

## ROFEL SHRI G.M. BILAKHIA COLLEGE OF PHARMACY

APPROVED BY PHARMACY COUNCIL OF INDIA (PCI) AND AFFILIATED TO GUJARAT TECHNOLOGICAL UNIVERSITY, AHMEDABAD

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## REPORT OF GUEST/EXTENSION LECTURE

**Title of Guest Lecture (Webinar):** Molecular Docking: A powerful approach for structure based drug discovery.

Speaker: Mrs. Jagruti Thakor, Academician, M.Pharm in Medicinal Chemistry.

Date & Venue: 20<sup>th</sup> June, 2022 on virtual platform through Google meet

No of Participants: 238

## **Summary Report:**

Mrs. Jagruti gave detailed concepts on new drug design along with the quantitative structural activity relationship. She explained about relationship between structural features of the compound and molecular response based on the experimental data. Mrs. Jagruti also explained the application of QSAR on drug design along with examples. Mrs. Jagruti had given an idea about the molecular ligand binding on the active site of the stable complex or receptor. He explained the change in configuration to give the proposed action. Mrs. Jagruti gave information about key and lock mechanism for molecular docking. She also covered the types of docking, types of interactions and different stages of docking. She also explained various examples to understand molecular docking process and how computer aided drug design becomes vital tool in drug discovery. Mrs. Jagruti explained all the vital fundamentals regarding the Molecular Docking to participants.



(Mrs. Jagruti Thakor delivered a session on Molecular Docking in drug discovery-2022)