REPORT ON

BASICS OF MOLECULAR DOCKING

The workshop aimed to introduce final year B. Pharmacy students to the "Basics of Molecular Docking and its transformative impact on drug discovery". Vishwanadham Yerragunta, Associate Professor at the School of Pharmacy, conducted the session, sharing his expertise on the topic and discussing its practical applications in pharmaceutical research on 01.02.2024 in Seminar Hall, NNRG School of Pharmacy.

Overview

1. **Introduction to Molecular Docking**
   - **Definition:** Molecular Docking is a method used to predict the interaction between a drug and its target protein.
   - **Importance:** It plays a crucial role in the early stages of drug discovery by helping scientists understand how drugs bind to their targets and predicting the efficacy of new compounds.
2. **Principles of Molecular Docking**
   - **Binding Affinity:** The strength of the interaction between the drug and its target.
   - **Scoring Functions:** Algorithms used to predict the binding affinity of a drug to its target.
   - **Docking Algorithms:** Techniques to explore the conformational space and predict the optimal binding pose.
3. **Applications in Drug Discovery**
   - **Lead Identification:** Finding potential drug candidates from a large pool of compounds.
   - **Lead Optimization:** Refining the chemical structure of drug candidates to improve their binding affinity and pharmacokinetic properties.
   - **Virtual Screening:** Using computational methods to screen large libraries of compounds quickly.
4. **Case Studies**
   - **Real-World Examples:** Discussion of successful applications of Molecular Docking in identifying new drug candidates.
   - **Challenges:** Addressed the limitations and challenges in Molecular Docking, such as accuracy of predictions and computational costs.
5. **Hands-On Demonstration**
   - **Software Tools:** Introduction to popular Molecular Docking software like AutoDock, GOLD, and Schrödinger.
   - **Practical Session:** A live demonstration on setting up a Molecular Docking experiment, including preparing the target protein and ligand, running the docking simulation, and interpreting the results.

Students were given the opportunity to ask questions regarding the concepts and applications of Molecular Docking.

- **Discussion Highlights:**
  - **Software Accessibility:** Queries about free vs. commercial software for Molecular Docking.
  - **Career Opportunities:** Questions about careers in computational drug discovery and necessary skills.

Positive Aspects:

- The workshop provided a comprehensive introduction to Molecular Docking.
- Students appreciated the practical demonstration and hands-on approach.
- The session highlighted the relevance of Molecular Docking in modern drug discovery.

Suggestions for Improvement:

- More in-depth coverage of specific software tools and their features.
- Additional time for hands-on practice and exploration of advanced topics.

Conclusion

The workshop on "Basics of Molecular Docking" successfully introduced final year B. Pharmacy students to the fundamental concepts and applications of Molecular Docking in drug discovery. It provided valuable insights and practical knowledge, equipping students with an understanding of this critical technology.

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