Workshop
on
In Silico Adventure in Natural Medicine - A Hands-on for Molecular Docking for Evidence-Based Approaches
(13-03-2024 to 16-03-2024)

The PG Department of Chemistry organized a four-day workshop titled "In Silico Adventure in Natural Medicine: A Hands-On Workshop for Molecular Docking for Evidence-Based Approaches" from 13-03-2024 to 16-03-2024 at MCA Lab

This workshop was specifically designed for MSc Organic and Analytical Chemistry students to provide them with practical skills in molecular docking and demonstrate its applications in natural medicine research.

Objectives:

1. To provide an introduction to molecular docking and its significance in natural medicine.

2. To offer hands-on training in using molecular docking software.

3. To explore evidence-based approaches for identifying bioactive compounds in natural products.

4. To facilitate knowledge sharing and collaboration among participants.

Sessions and Activities

Session 1: Introduction to Molecular Docking

The workshop began with an introductory lecture by Sri G.Gnasna Bhaskar G.S Phyto labs an expert in bioinformatics and molecular docking.

He provided an overview of molecular docking, explaining its principles, methodologies, and importance in drug discovery.

The session covered key topics such as the interaction between ligands and receptors, scoring functions, and the use of docking to predict the binding affinity of natural compounds.

Session 2: Software Tools and Setup

In this session, participants were introduced to various molecular docking software tools, including AutoDock, PyRx, and Vina.

Sri G.Gnasna Bhaskar provided a step-by-step guide on how to install and configure these tools, ensuring that all participants had the necessary software setup on their laptops.

Session 3: Hands-On Molecular Docking Exercise

Participants engaged in a hands-on exercise where they performed molecular docking experiments using a provided dataset of natural compounds and target proteins.

Under the guidance of Sri G.Gnasna Bhaskar and a team of assistants, attendees learned how to prepare ligand and receptor files, run docking simulations, and interpret the results. This practical session emphasized the importance of accuracy and reproducibility in molecular docking studies.

Session 4: Case Studies and Applications

Several case studies were presented to demonstrate the application of molecular docking in natural medicine research:

This session focused on the analysis and interpretation of docking results.

Sir explained how to evaluate binding affinities, visualize docking poses, and validate docking predictions. Participants were encouraged to discuss their findings and troubleshoot any issues encountered during the practical exercises.

The "In Silico Adventure in Natural Medicine: A Hands-On Workshop for Molecular Docking for Evidence-Based Approaches" was a successful event that equipped participants with valuable skills and knowledge in molecular

docking. The hands-on exercises and case studies demonstrated the potential of in silico methods to advance natural medicine research. Participants left with a deeper understanding of molecular docking and its applications, ready to apply these techniques in their own research endeavors.

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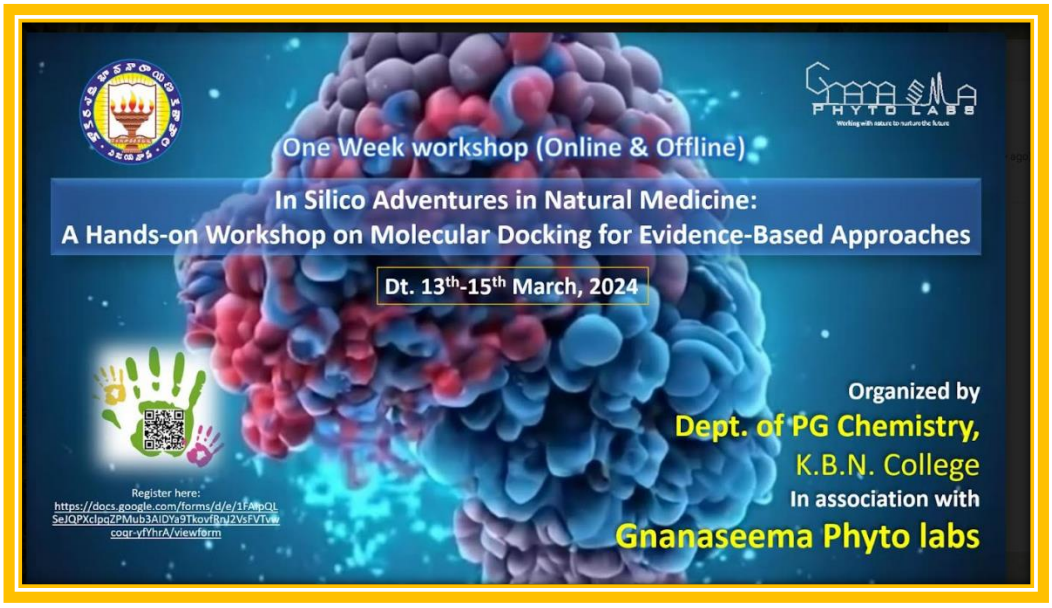


In Silico
Hands-on Workshop
KBN College,
Phyto labs