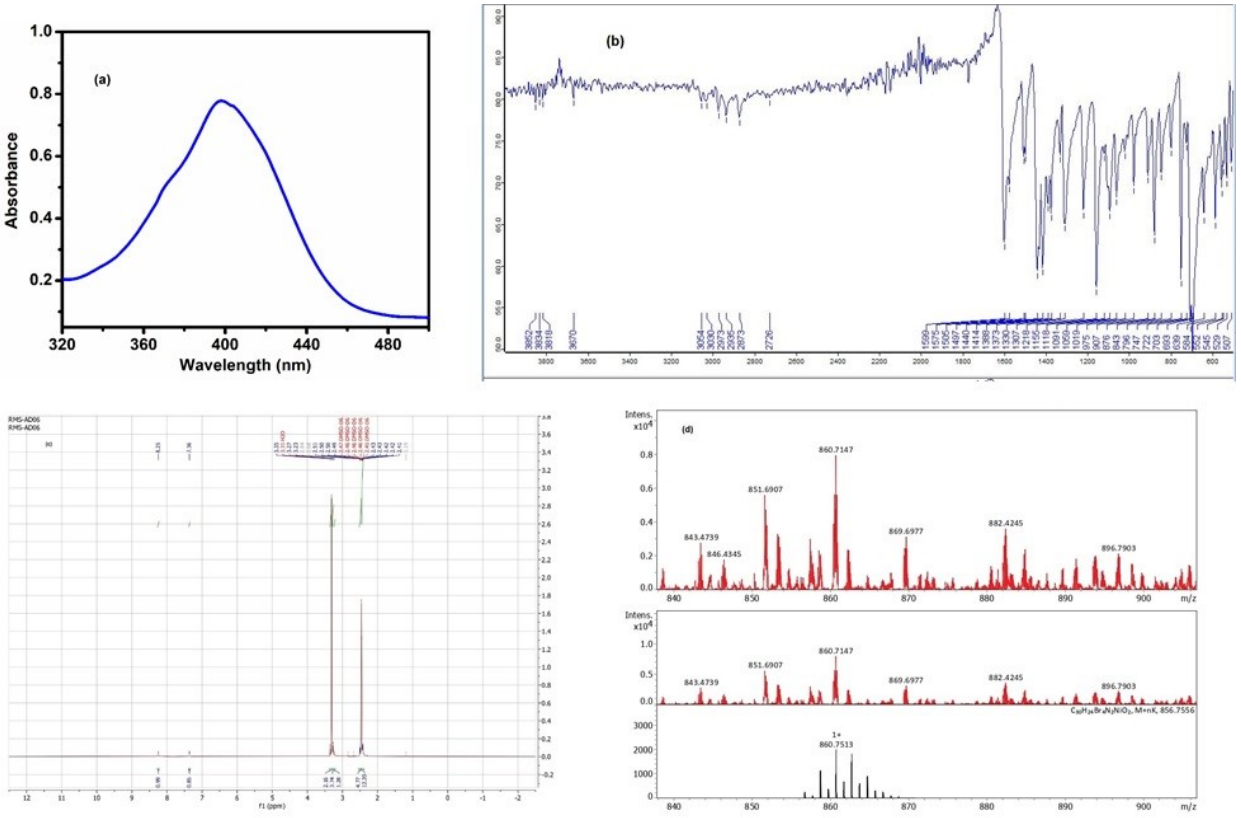

Figure S2 (a) UV-Vis and (b) FTIR (c) 1H NMR (d) Mass spectra of the complex

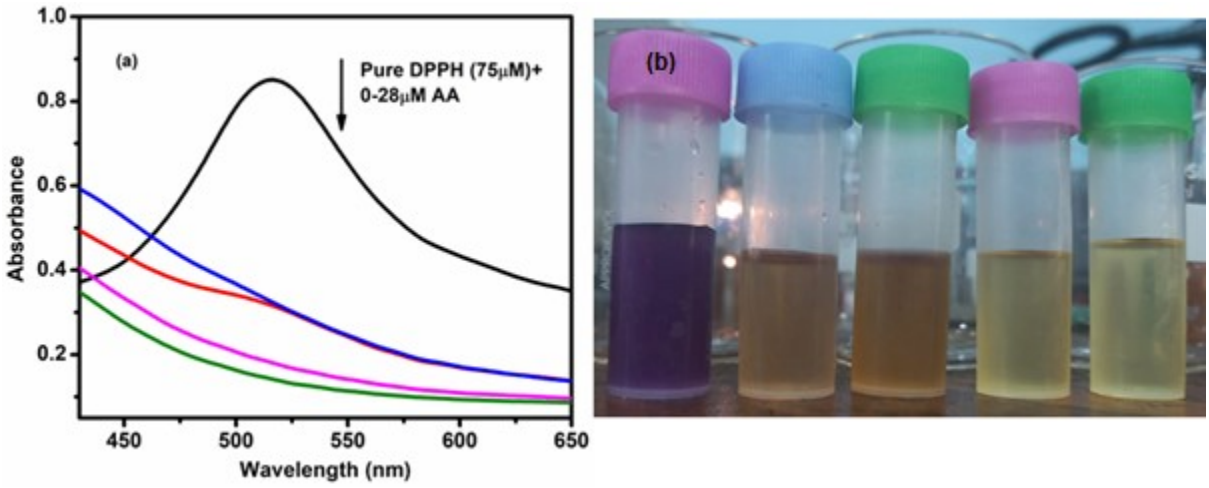

Figure S3 (a) Decrease in absorbance of DPPH with addition of ascorbic acid (b) Colour changes of pure DPPH solution with gradual addition of ascorbic acid

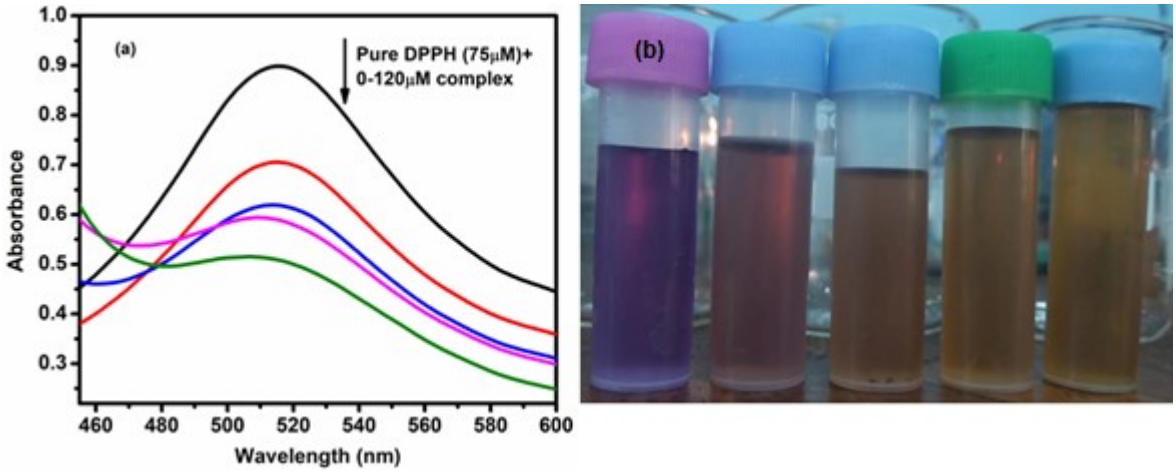

Figure S4 (a) Decrease in absorbance of DPPH with addition of complex (b) Colour changes of pure DPPH solution with gradual addition of complex

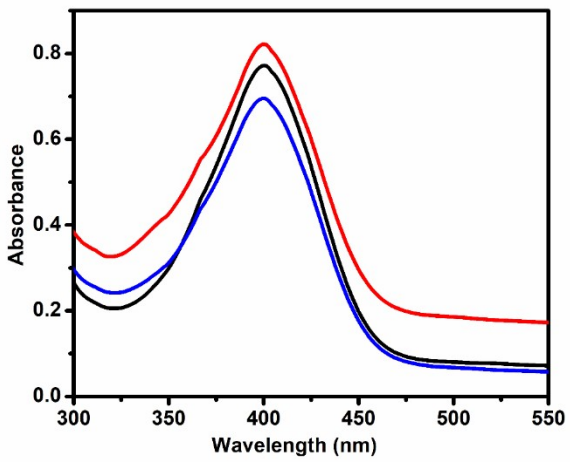

Figure S5 UV spectra of the complex at day 1, 7 and 14

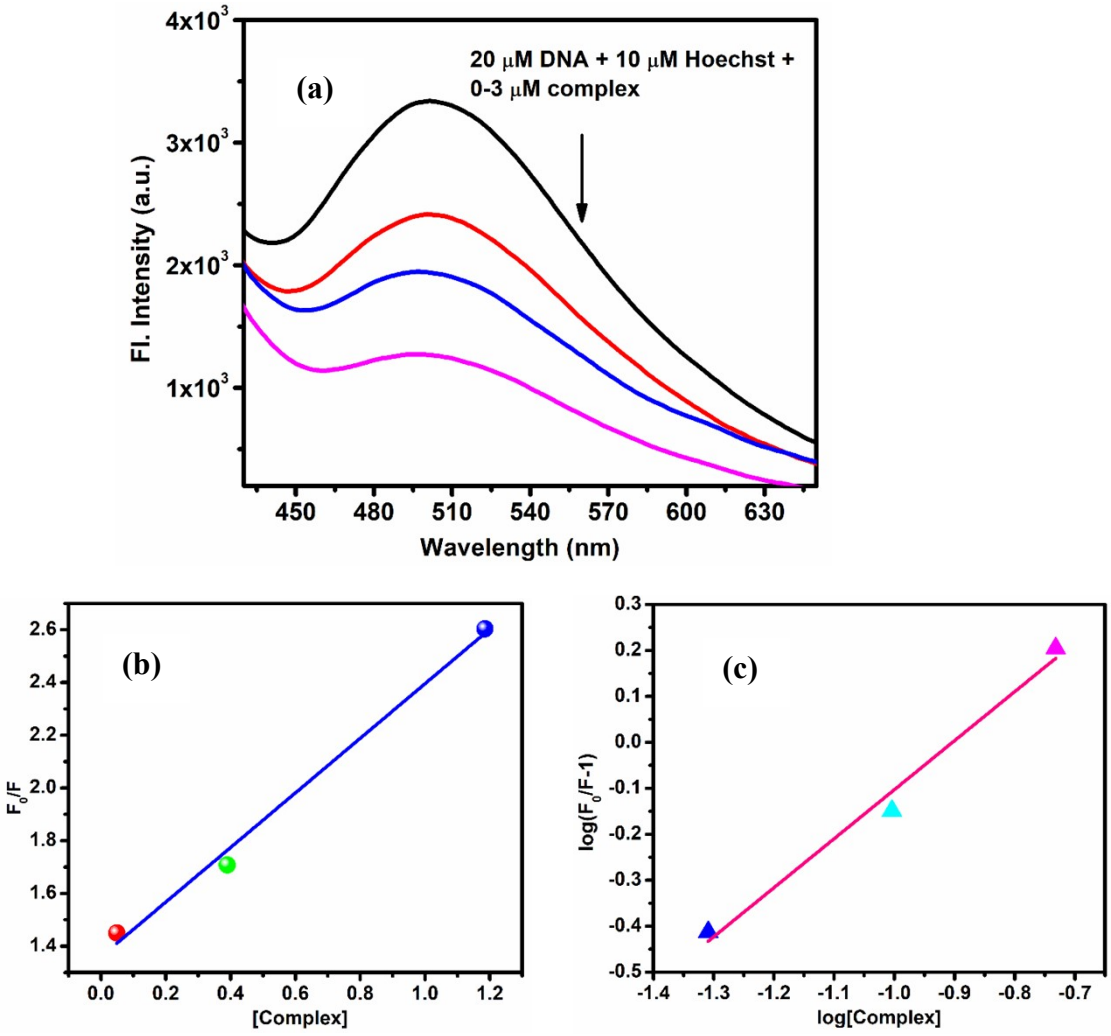

Figure S6 (a) Fluorescence quenching of DNA- Hoechst adduct by the complex (b) Stern Volmer plot (c) Scatchard plot at 303 K

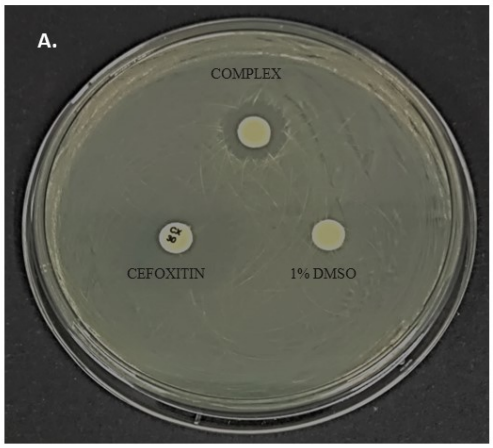

Figure S7 Antibacterial activity of complex against Gram positive MRSA through disc diffusion assay. Standard antibiotic Cefoxitin (cx30) and 1% DMSO was used as control. Complex shown a significant zone of inhibition (14mm) whereas control demonstrated the zone of inhibitions <6mm.

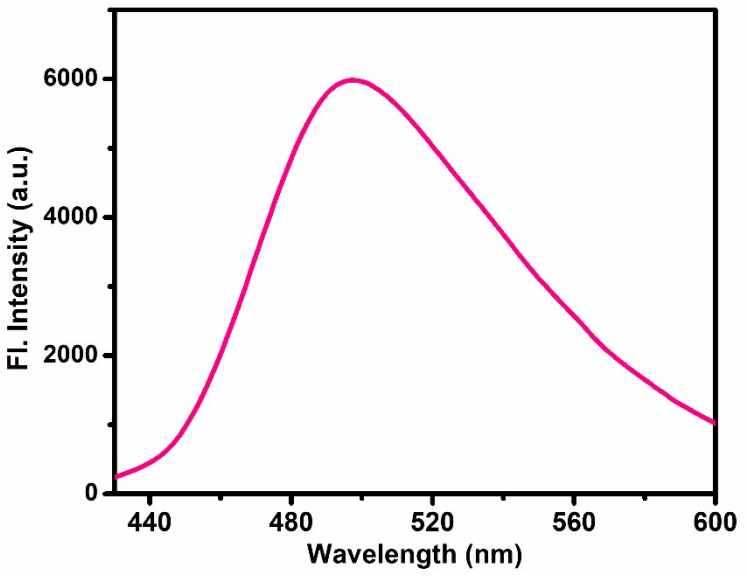

Figure S8 Fluorescence spectrum of the pure complex

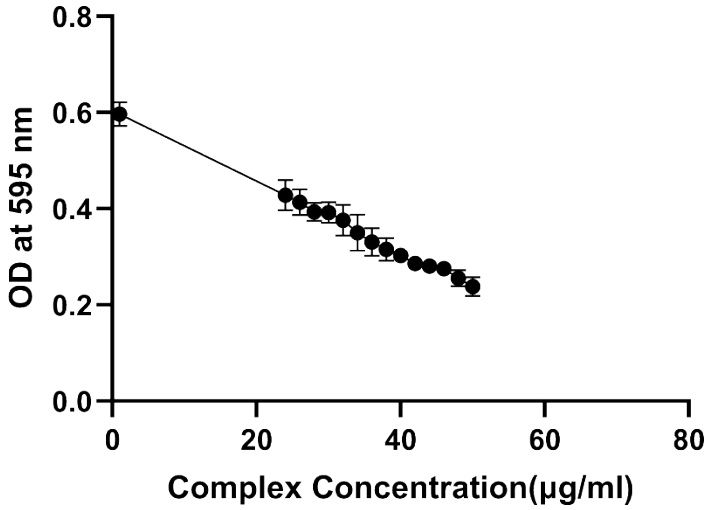

Figure S9 Determination of minimum inhibitory concentration (MIC) >50µg/ml of complex against KP (BAA1705)

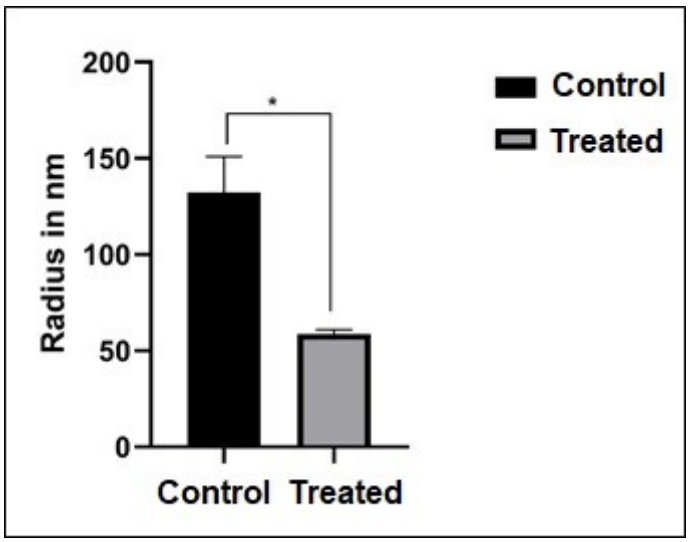

Figure S10 Quantification of cell radius for control before and after treated with complex. Treated MRSA cells shows reduce radius size than control cells. The radius was measured by ImageJ software. The data provided is the mean ± standard deviation of triplicate experiments and statistically significant.

Table S1 Bond distances (Å) and angles (º) for complex [Ni(L_2)]

Bond lenghts		**Bond angles**	
Ni1-N1	2.017(7)	N1-Ni1-N1i	115.8(4)
Ni1-N1i	2.017(7)	N1-Ni1-O1	92.8(3)
Ni1-O1	1.903(6)	N1-Ni1-O1i	106.8(3)
Ni1-O1i	1.903(6)	N1i-Ni1-O1	106.8(3)
Br1-C2	1.931(8)	N1i-Ni1-O1i	92.8(3)
Br2-C4	1.907(8)	O1-Ni1-O1i	143.0(4)
N1-C7	1.274(12)		
N1-C8	1.485(11)		

i=-x+1, y, -z+1