REPORT ON HAND-ON WORKSHOP ON "COMPUTER AIDED DRUG DESIGN"

Two days hands on workshop on "Computer aided drug designing"(CADD) was organized by the department of Biochemistry of Maharani Lakshmi Ammanni College for women, autonomous, Bangalore, for 25 students of III year CZM students of mLAC to enhance the skill sets of drug discovery

The workshop was held on 3rd and 4th May 2021 on online mode using Google meet platform. The focus of the workshop was to provide an insight on the recent advances CADD and to explore its possible diverse application in various research areas.

The conference was inaugurated by welcoming all the participants and invited speakers to the virtual conference by **Dr.Kamala,** Associate professor, HOD, Department of Biochemistry. A formal welcome address was delivered by **Dr. Shashikala A**, Principal, mLAC, a brief introduction about the Department of Biochemistry was presented by Dr. Kamala A, Associate professor, HOD, Department of Biochemistry and the inaugural address was delivered by **Dr. Girinath Pillai,** Senior Research scientist, Zastra Innovations Pvt Ltd Chief Guest, delivered the keynote address on the theme of the conference and highlighted the complete process of CADD.

The first technical session began at 10.05 am with a talk on "**Insights into Molecular Docking**" by **Dr. Girinath Pillai.** He started with an overview of Drug discovery and gave detailed information regarding the various stages, loopholes, and development in CADD. His talk was very informative. He also clarified the queries of the students regarding additional courses to be taken up UG students to enhance their skill sets.

The second technical session and hand-on session started at 11.00 am with lecture on "**Identification of a cellular target**" by **Ms.Usha.T,** Associate professor, Department of Biochemistry. Her talk was focused on how to identify a biological protein or DNA target for Drug discovery process followed by practical session for the same.

The post lunch technical session started with a lecture on "**Small molecules in Molecular docking and determining their drug likeliness**" by **Dr. Sushil kumar Middha**, Associate professor, Department of Biotechnology at 1.30. Followed by a session on "Retrieval of 3D structure of protein and understanding its properties" by Dr. Sushil kumar Middha, Associate professor, Department of Biotechnology mLAC

The second day of the workshop started with third technical session started at 09.40 am with lecture on "**Types of Docking**" by **Dr. Vivekchandramohan**, Associate professor, SIT. His talk was focused on various types of docking, software. Followed by a practical session by **Mr. Avijeeth Maity**, Research Associate, Bangalore university at 10.50

The second technical session and handon session started at 12.45pm post lunch with lecture on "**Homology modelling**" by **Ms.Usha.T,** Associate professor, Department of Biochemistry. Followed by practical session Building of 3D structure of protein using swiss PDB modeler.

Final session was at 4.00 pm by **Dr. Sushil kumar Middha**, Associate professor, Department of Biotechnology on "**Molecular Docking- Dissecting research papers**" to brief about how the

knowledge obtained through the two day workshop can be utilized to start a project in CADD and can be published I scientific journals.We have received an excellent feedback from the all the 25 participants and others in the class also want the same type of workshop to be extended to them.

Certificate of participation