Date/Day*:* 7 August 2025 (Thursday)

Title: Workshop on Application of Molsoft software for Molecular modelling, Docking and Virtual screening

Organized by: Department of Pharmaceutical Chemistry. The event was coordinated by Ms.Rachel Britto, Ms. Sayli Sawant, Ms. Shenaz Saksena, Dr. I. Ramya and Mr. Prathmesh.

Objectives:

1. To familiarize with the Molsoft ICM software interface and tools
2. To enhance understanding of structure-activity relationships (SAR)
3. To demonstrate how to dock ligands into target proteins and interpret binding interactions and scoring.

Program Outcome: PO1, PO2, PO6, PO8, PO9, PO11.

Resource Person: The speaker of the session was Dr. Shamshair Singh Sardar, Senior Application Scientist, Advent Informatics Pvt. Ltd.

Participant details*:*

Total no. of college students: 8 0

Total no. of Faculty: 06

Summary of the activity

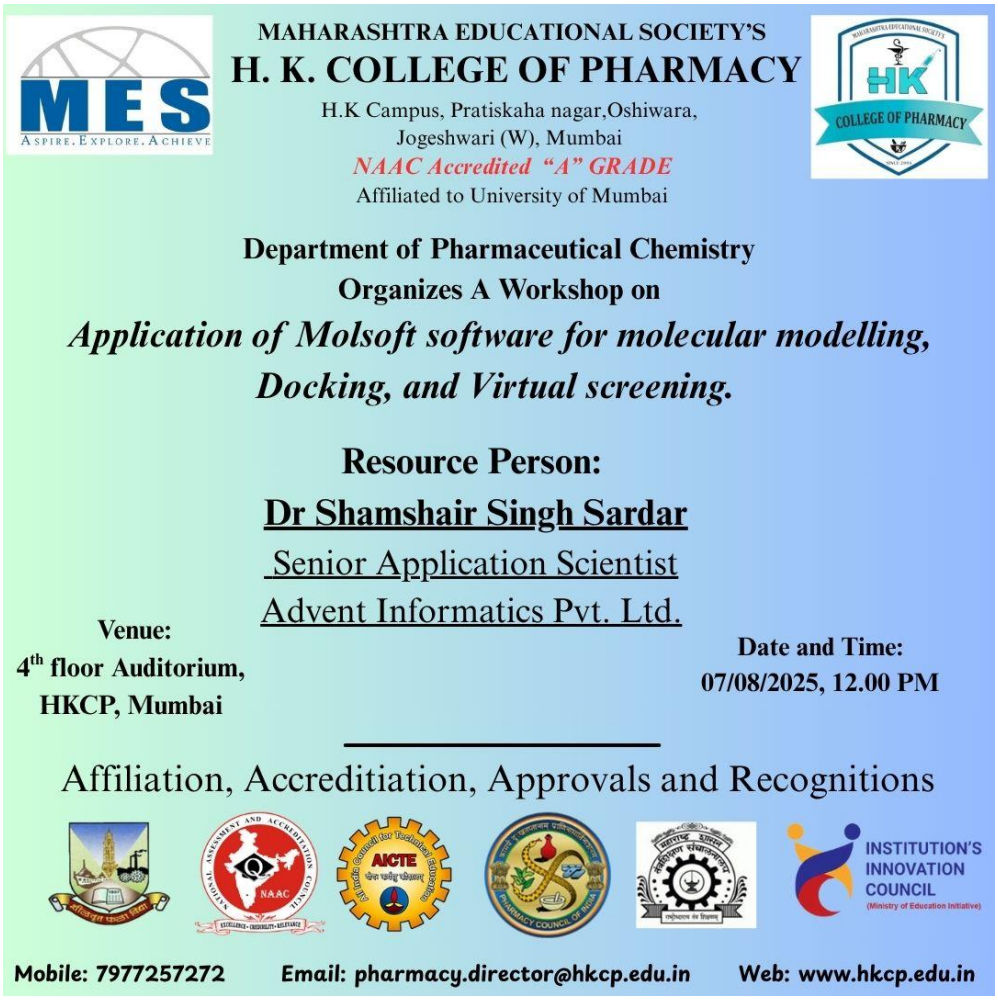
On 7thAugust 2025, Department of Pharmaceutical Chemistry, Humera Khan College of Pharmacy, in collaboration with Dr. Shamshair Singh Sardar, Senior Application Scientist, Advent Informatics Pvt. Ltd. Organized a workshop on Application of Molsoft software.

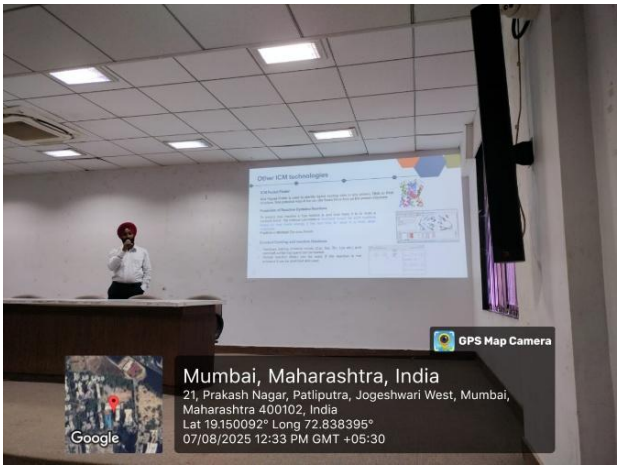
The speaker Dr. Shamshair Singh Sardar provided an in-depth overview of Molsoft's ICM (Internal Coordinate Mechanics) software, highlighting its powerful capabilities in molecular modeling, docking, and virtual screening. He emphasized academic and commercial collaborations that have led to impactful drug discovery projects and shared notable success stories where ICM software has contributed to high-impact publications, including in Nature.

Atomic Property Fields (APF) for pharmacophore modeling and ligand-based screening, RTCNN score for enhanced docking accuracy using deep learning and induced fit docking and 4D docking for accounting for receptor flexibility were some of the key points discussed by the presenter.

Dr. Shamshair highlighted the importance of SCARE method for generating receptor conformations and use of Fast Fourier Transform (FFT) in molecular alignment. He accentuated the implementation of tools like Optimal Docking Area (ODA) to identify favorable docking regions and ICM Pocket Finder, for detecting potential binding sites on protein surfaces.

Brochure/ Photo gallery:





Key outcome of the activity:

1. Participants gained insights into how ICM's integrated tools support advanced modeling workflows, from binding site prediction to virtual screening, making it an asset in both academic research and industrial drug discovery**.**
2. The workshop also highlighted real-world applications and success stories, enhancing students' ability to apply these tools in academic research.
3. The workshop highlighted Molsoft's role in antibody design and its performance in benchmarks with Pfizer, demonstrating the software's reliability and success in both academic and industrial settings.

Link for social media:

LinkedIn:	https://www.linkedin.com/posts/h-k-college-of-pharmacy-mumbai-303524222_a-workshop-was-organized-by-department-of-activity-7359791662140637185-zEKI?utm_source=share&utm_medium=member_desktop&rcm=ACoAADf2WrMBUFgAeZVznddoMfc3VtpDnyqdS4Y
Facebook:	https://www.facebook.com/photo/?fbid=1224267386379568&set=a.470185965121051

Instagram:	https://www.instagram.com/p/DNHplztIxOT/?utm_source=ig_web_copy_link&igsh=MzRlODBiNWFlZA==

Prepared by	**IQAC coordinator**	**Principle**
Dr. I.Ramya	Dr. Archana Upadhya	Dr. Tushar N. Lokhande

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