MS14-P19 | SYNTHESIS, SPECTROSCOPIC PROPERTIES, CRYSTAL STRUCTURE, ANTIMICROBIAL PROPERTIES AND MOLECULAR DOCKING STUDIES OF THE COMPLEX (1) $3(C_{36}H_{24}MnN_6)$ $6(PF6)$ $0.5H_2O$

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The complex (1) of general formula $3(C_{36}H_{24}MnN_6)$ $.6(F_6P)$. $0.5H_2O$ was prepared and characterized by IR, UV-visible spectroscopy and single crystal X-ray structure analysis. The complex (1) is crystallized in the monoclinic system (z = 2) with space group of P 2/c, the unit cell parameters are a =15.1490(3) Å, b= 15.2154(2) Å, c = 23.1114(3) Å, b = 90.5152[1], and V = 5326.92 Å3. The asymmetric unit contains one and a half Manganese (II) complex (2) $[Mn(II)(C_{12}H_8N_2)_3]^{2+}$; one of the cations having crystallographic twofold rotational symmetry. Each Mn (II) is pseudo-octahedrally coordinated by three 1,10-phenanthroline molecules with Mn-N distances included between 1.96 and 1.99 Å. Besides, the intermolecular hydrogen bonds: C-H/F, C-H/O and π-π interactions are together playing a vital role in the stabilization of the crystal packing. In addition, the antibacterial activity of the complex (1) was evaluated against some bacterial species: Escherichia coli, Staphylococcus aureus, Klebsiella pneumonia, Bacillus Spp, Serratia marcescens, Acinetobacter Bounannue, Staphylococcus saprophiticus; and the antifungal activity against: Aaspergillus niger, Aspergillus spp, Aspergillus nidulans and Candida albicanse. Finally, the 1,10-phenanthroline was docked against various target proteins from diverse bacterial species 1E15 (S. marcescens), 3BU2 (S. saprophiticus), 3GFX (klipsila pnumani), 1BY3 (E. coli) and 5IDV (acinetobacter baumannii) to confirm those obtained results from antibacterial activity. In short, the results of synthesized complex (1) can be exploited in medical field.