Synthesis and characterization of (E)-N-carbamimidoyl -4 and (E)-4-benzenesulfonamides; biological study, DFT, molecular docking and ADMET predictions

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Table S_1: [a]MIC and MBC values (μg/mL) for the sulphonamide Schiff bases.

Compounds	MIC	MBC
L_1	1.25	2.5
L_2	0.625	1.25

[a]MIC and MBC correspond to the minimum inhibitory concentration and minimum bactericidal concentration respectively.

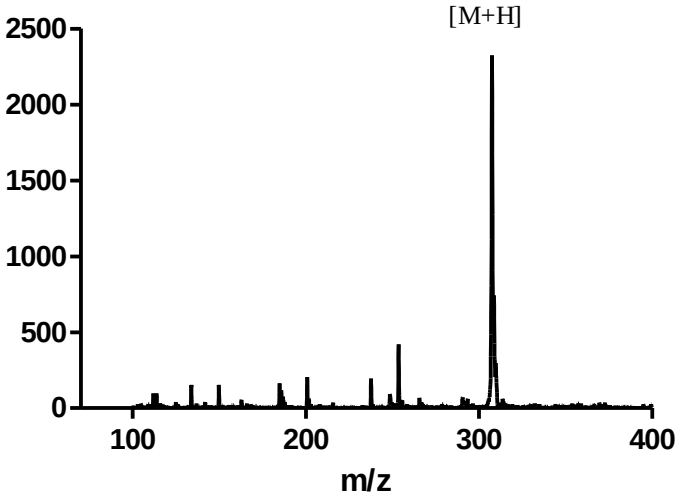

Fig. S_1: Mass spectrum for L_1 showing [M+1] ion as the base peak.

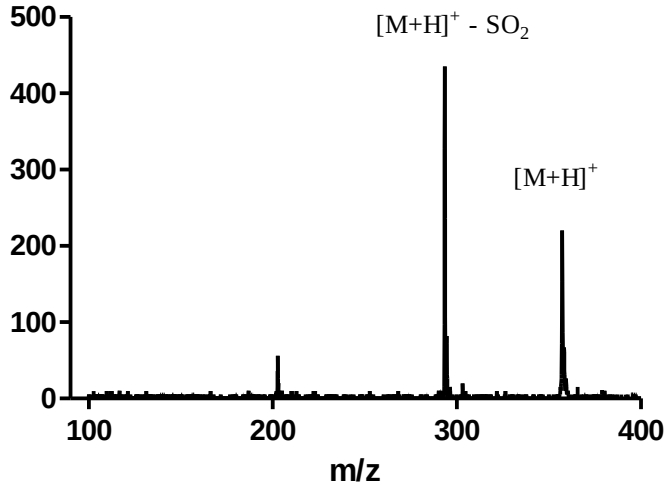

Fig. S_2: Mass spectrum for L_2 showing ([M+1]-SO_2) ion as the base peak and [M+1] ion as the molecular ion.

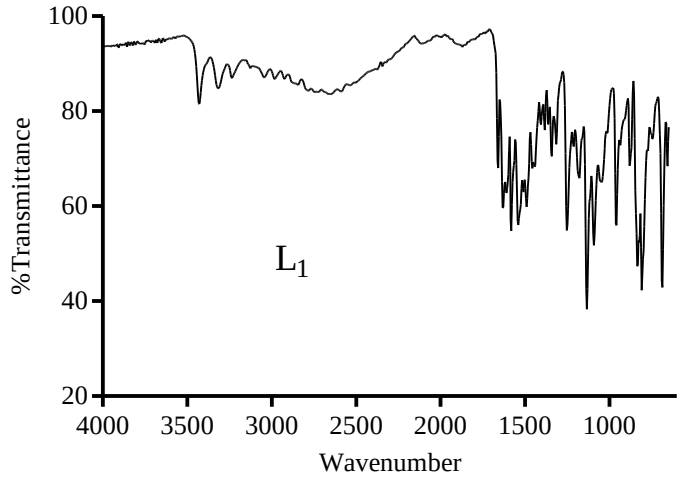

Fig. S_3: FT-IR spectrum for L_1 showing the different vibrational bands for the sulfaguanidine Schiff base compound.

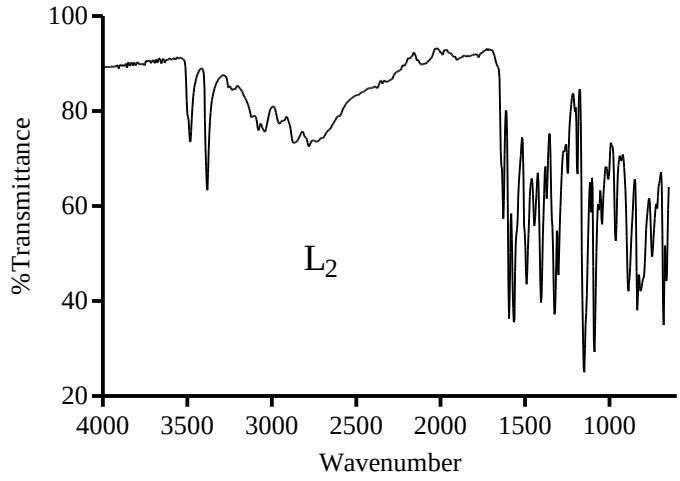

Fig. S_4: FT-IR spectrum for L_2 showing the different vibrational bands for the sulfamerazine Schiff base compound.

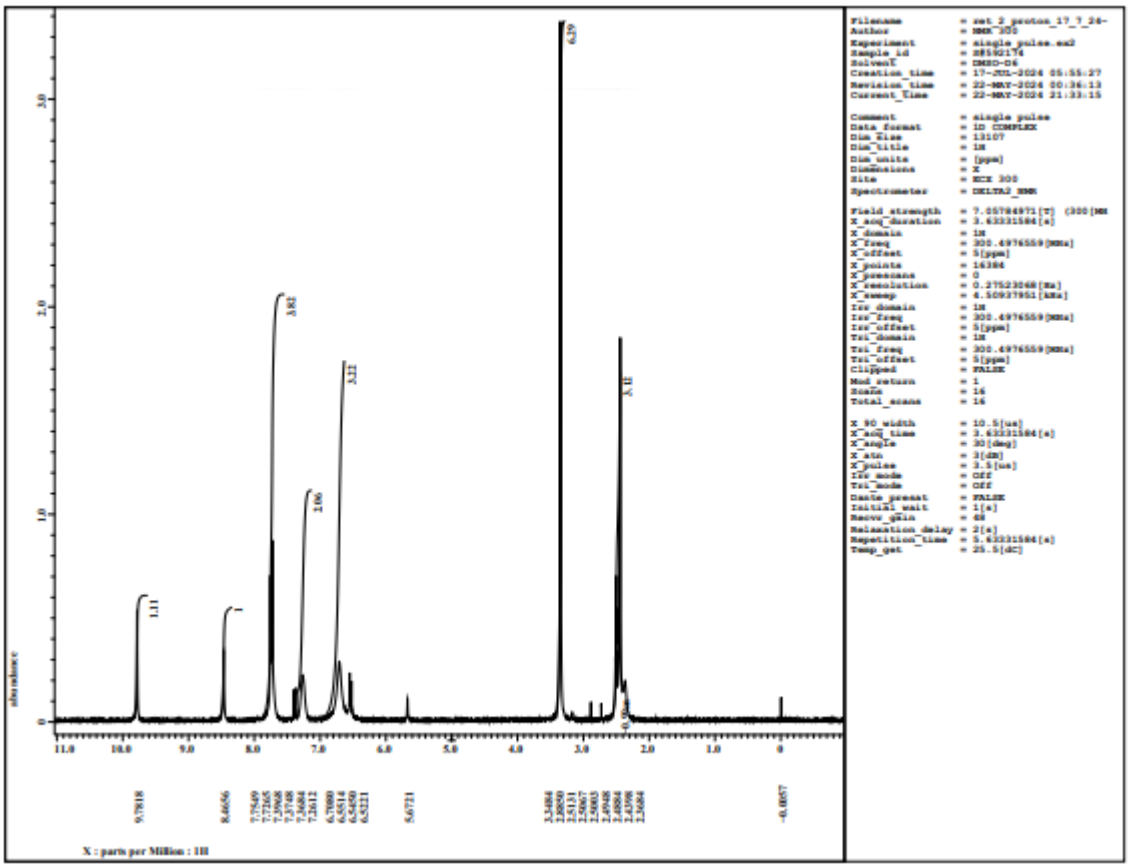

Fig. S_5: ^{1}H-NMR spectrum of Compound L_1 showing the numbers of protons in different chemical environment.

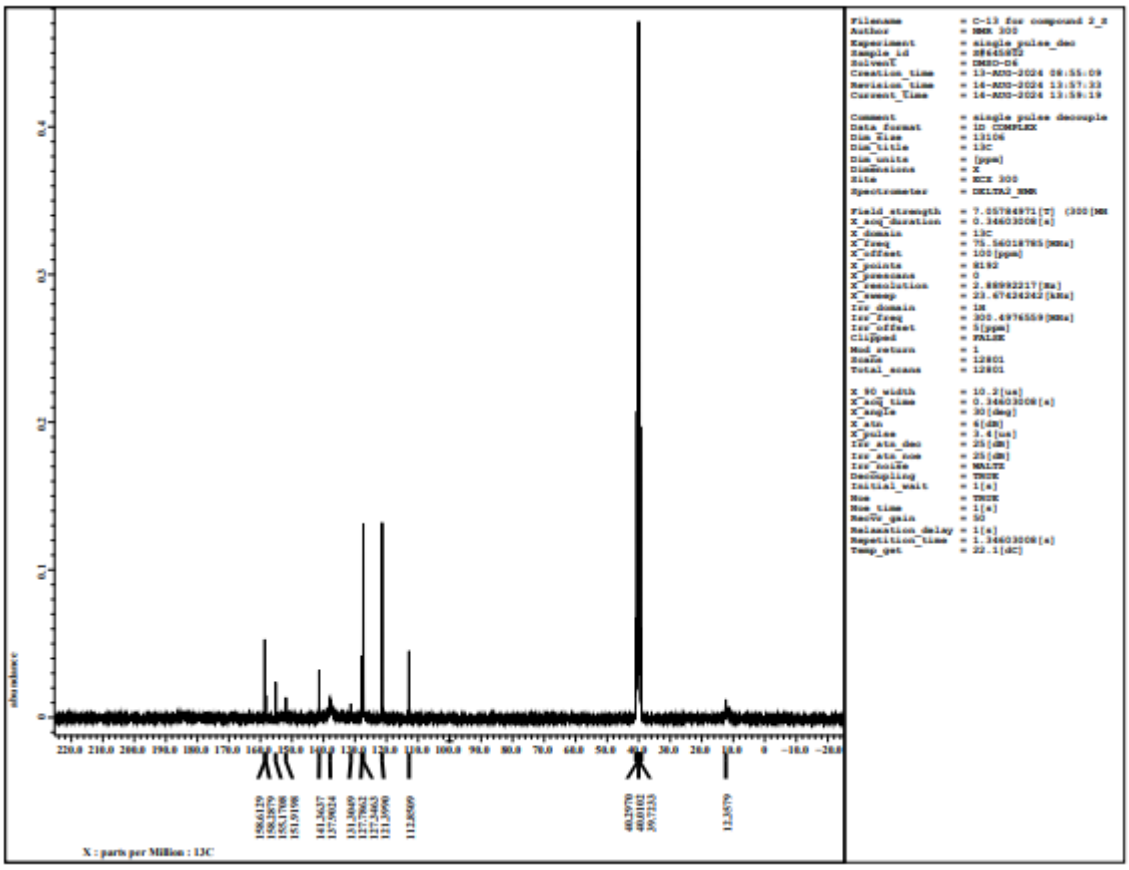

Fig. S_6: ^{13}C-NMR spectrum of Compound L_1 showing the carbon atoms in different chemical environment.

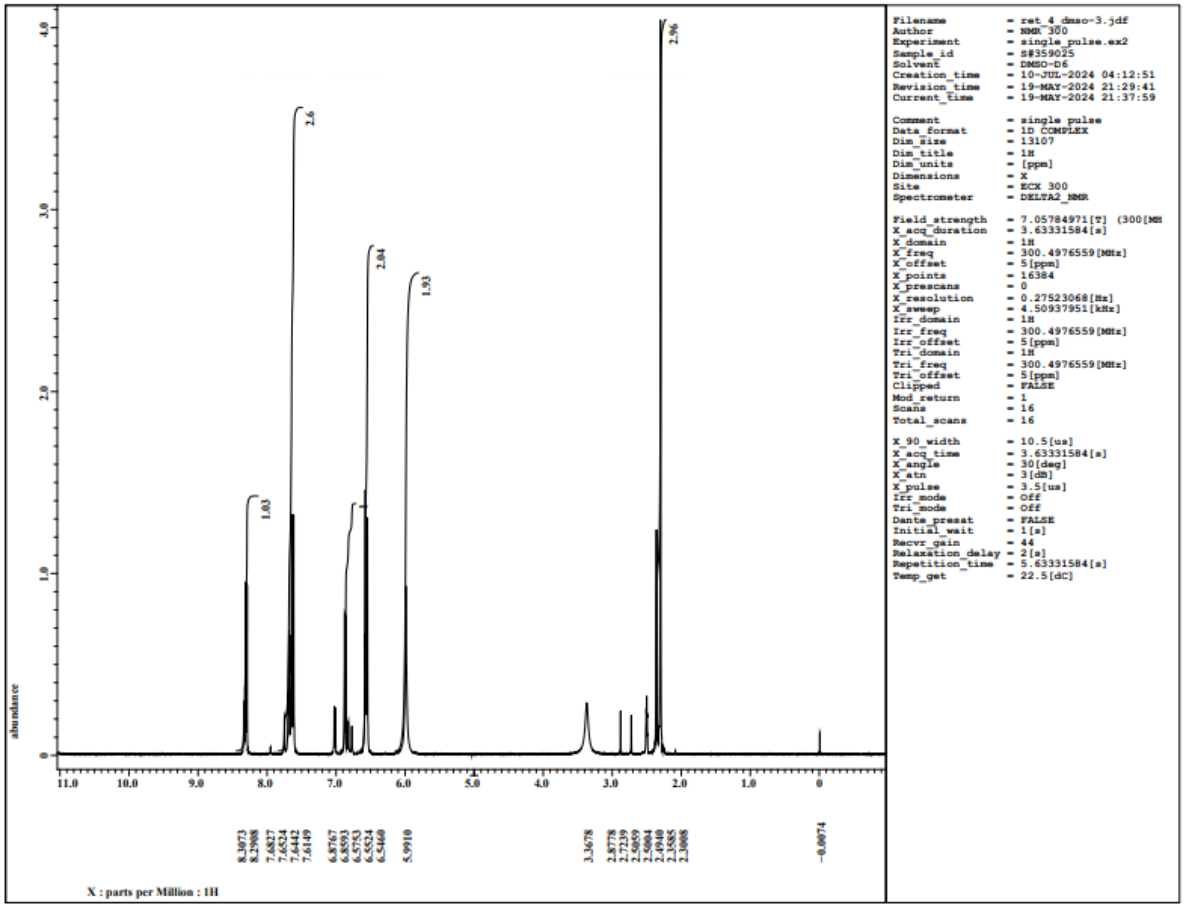

Fig. S_7: ^{1}H-NMR spectrum of Compound L_2 showing the numbers of protons in different chemical environment.

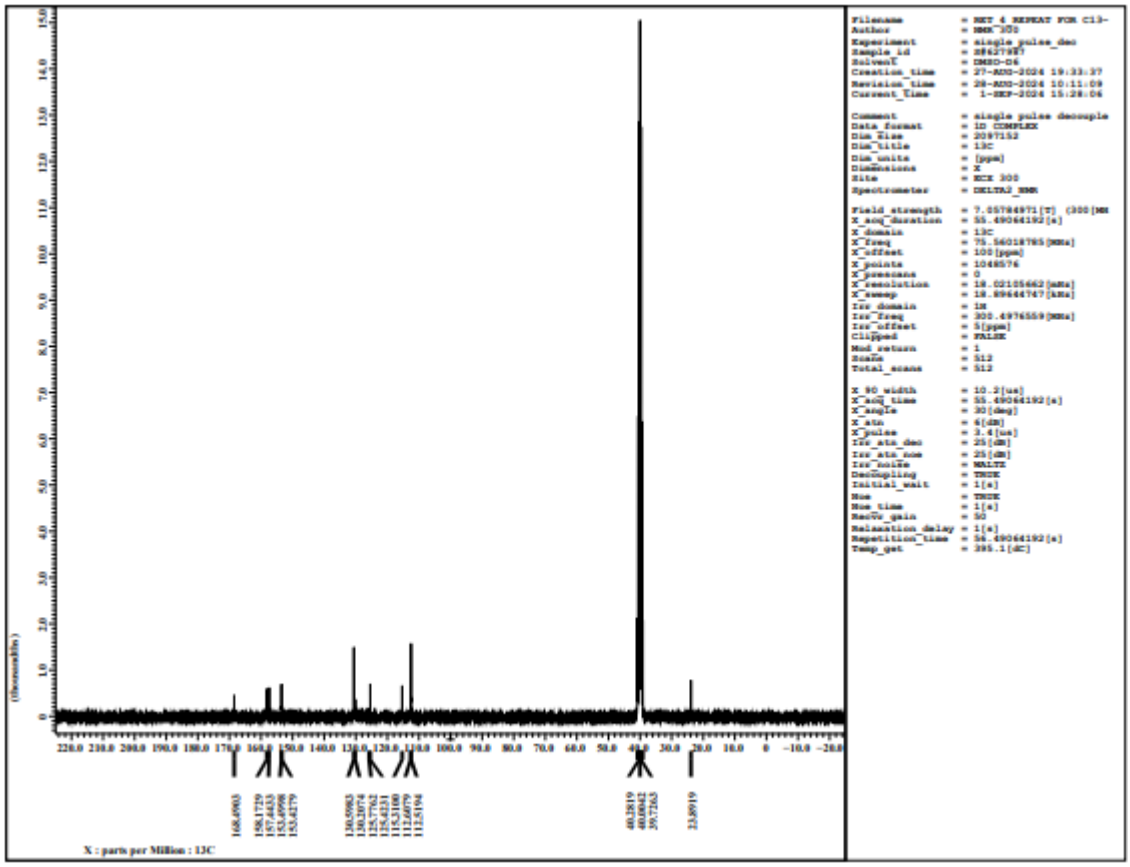

Fig. S8: ^{13}C-NMR spectrum of Compound L_2 showing the carbon atoms in different chemical environment.

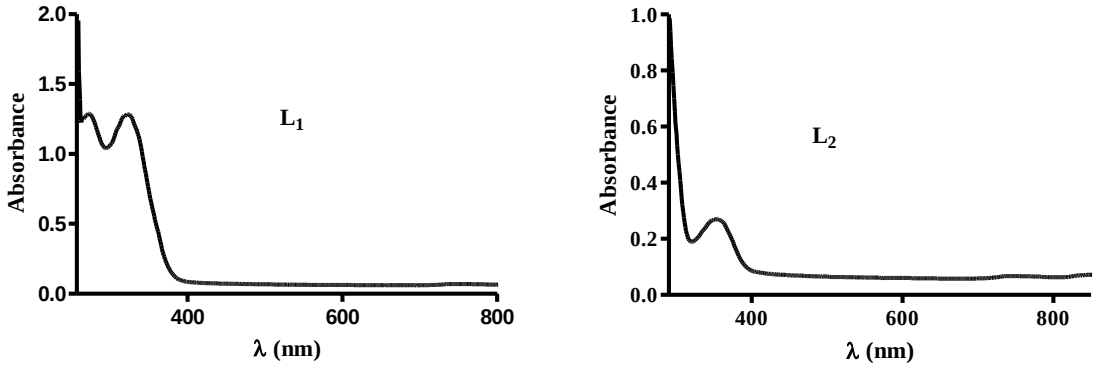

Fig. S_9: Electronic spectra showing the absorption bands for L_1 & L_2.

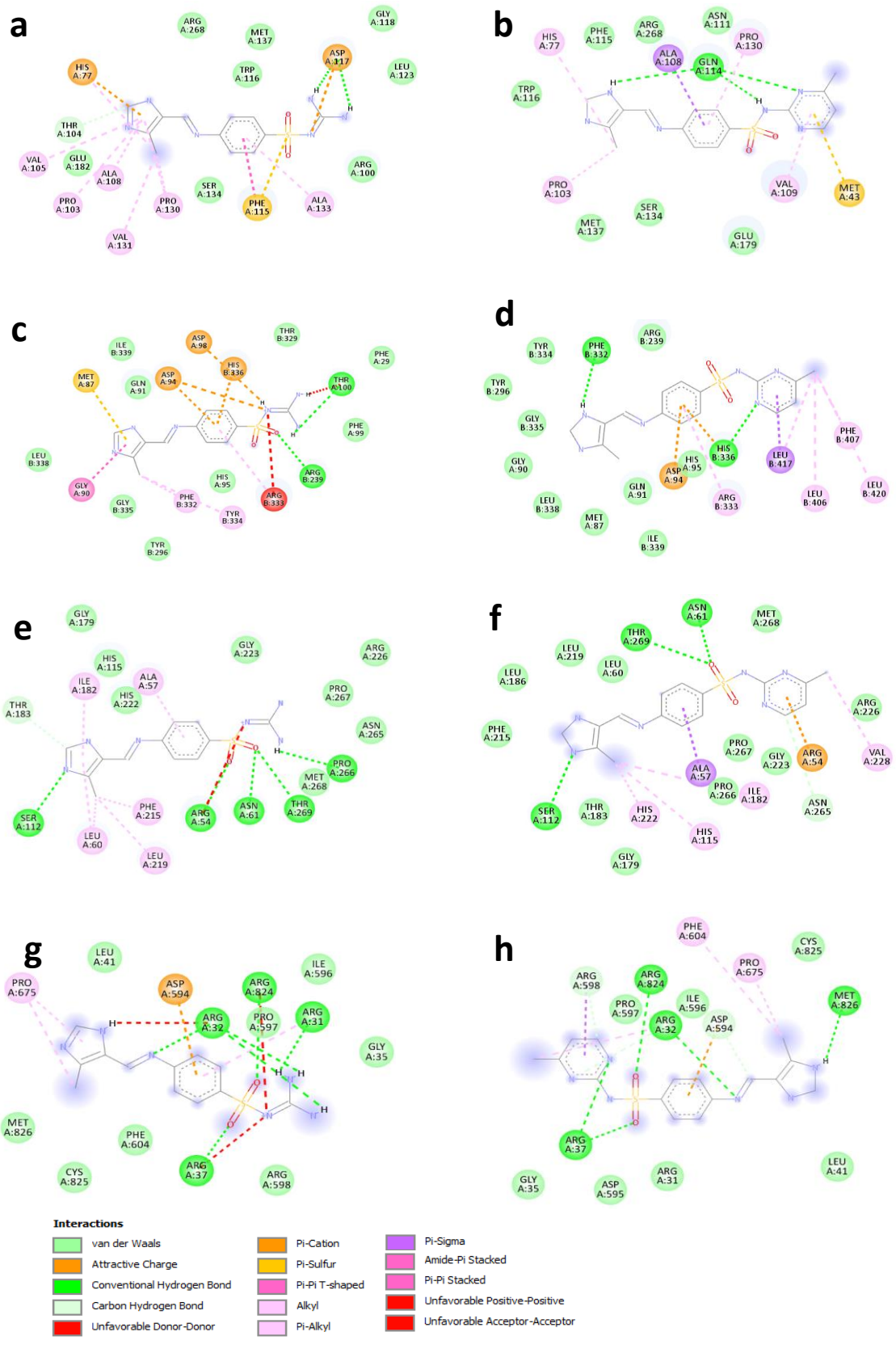

Fig. S_{10}. Binding interactions of compounds L1 and L2 with antimicrobial target enzymes: cytochrome peroxidase (PDB ID: 4AAO), myeloperoxidase (PDB ID: 6WY7), NADPH oxidase (PDB ID: 7U8G), and xanthine oxidase (PDB ID: 1N5X). Amino acid residues of each protein are represented as discs, while ligands L1 and L2 are depicted as lines. Intermolecular interactions are colored according to the type of interactions. (a) L1-4AAO (b) L2-4AAO (c) L1-6WY7 (d) L2-6WY7 (e) L1-7U8G (f) L2-7U8G (g) L1-1N5X and (h) L2-1N5X.

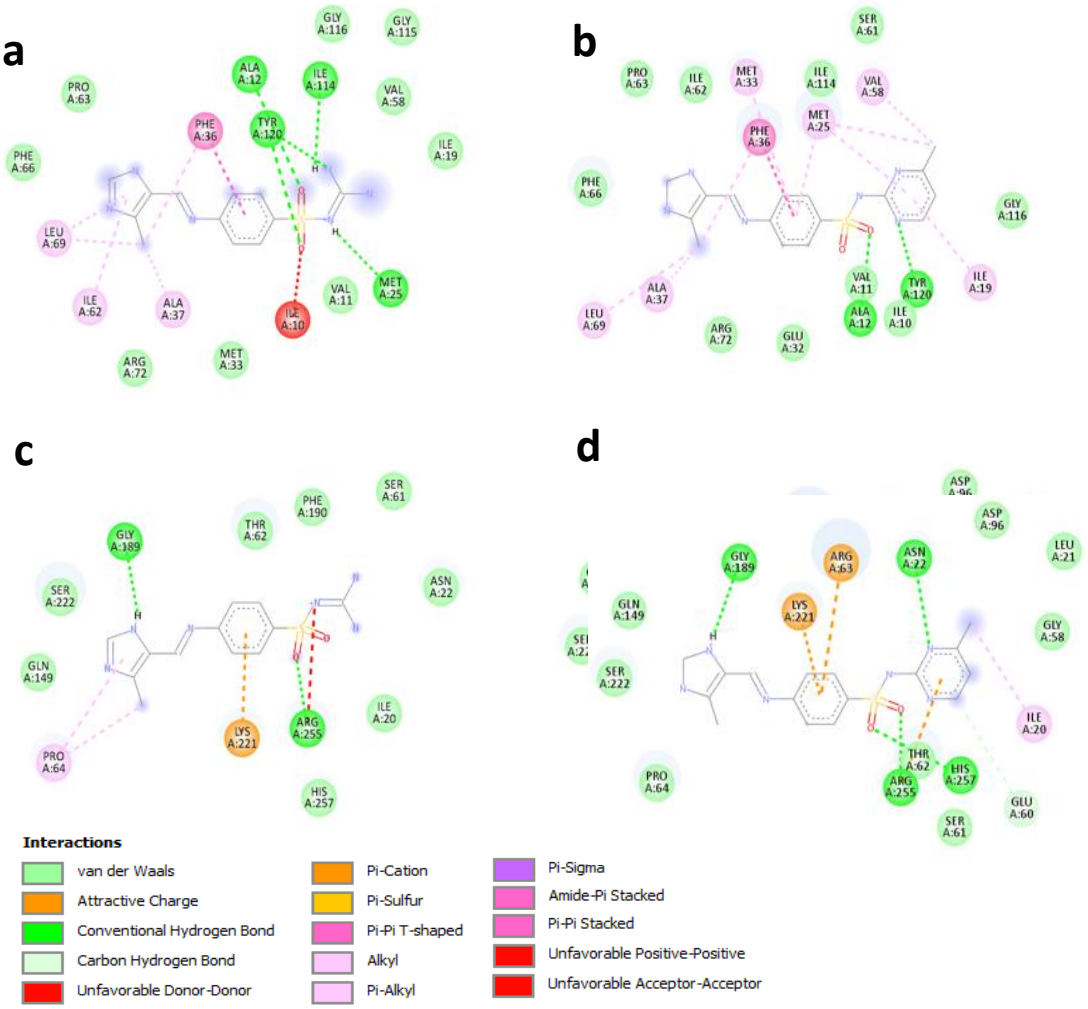

Fig. S_{11}: Binding interactions of compounds L1 and L2 with antioxidant target enzymes: DHFR (PDB ID: 4E4F) and DHPS (PDB ID: 5V7A). Amino acid residues of each protein are represented as discs, while ligands L1 and L2 are depicted as lines. Intermolecular interactions are colored according to the type of interactions. (a) L1-4E4F (b) L2-4E4F (c) L1-5V7A and (h) L2-5V7A.