

Course Title:

"Next Generation Sequencing, Data Analysis and Drug Design"

Resource Person: Dr. Mureed Hussain Starting Date: June, 2023 Duration: Five Weeks (Wednesday and Friday; 5-7 PM) Fee: UMT Students 5000, Faculty 8000, Others 6000. Email: <u>mureed.hussain@umt.edu.pk</u>

Introduction:

Sequencing of human genome has opened a new era of finding disease-causing variations in human DNA. Next generation is the modern-day cutting-edge technology to sequence human genome. Analysis and interpretation of sequencing data is a challenge. This course and training offer the trainee to learn about next generation sequencing (NGS) data analysis and sort out disease causing variations.

Conventional drug discovery strategies consume a lot of time and resources where hit and trial experiments are conducted for finding a suitable drug. In the recent times, the strategies of drug discovery have changed. Now a days, computational biology usage has minimized the time and resources for finding a potential drug against a specific disease.

Looking into the importance of NGS data analysis and drug design, some of the key areas where the field of study has made significant contributions include, but not limited to:

i. *RNA Seq Data Analysis*: RNA sequence data analysis using Linux (Bash scripts & R programing)



- ii. *Human Genome Analysis*: Using UCSC genome browser, analysis of NGS data and interpretation of deleterious variations & their probable effect on protein structure and function
- iii. Drug Design: Selection of pathogenic proteins, binding sites and potential ligands,
- iv. *Molecular Docking and Analysis*: Molecular Docking with potential drugs and analysis using Chimera, Autodoc, Discovery Studio, DFT, and MD simulation

Objectives:

- 1. Understanding the basics of NGS technology: The course can provide a comprehensive understanding of the principles, methods, and applications of NGS technology in genomics, transcriptomics, and epigenomics. Participants can learn about the sequencing platforms, library preparation, sequencing runs, and data analysis pipelines.
- 2. *Analyzing NGS data*: Participants can learn about the tools and methods for data analysis, including alignment, variant calling, gene expression analysis, and pathway analysis.
- 3. *Designing drugs*: Participants can learn about the computational methods for drug design, including molecular docking, virtual screening, and molecular dynamics simulations.
- 4. *Collaboration and networking*: The course can also provide an opportunity for participants to network with each other and with experts in the field, fostering collaboration and new partnerships for future research and development.

Overall, the training course can aim to equip participants with the knowledge, skills, and tools to apply NGS technology to drug discovery and development.

Learning Outcomes:

1. *Improved problem-solving skills:* Participants would develop problem-solving skills by working on case studies and projects related to NGS and drug design, which would enhance their ability to apply their knowledge to real-world scenarios.



- 2. *Analyzing NGS data:* Participants would learn how to handle and analyze NGS data using different bioinformatics tools and software.
- 3. *Ability to use computational tools for drug design:* Participants will learn how to use computational tools such as molecular docking, virtual screening, and molecular dynamics simulations to design and optimize drug molecules.
- 4. *Knowledge of current trends and future directions in drug design*: Participants will gain an understanding of the latest trends and future directions in drug design, including the use of artificial intelligence, machine learning, and big data in drug discovery.

Overall, the educational outcomes of a Certificate course on NGS and drug design would be an improved understanding of the technologies, enhanced skills in data analysis, and a deeper understanding of the drug discovery process and its integration with NGS technology.

Duration:

Duration: 05 Weeks Number of Days/Week: 02 Number of hours/day: 02 Total Contact Hours: 20

Eligibility Criteria:

The course is designed for the large group of audience including graduate students (Currently enrolled in 4th semester and above), research scholars, and faculty members.

Course Outline:

SN	Content	Week
1	Human Genome Analysis using UCSC genome browser	1
2	Exploration of databases containing human DNA sequencing data	



3	Retrieval and analysis of pathogenic proteins	2
4	Prediction of deleterious variations in the non-protein coding regions of human DNA	
5	RNA Seq Data Analysis using Linus (Bash Scripts)	3
6	RNA Seq Data Analysis using R Programing	
7	Drug Databases and Repositories	4
8	Screening of drug like compounds	
9	Molecular docking and validation	5
10	Visualization using Discovery studio visualizer	

Evaluation Criteria:

Class Participation/Attendance:	10%
Quizzes:	20%
Assignments:	20%
Final/Project:	50%

Readings

- Bioinformatics: A Practical Handbook of Next Generation Sequencing and Its Applications, by Lloyd Low & Martti Tammi. World Scientific, New Jersey, 2017
- Database annotation in molecular biology, principles and practices, by Arthur M. Lesk. John Wiley & Sons, Chichester, 2005
- Bioinformatics: Databases and Systems, by Stanley I. Letovsky. Springer US, Boston, MA, 2002
- Bioinformatics Databases: Design, Implementation, and Usage, by Sorin Draghici. CRC ; Taylor & Francis [distributor], Boca Raton, Fla., London, 2008