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ROFEL SHRI G.M. BILAKHIA COLLEGE OF PHARMACY

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ROFEL NAMDHA CAMPUS, Vapi-Namdha Road, P.B. No. 11, Vapi (West) - 396191, Dist.- Valsad (Gujarat)

Tel: 9727723722 | 42 | 62; Email: rofelpharm@gmail.com; website: www.rofelpharmacy.ac.in

REPORT ON GUEST / EXTENSION LECTURE

Title of Guest Lecture (Webinar): Computational methods in Drug Design and Discovery Process

Speaker: Dr. Ashish Shah, Associate Professor, Sumandeep Vidyapeeth, Gujarat

Date & Venue: 31st July 2021, virtual platform

Coordinator: Dr. Ankit Merai, Associate Professor

Summary Report:

Dr. Ashish gave detailed concepts on computational methods in drug design and discovery process. He explained about pharmacophore and pharmacophore based drug design. Dr. Ashish also explained the protein ligand docking with examples. Dr. Ashish had given an idea about the classification of computer added drug delivery and he explained briefly about ligand and structural based design, He highlighted the types of CADD techniques used in drug discovery. Dr. Ashish explained the various strategies of molecular binding with ligand. He gave detailed information about the QSAR and its applications.

Classification of CADD

CADD can be classified into two general categories:

- Ligand-based**
Ligand-based CADD exploits the knowledge of known active and inactive molecules through
 - chemical similarity searches
 - construction of predictive, quantitative structure-activity relation (QSAR) models.
- Structure-based**
Structure-based CADD relies on the knowledge of the target protein structure to select compounds based on their binding energies.

Ligand-Based Drug Design Structure-Based Drug Design

Construction of a QSAR model that predicts biologic activity from chemical structure

Set of Compounds

Activity Data (Y) Molecular Descriptors (X_i)

QSAR
 $Y = f(X_i)$

Prediction Interpretation

Session Proceedings and content delivery by Dr. Ashish Shah

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