DEPARTMENT OF PHARMACEUTICAL CHEMISTRY

"Molecular Properties Prediction Softwares: A Primer for Researchers"

Date of Seminar: 10th January 2025

Time: 3:00 PM

Target Audience: B.Pharm IIIrd Year Students

Venue: SNVPMV -Auditorium

Objective of the Seminar:

The primary objective of the seminar was to provide an introduction and hands-on understanding of various molecular properties prediction softwares, an essential tool for researchers in the field of pharmaceutical chemistry. Dr. K. Vinuta, Associate Professor, conducted the session, highlighting key software used in molecular modeling, as well as their applications and significance in pharmaceutical research.

Session Overview:

The seminar began at 3:00 PM with Dr. K. Vinuta welcoming the students and faculty members. She provided an overview of the importance of molecular property prediction in research, particularly in drug design and development. Dr. Vinuta discussed the underlying principles of molecular modeling, software tools available for property prediction, and their practical uses in the research setting.

Key topics covered included:

- Introduction to molecular properties prediction
- Overview of popular molecular modeling software (e.g., ChemDraw, Spartan, AutoDock, Gaussian)
- Application of prediction tools in drug design, ADMET studies, and QSAR modeling
- Step-by-step demonstration of software tools for various molecular predictions

Dr. Vinuta also emphasized the role of computational chemistry in modern pharmaceutical research and how such software can enhance the efficiency of researchers in evaluating molecular behavior, solubility, toxicity, and other critical properties.

Key Learning Outcomes:

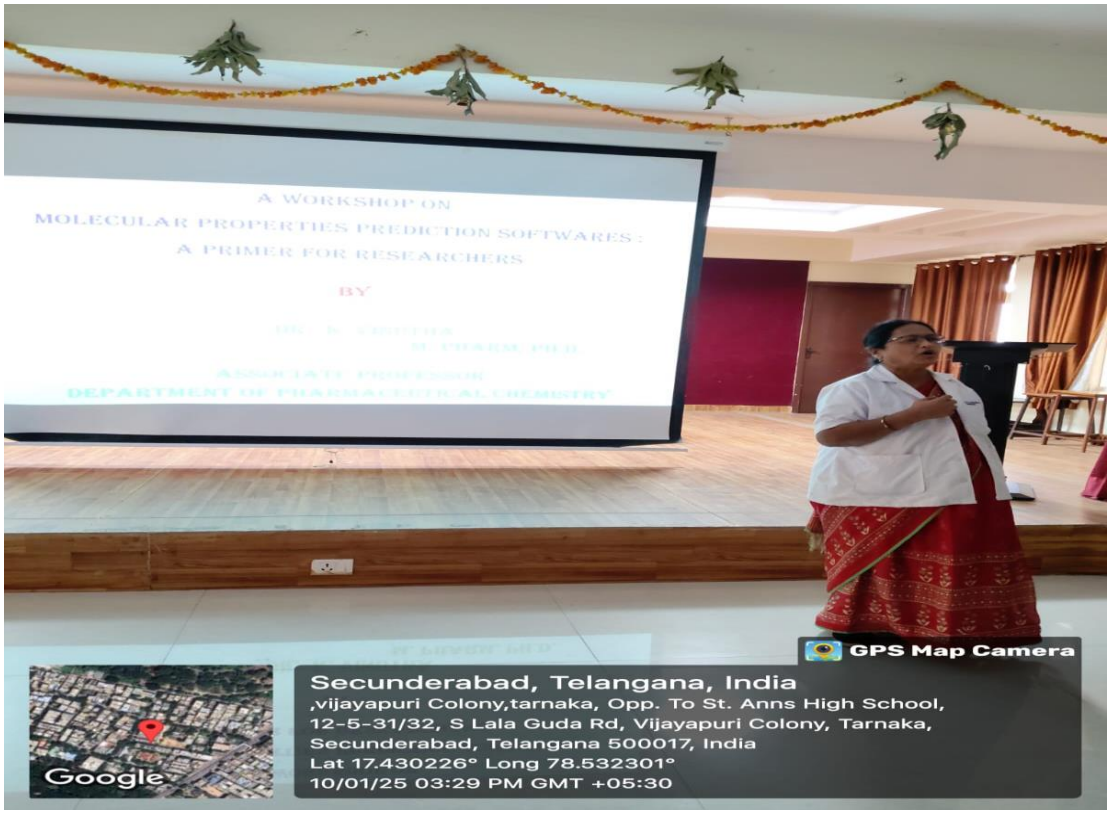
- **In-depth Knowledge:** Students gained significant insight into molecular property prediction, including the practical use of computational tools in drug research.
- **Hands-On Experience:** A detailed demonstration helped students familiarize themselves with the functionalities of the software.
- **Research Application:** Students were able to grasp the connection between theoretical chemistry concepts and practical, real-world applications in pharmaceutical research.

Faculty Involvement:

- **Dr. S. Hemalatha** and **Mrs. P. Kavitha** were present during the seminar and contributed to the discussion by answering students' queries and providing additional perspectives on the use of computational tools in research.

Conclusion:

The seminar proved to be highly beneficial for the B.Pharm IIIrd-year students, enhancing their understanding of molecular property prediction softwares and their role in pharmaceutical research. The students left with valuable knowledge that will aid them in their academic and research pursuits, and the session received positive feedback from the attendees.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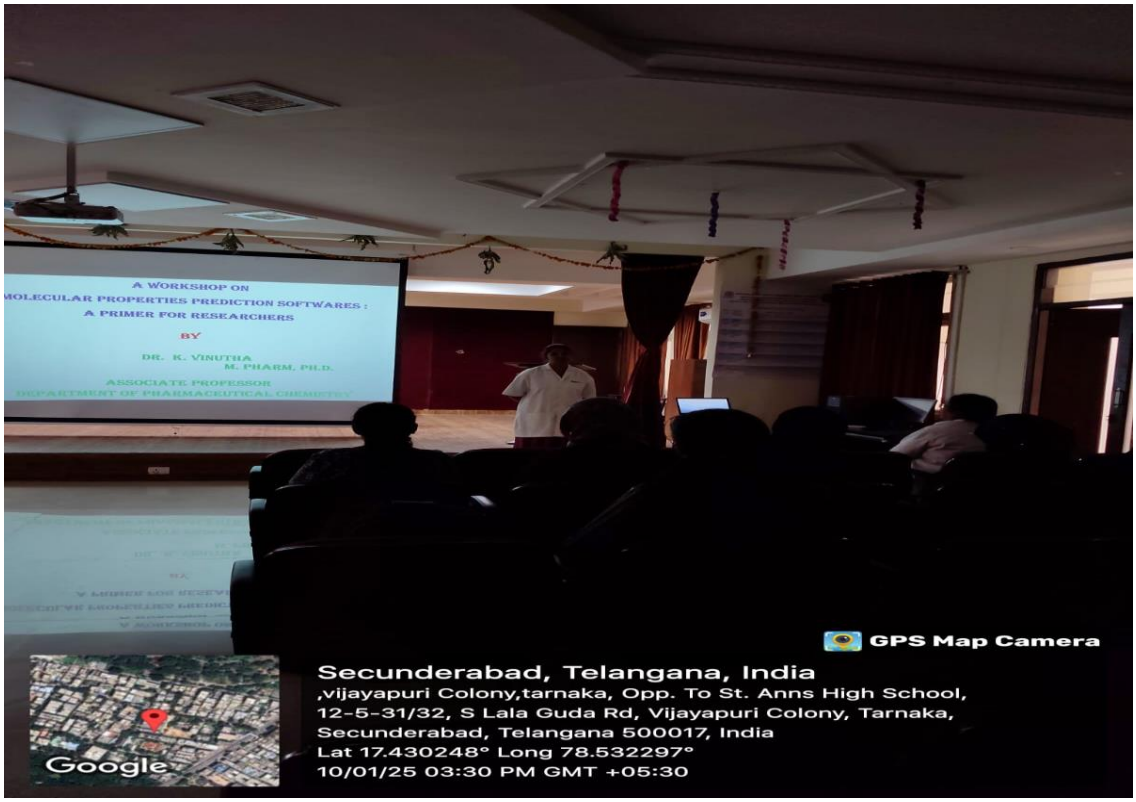
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