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Molecular Decoding drug molecule mutant protein Periphilin -1 Blood Cancer through Molecular Docking

INTRODUCTION

- Blood cancer remains a formidable challenge, with periphilin-1 emerging as a key mutant protein target. Molecular docking provides a promising avenue for understanding drug molecule interactions with periphilin-1
- Periphilin-1's role in blood cancer underscores the need for precise molecular insights. Molecular docking simulates drug-protein interactions, revealing binding affinity and mode of action.
- Understanding periphilin-1's structure and function is vital. Mutations in periphilin-1 disrupt cellular processes, driving cancer progression. Docking elucidates how drug molecules interact with mutant periphilin-1, aiding drug design.
- Docking facilitates screening and evaluation of drug candidates. By analyzing binding patterns, researchers identify compounds to modulate periphilin-1 activity and inhibit cancer.
- Innovative approaches offer hope in blood cancer research. Molecular docking, coupled with multidisciplinary efforts, promises effective therapies for patients.

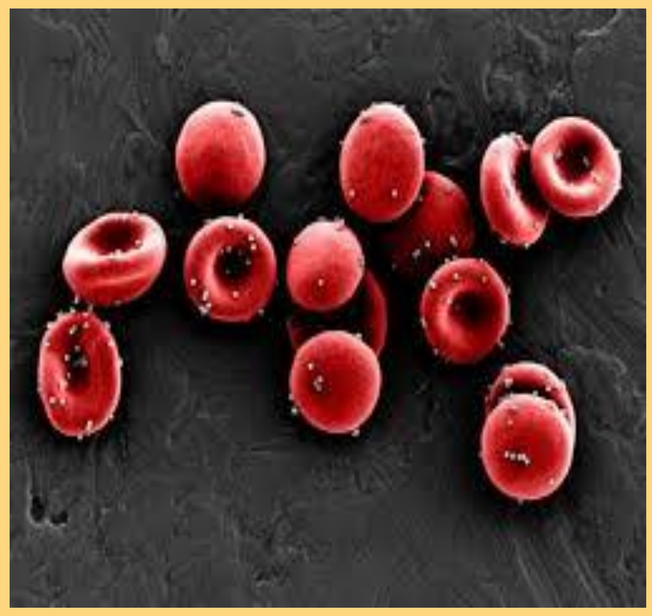
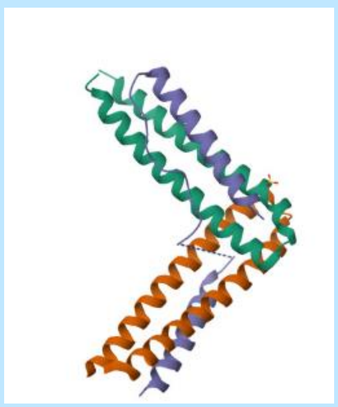
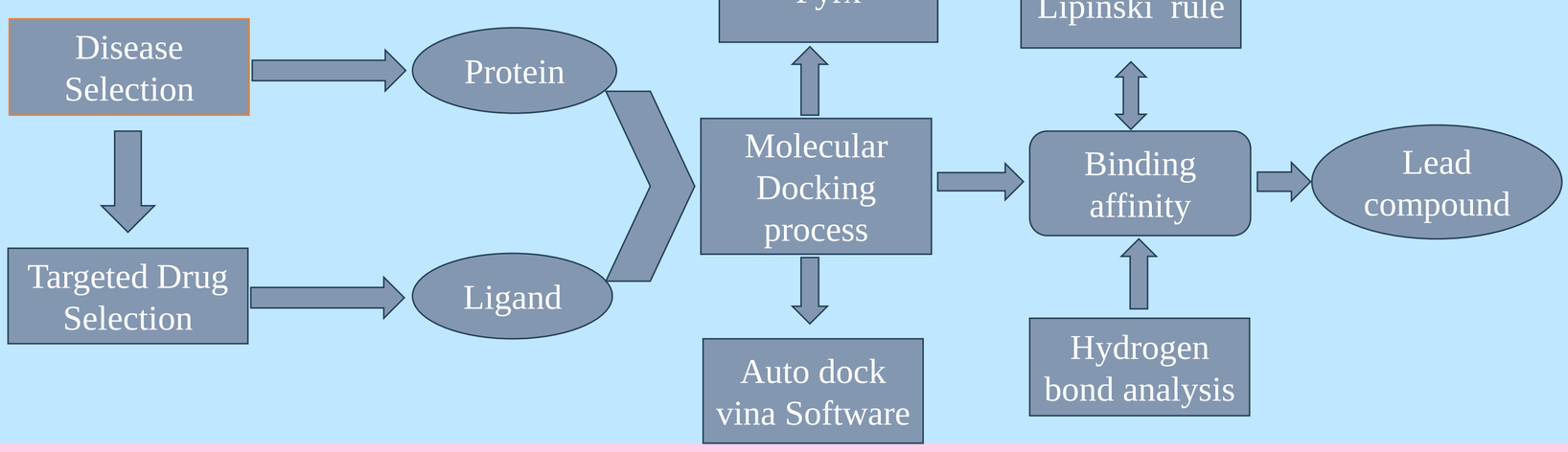


Fig. 1. RBC Blood Cancer Cells

MATERIALS AND METHODS



Periphilin-1



Drug Molecule

RESULTS

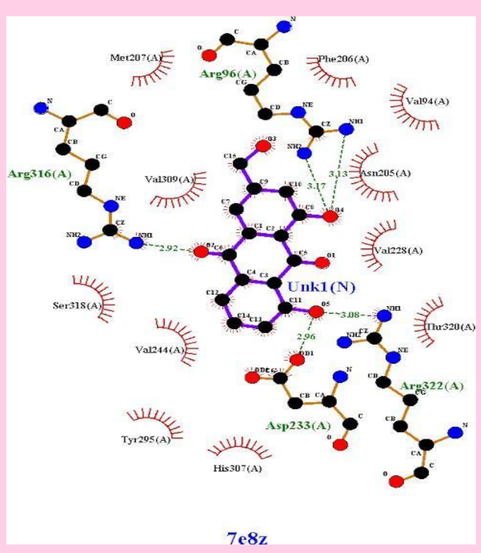


Fig. 2. LIGPLOT

Table 1. LIGPLOT .hhb output

Donor			Acceptor			Distance
SER A	167	OG	UNK	0	01	33.97
GLN A	72	ND2	UNK	1	06	4.07
ASN A	1854	N	UNK	1	03	4.37
UNK	1	06	TYR A	1787	0	3.12
UNK	1	04	TYR A	1787	0	4.09
UNK	1	04	ASN A	1771	OD1	3.03

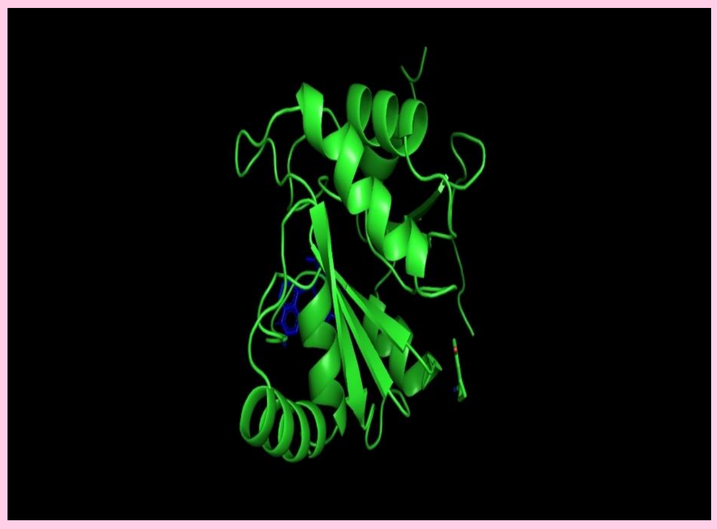


Fig. 3. Protein-ligand interaction in PYMOL

Hydrogen bond analysis through LIGPLOT software and visualization of protein-ligand interaction using PYMOL software.

DISCUSSION AND CONCLUSION

- The binding affinity and specificity of ligands to proteins rely significantly on hydrogen bonds, crucial for molecular recognition. Interactions between hydrogen atoms and electronegative atoms like oxygen or nitrogen play pivotal roles.
- Various forms of interactions, including hydrogen bonding, hydrophobic interactions, and electrostatic interactions, shape ligand-protein binding. Examples include:
  - ❑ - A score of -8.0 with 9 hydrogen bonds.
  - ❑ - A score of -8.6 with 10 hydrogen bonds.
- The PubChem coordinate type of ligand is 8,11,13. Lipinski's rule of 5 properties retrieved from ADMET LAB 2.0 guide ligand selection.
- Using molecular docking, the ligand scoring -8.0 shows promise in targeting 5Y6J for treating fusarium wilt in plants. However, further experimental validation is essential to confirm its therapeutic potential.

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