

*Hydrogen bonding interaction of 4-AP metal complex with proteins*Lalitha Ponsankarar¹, A.Sinthiya¹, V.Rashmi²¹Physics And Srimad Andavan Arts And Science College, Trichy, India, ²Microbiology and Srimad Andavan Arts and Science College, Trichy, India

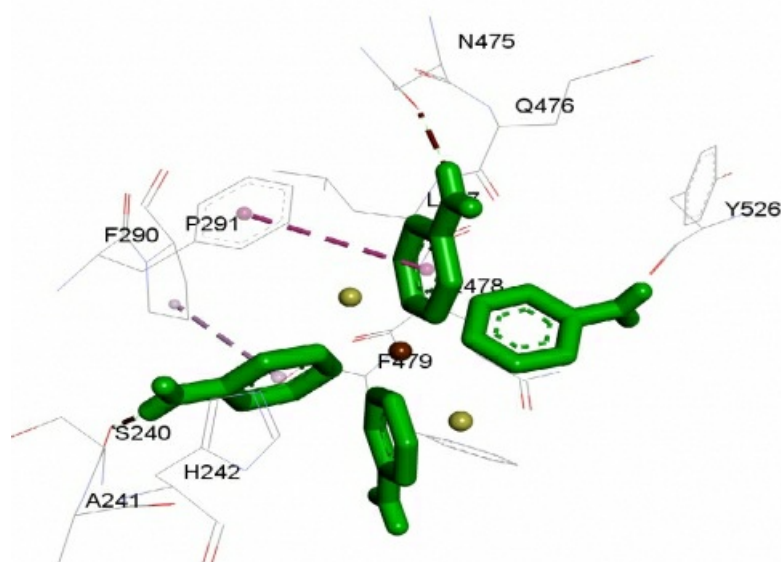
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The hydrogen bond occurred between the Tetrakis (4-aminopyridine- kN1) di chloride copper (II) monohydrate and Human Serine Racemase and Sphingosine 1-phosphate (S1P) lyase identified using molecular docking tool (Auto dock tools) to understand the drug-drug interaction. Based on the crystallographic structure of Tetrakis (4-aminopyridine- kN1) di chloride copper (II) monohydrate with enzyme and protein obtained using Auto dock tools and analysis through hirshfeld surface show that the Hydrogen bonding interaction is restricted by N-H...O hydrogen bonding and both the molecular structure show the hydrophilic interactions. Docked structure of S1P and HSR with ligand closely contact protein interactions of N....H....O and N-H...O hydrogen bonding shows on the complex function of hirshiefeld surface in molecular goemetry. It shapies relies on the interactions between Macromelecule of protein-ligand as well as atoms using crystal explorer The human serine racemase and the ligand interact through N(4-aminopyridine)-H...O(Serine) and N(4-aminopyridine)-H...O(Asparagine) hydrogen bonding with bond distance 2.05Å and 2.07Å respectively and the estimated Free Energy of Binding is -5.81 kcal/mol and estimated Inhibition Constant, Ki is 54.66 µM (micro molar) [Temperature = 298.15 K].The Sphingosine 1-phosphate (S1P) lyase and the ligand interact through N(4-aminopyridine)-H...O(Glutamine) and N(4-aminopyridine)-H...O(Valine) hydrogen bonding with bond distance 1.97Å and 1.91Å respectively and the estimated Free Energy of Binding is -5.32 kcal/mol and estimated Inhibition Constant, Ki is 126.74µM (micromolar) [Temperature = 298.15 K].The antibiotic sensitivity study of Tetrakis (4-aminopyridine- kN1) di chloride copper (II) monohydrate with the micro-organisms like Escherichia coli and Streptomycetes show that it has less antibiotic sensitivity with these microorganisms. These studies identify the possibilities of Tetrakis (4-aminopyridine- kN1) di chloride copper (II) monohydrate to act as drug with required changes in its molecular structure. These analysis are recently application of inhibitory action of therapeutic target for treatment of Multiple Sceloris(MS). 4-Aminopyridine metal complex increase neurological effects in pottasium(K+) channel blockade. In the field of antineoplastic drug development the transition metals are dynamic in electron affinity, reactivity and geometry . For the drug chemist the usage of transition metals act as a effective tool to develop and study molecules - drug interactions.

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