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Molecular Decoding drug molecule mutant Protein FAM168A on Blood Cancer through molecular docking

INTRODUCTION

- FAM168A, a mutant protein associated with blood cancer, presents a formidable challenge in drug development. Molecular docking provides essential insights into how drug molecules interact with FAM168A, guiding targeted therapy design.
- Understanding the structure and function of FAM168A is crucial, as its mutations drive cancer progression. Molecular docking reveals precise interactions between drugs and mutant FAM168A, aiding in therapeutic development.
- Through molecular docking, researchers screen and evaluate drug candidates, identifying compounds capable of modulating FAM168A activity to inhibit cancer growth.
- Interdisciplinary collaboration among molecular biologists, computational biologists, and biotechnologists is vital for translating research into effective treatments for blood cancer patients.
- Innovative approaches like molecular docking, combined with interdisciplinary efforts, offer hope for improved therapies in blood cancer research.

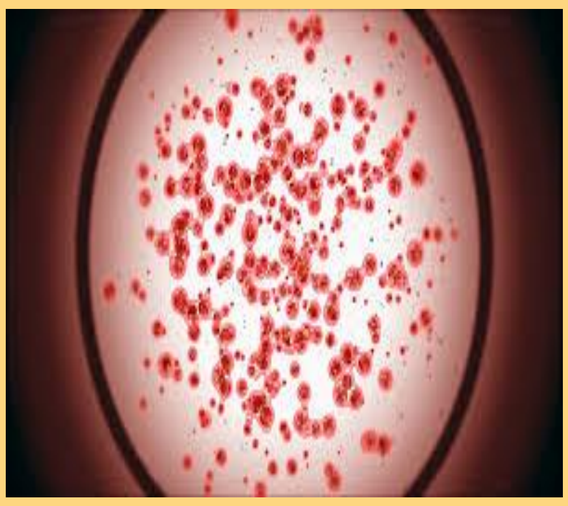
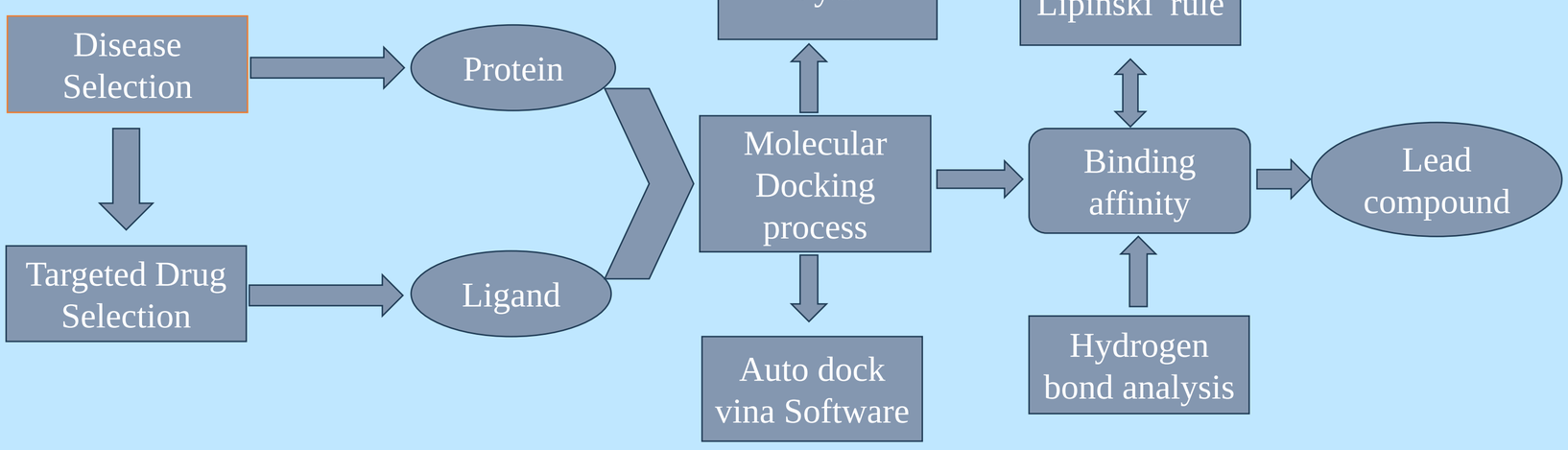


Fig. 1 RBC Blood Cancer Cells

MATERIALS AND METHODS

FAM 168A



Drug Molecule

RESULTS

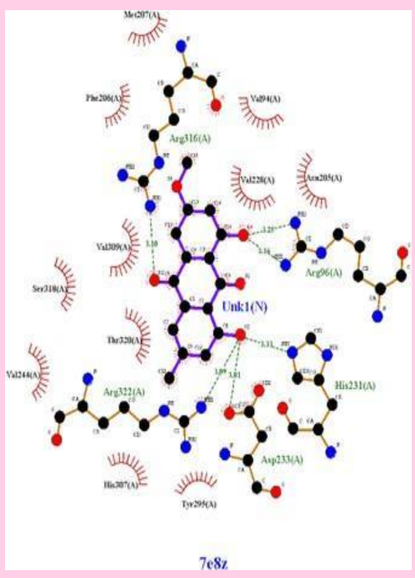


Fig.2 LIGPLOT

Table .1 LIGPLOT .hhb output

Donor			Acceptor			Distance
SER A	171	OG	UNK	0	01	32.179
GLN A	69	ND2	UNK	1	06	3.87
ASN A	1771	N	UNK	1	03	4.12
UNK	1	06	TYR A	1697	0	3.91
UNK	1	04	TYR A	1697	0	4.67
UNK	1	04	ASN A	1665	OD1	3.33

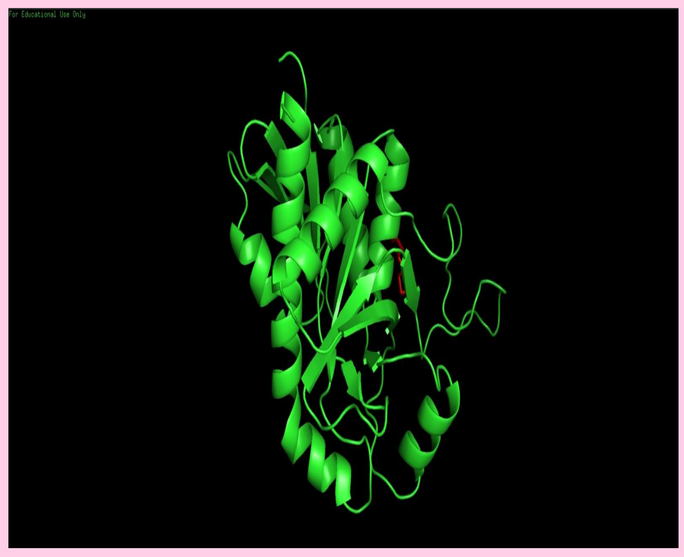


Fig.3 protein-ligand interaction in PYMOL

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

DISCUSSION AND CONCLUSION

- The effectiveness of ligands in binding to proteins hinges significantly on hydrogen bonds, pivotal for molecular recognition. Interactions between hydrogen atoms and electronegative atoms such as oxygen or nitrogen are central to this process.
- Various types of interactions, including hydrogen bonding, hydrophobic interactions, electrostatic interactions, contribute to shaping ligand-protein binding. For instance:
  - ❑ - A ligand scoring -8.0 exhibits 9 hydrogen bonds.
  - ❑ - Another ligand scoring -8.6 forms 10 hydrogen bonds.
- The PubChem coordinate type of ligand is specified as 8,11,13. Lipinski's rule of 5 properties, retrieved from ADMET LAB 2.0, guides the selection of ligands.
- Using molecular docking, the ligand scoring -8.0 demonstrates promise in targeting the mutant protein FAM168A for potential treatment of blood cancer. However, further experimental validation is imperative to ascertain its therapeutic efficacy.

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