

CANCER GENOMICS WITH NGS

Submitted in partial fulfilment of the required for the award of
Master of Science Degree in Bioinformatics and Data Science

By

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**DEPARTMENT OF BIOINFORMATICS AND DATA
SCIENCE**

SCHOOL OF BIO AND CHEMICAL ENGINEERING

SATHYABAMA

INSTITUTE OF SCIENCE AND TECHNOLOGY
(DEEMED TO BE UNIVERSITY)

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BONA FIDE CERTIFICATE

This is to certify that this Project Report is the bonafide work of A.SHALINI(43739013) who carried out the project entitled "CANCER GENOMICS WITH NGS" under my / our supervision from January 2024 to April 2024

Internal Guide

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Submitted for Viva voce Examination held on_____

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DECLARATION

I, **A. SHALINI (43739013)**, hereby declare that the Project Report entitled “CANCER GENOMICS WITH NGS” done by me under the guidance of **Dr. JEMMY CHRISTY** is submitted in partial fulfilment of the requirements for the award of Master of Science degree in Bioinformatics and Data Science.

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(A. SHALINI)

ABSTRACT

This workshop titled "Cancer Genomics with NGS" encompasses a comprehensive exploration of cancer genomics using Next-Generation Sequencing (NGS) technology. The workshop begins with an introduction to Linux command line basics, followed by advanced commands and the Festival OFF tool. Subsequent sections cover Bash scripting, R programming, and data retrieval from cancer databases such as TCGA. The report delves into Next-Generation Sequencing, covering various file formats like FASTA, SAM/BAM, GFF/GTF, BED, and VCF. Additionally, it discusses RNA-seq analysis, variant calling with GATK, somatic copy number alterations, and GISTIC analysis. Fusion transcript detection and basic machine learning concepts for disease subtype classification are also covered. The workshop concludes with building a machine learning model to predict disease subtypes from genomic data.

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1. CANCER GENOMICS WITH NGS

1.1 OVERVIEW

The project titled "Cancer Genomics with NGS" provides an in-depth exploration of cancer genomics utilizing Next-Generation Sequencing (NGS) technology. This report aims to cover a wide range of topics essential for understanding and analyzing cancer genomic data. It begins with an introduction to the Linux command line, covering basic commands and gradually advancing to more complex ones. The usage of the Festival OFF tool is also discussed for text-to-speech synthesis. Subsequent sections delve into Bash scripting and R programming, essential skills for automating tasks and data analysis in bioinformatics.

Furthermore, the report covers the retrieval of genomic data from cancer databases such as The Cancer Genome Atlas (TCGA), which serves as a valuable resource for cancer research. Next, the fundamentals of Next-Generation Sequencing (NGS) are explored, including various file formats such as FASTA, SAM/BAM, GFF/GTF, BED, and VCF commonly encountered in cancer genomics. The report then progresses to RNA-seq analysis, variant calling with GATK, somatic copy number alterations, and GISTIC analysis, providing insights into genetic variations and alterations associated with cancer.

Moreover, the project includes discussions on fusion transcript detection, introducing machine learning concepts for disease subtype classification from genomic data. The final section focuses on building a machine learning model to predict disease subtypes based on genomic features, highlighting the potential of computational approaches in cancer research and personalized medicine.

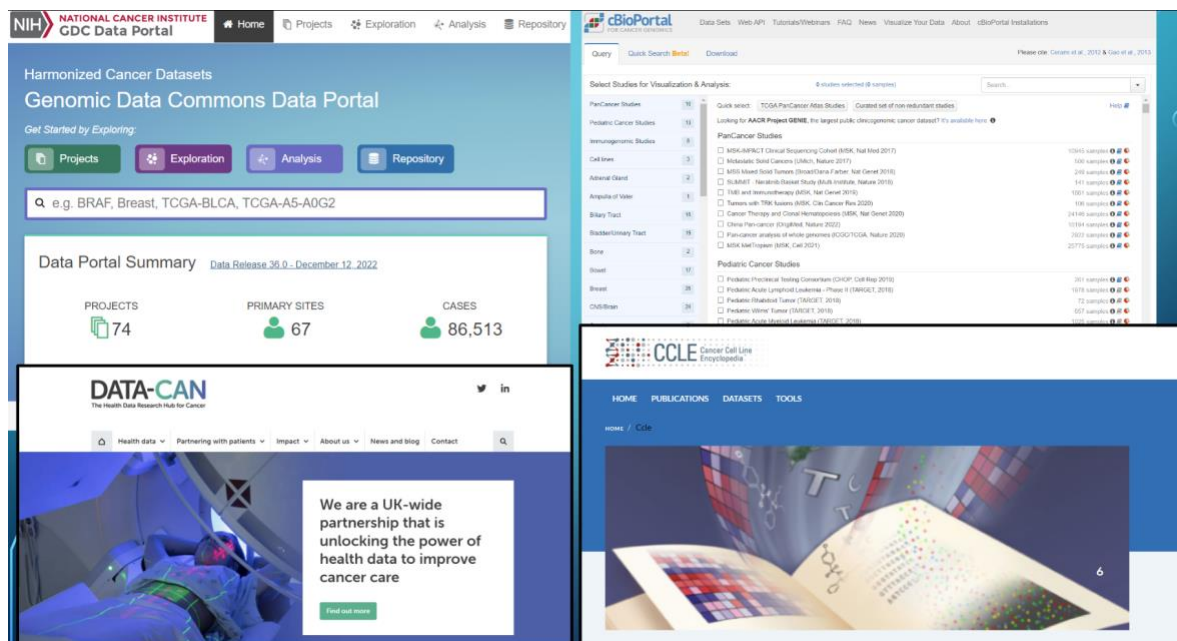


Fig1.1: Cancer Genomics Hubs

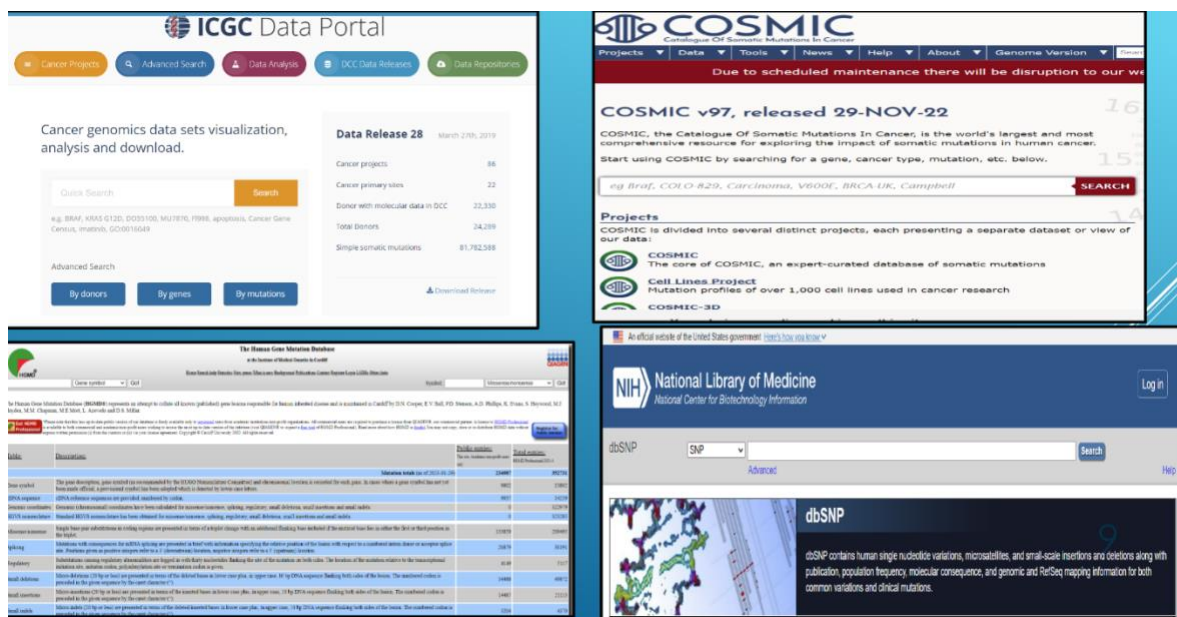


Fig 1.2: Mutation Related Databases

“Best Practices” for DNA-Seq variant calling

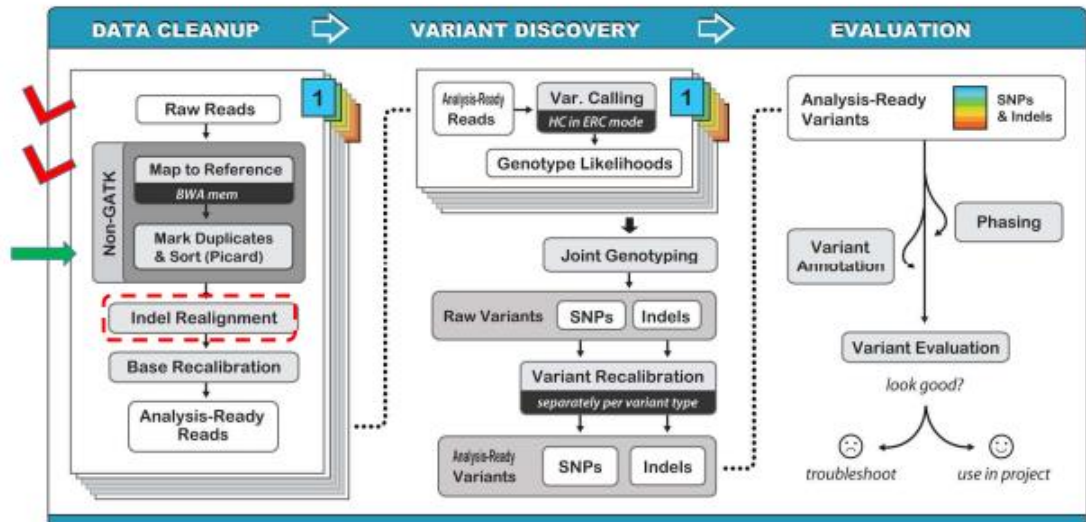


Fig 1.3: DNA-Seq variant calling

1.2 OBJECTIVES

- Develop proficiency in using the Linux command line for data manipulation and analysis.
- Acquire essential bioinformatics skills such as Bash scripting and R programming.
- Learn how to retrieve and manage genomic data from cancer databases like TCGA.
- Understand Next-Generation Sequencing (NGS) fundamentals, including different file formats and analysis techniques.
- Gain insights into genomic alteration analysis, including somatic copy number alterations and fusion transcript detection.
- Introduce machine learning concepts for disease subtype classification from genomic data.
- Learn how to build and evaluate machine learning models for predicting disease subtypes based on genomic features.

1.3 LEARNING OUTCOMES

Technical Proficiency:

I have mastered the use of the Linux command line, acquiring both basic and advanced commands necessary for efficient data manipulation and analysis in bioinformatics. This proficiency enables to navigate and manipulate large datasets, perform complex analyses, and automate repetitive tasks, thereby enhancing their productivity and effectiveness in genomic research.

Bioinformatics Skills:

Through the project, I have developed essential bioinformatics skills in Bash scripting and R programming. I am now capable of automating tasks and implementing advanced data analysis techniques, such as statistical modeling, visualization, and machine learning, to extract meaningful insights from genomic data and contribute to cancer research effectively.

Data Retrieval and Management:

Participants have learned how to retrieve, manage, and analyze genomic data from cancer databases like TCGA. This skill enhances understanding of cancer genomics and its applications, allowing to access a wealth of valuable data for research purposes and contribute to advancements in cancer diagnosis, treatment, and prevention.

Next-Generation Sequencing (NGS) Fundamentals:

Understanding NGS fundamentals, including different file formats (FASTA, SAM/BAM, GFF/GTF, BED, VCF), RNA-seq analysis, and variant calling with tools like GATK, equips participants with the knowledge and tools necessary to process and analyze genomic data generated from NGS experiments accurately. This knowledge forms the foundation for advanced genomic analysis and interpretation.

Genomic Alteration Analysis:

Participants have gained insights into somatic copy number alterations, GISTIC analysis, and fusion transcript detection, crucial for understanding the genetic

variations associated with cancer. This understanding allows to identify potential biomarkers, therapeutic targets, and pathways involved in cancer development and progression.

Introduction to Machine Learning:

The workshop has introduced to machine learning concepts for disease subtype classification from genomic data. By understanding machine learning algorithms, techniques, and applications in cancer research, participants can explore the potential of computational approaches to address complex problems and make predictions based on genomic features.

Model Building and Evaluation:

I have learned how to build and evaluate machine learning models for predicting disease subtypes based on genomic features. This skill enables them to develop accurate and reliable predictive models that can guide personalized medicine and precision oncology, leading to more effective cancer treatments and improved patient outcomes.

1.4 CONCLUSION

In conclusion, the project "Cancer Genomics with NGS" has equipped participants with a diverse set of skills and knowledge essential for conducting cutting-edge research in cancer genomics. By gaining technical proficiency in the Linux command line, mastering bioinformatics skills such as Bash scripting and R programming, and learning how to retrieve and manage genomic data from databases like TCGA, participants are now well-prepared to analyze and interpret complex genomic datasets.

Furthermore, our understanding of Next-Generation Sequencing (NGS) fundamentals, including different file formats and analysis techniques, has provided them with the tools necessary to process and analyze genomic data accurately. This knowledge, coupled with insights into genomic alteration analysis and machine learning concepts for disease subtype classification, enables participants to explore the intricate genetic variations associated with cancer and develop predictive models for personalized medicine.

In the future, these skills and knowledge will undoubtedly contribute to advancements in cancer research, diagnosis, and treatment. By leveraging computational approaches and machine learning techniques, researchers can uncover novel biomarkers, therapeutic targets, and pathways, ultimately leading to improved cancer therapies and better patient outcomes. Overall, the project has empowered participants to make significant contributions to the field of cancer genomics and pave the way for a deeper understanding of cancer biology and personalized oncology.

1.5 WORKSHOP DURATION: 1 MONTH

2. NPTEL COURSE

COMPREHENSIVE MOLECULAR DIAGNOSTICS AND ADVANCED GENE EXPRESSION ANALYSIS

2.1 INTRODUCTION:

This NPTEL course has been a journey through the fascinating world of molecular biology, equipping me with the knowledge and skills needed to understand and apply cutting-edge techniques in molecular diagnostics.

Throughout the course, I delved into the central concepts of molecular biology, including the central dogma, nucleic acid structure, DNA replication, RNA transcription, and protein synthesis. These foundational understandings provided me with a solid framework upon which to build my knowledge of advanced techniques and applications in molecular diagnostics.

One of the key highlights of the course was mastering essential techniques such as Polymerase Chain Reaction (PCR), Next-Generation Sequencing (NGS), and CRISPR-Cas9 technology. Through hands-on exercises and theoretical modules, I gained proficiency in performing these techniques, understanding their underlying principles, and analyzing the data they produce.

Furthermore, the course offered a comprehensive exploration of the clinical applications of molecular diagnostics in various medical fields. From infectious diseases to cancer management and genetic disorders, I learned how molecular techniques are used to diagnose, monitor, and treat a wide range of conditions, leading to personalized treatment strategies and improved patient outcomes.

Ethical considerations and future trends in molecular diagnostics were also thoroughly discussed. I gained an understanding of the importance of ethical practices in research and healthcare, as well as the potential impact of emerging technologies such as artificial intelligence, nanotechnology, and multi-omics integration on the field.

2.2 OBJECTIVES:

1. Understand the fundamental principles of molecular biology, including the central dogma, nucleic acid structure, and protein synthesis.
2. Explore the historical developments and advantages of molecular diagnostics over traditional methods.
3. Master key techniques such as PCR, NGS, CRISPR-Cas9, and proteomics for gene expression analysis and manipulation.
4. Examine the clinical applications of molecular diagnostics in infectious diseases, cancer management, genetic disorders, and various medical specialties.
5. Navigate ethical considerations and future trends in molecular diagnostics, including quality control, AI, nanotechnology, and multi-omics integration.

2.3 LEARNING OUTCOMES:

1. **Foundational Understanding:** Gain a comprehensive understanding of fundamental concepts in molecular biology, including the central dogma, nucleic acid structure, DNA replication, RNA transcription, and protein synthesis. This knowledge forms the basis for further exploration of advanced techniques and applications in molecular diagnostics.
2. **Technical Proficiency:** Develop proficiency in essential techniques such as Polymerase Chain Reaction (PCR), Next-Generation Sequencing (NGS), and CRISPR-Cas9 technology for gene expression analysis and manipulation. Learners will become adept at performing these techniques in laboratory settings, understanding their principles, and troubleshooting common issues.
3. **Clinical Applications:** Explore the clinical applications of molecular diagnostics in infectious diseases, cancer management, genetic disorders, and various medical specialties. By understanding how molecular techniques are applied in real-world scenarios, learners will be equipped to interpret clinical data, contribute to research, and make informed decisions regarding patient care and treatment strategies.
4. **Advanced Analysis Skills:** Develop the ability to analyze complex data generated from NGS, proteomic analyses, and other molecular techniques. This includes proficiency in bioinformatics tools and software for data interpretation, allowing learners to extract meaningful insights from large datasets and identify biomarkers, genetic mutations, and disease signatures.
5. **Ethical Awareness and Future Trends:** Understand the importance of ethical considerations in molecular diagnostics, including patient privacy, data security, and responsible research practices. Additionally, stay informed about future trends and emerging technologies shaping the field, such as quality control measures, artificial intelligence (AI), nanotechnology, and multi-omics integration. By staying ahead of these trends, learners can contribute to advancements in molecular diagnostics and ensure the ethical and responsible use of technology in healthcare.

2.4 CONCLUSION:

In conclusion, the NPTEL course on "Comprehensive Molecular Diagnostics and Advanced Gene Expression Analysis" has been a transformative learning experience that has enriched my understanding of molecular biology and its applications in healthcare. Through this course, I have gained a deep understanding of fundamental concepts such as the central dogma, nucleic acid structure, and protein synthesis, as well as advanced techniques like PCR, NGS, and CRISPR-Cas9 technology.

The course has equipped me with the knowledge and skills needed to navigate the complex world of molecular diagnostics, enabling me to analyze clinical data, interpret genetic information, and contribute to personalized treatment strategies. Additionally, the exploration of ethical considerations and future trends in molecular diagnostics has broadened my perspective on the ethical implications of scientific research and the potential impact of emerging technologies on healthcare.

Overall, this course has been instrumental in shaping my understanding of modern healthcare, molecular bioinformatics, and precision medicine. It has provided me with a solid foundation upon which to build my career in the field of molecular biology, and I am excited to continue exploring the frontiers of medical science in the future.

2.5 COURSE DURATION: 12 WEEKS

3. NPTEL COURSE

INTRIDUCTION TO INTERNET OF THINGS

3.1 INTRODUCTION:

Embarking on the NPTEL course on the Internet of Things (IoT) has been an enlightening journey into the realm of connected technology. Throughout the course, I have explored the fundamental concepts and practical applications of IoT, gaining insights into its transformative potential across various domains.

In the initial weeks, I focused on understanding the basics of IoT, including its architecture, components, and applications. This laid the groundwork for my exploration into more advanced topics. We delved into networking protocols, learning how devices communicate in IoT networks.

As the course progressed, we deepened our understanding of sensor networks, exploring the diverse range of sensors used in IoT applications. I learned about deployment considerations, data processing techniques, and the role of sensors in collecting valuable data. Additionally, we had the opportunity to work on hands-on projects using platforms like Arduino and Raspberry Pi. These projects helped solidify my understanding of IoT concepts and gave me practical experience in building IoT solutions.

One of the highlights of the course was exploring real-world applications of IoT through case studies and examples. From precision agriculture to remote patient monitoring, I saw how IoT is revolutionizing processes and improving efficiency across various industries.

3.2 OBJECTIVES:

1. **Understand IoT Fundamentals:** Gain a comprehensive understanding of IoT concepts, architecture, and applications across various domains.
2. **Explore Networking Principles:** Learn about networking protocols, communication models, and standards relevant to IoT for seamless connectivity and data exchange.
3. **Master Sensor Technologies:** Understand the principles of operation, deployment considerations, and data processing techniques of sensors used in IoT applications.
4. **Hands-on Experience:** Acquire practical skills in building IoT solutions through hands-on projects using platforms like Arduino and Raspberry Pi.
5. **Real-world Applications:** Explore case studies showcasing real-world applications of IoT in agriculture, healthcare, industrial automation, and smart cities.
6. **Cloud Computing and Analytics:** Understand cloud computing platforms and services for IoT data storage, processing, and analytics, and their role in scaling IoT solutions.
7. **Explore Emerging Trends:** Stay updated on emerging IoT trends like fog computing, edge computing, and machine learning, and understand their implications for future applications.
8. **Critical Thinking and Problem Solving:** Develop critical thinking skills to analyze IoT challenges and find appropriate solutions considering scalability, security, and interoperability.
9. **Collaboration and Communication:** Foster collaboration and communication skills through interactions with peers and industry experts, facilitating the exchange of ideas and best practices.
10. **Application of Knowledge:** Apply acquired knowledge and skills to design, develop, and implement IoT solutions tailored to specific use cases and industry requirements, contributing to innovation and efficiency improvements.

3.3 LEARNING OUTCOMES:

Introduction to IoT

- Understand the fundamental concepts of IoT, including its architecture, components, and applications.
- Recognize the importance of IoT in various domains such as healthcare, agriculture, and industrial automation.
- Identify the challenges and opportunities associated with IoT adoption and implementation.

Basics of Networking and Communication Protocols

- Explain the basics of networking, including network architectures, protocols, and communication models.
- Describe the OSI and TCP/IP models and their relevance to IoT networking.
- Understand various communication protocols used in IoT and their roles in enabling seamless communication between devices.

Sensor Networks and Machine-to-Machine Communications

- Define sensor networks and their applications in IoT.
- Identify different types of sensors, deployment considerations, and data processing techniques.
- Explain machine-to-machine (M2M) communications and the protocols and architectures used for enabling communication between IoT devices.

Interoperability, Arduino Programming, and Raspberry Pi

- Discuss the challenges and solutions for achieving interoperability in IoT ecosystems.
- Apply Arduino programming skills to interface sensors and actuators with Arduino boards.
- Utilize the Raspberry Pi platform to implement IoT projects and integrate sensors, actuators, and communication modules.

Python Programming and Cloud Computing

- Apply Python programming skills to develop IoT applications and scripts.
- Describe the role of cloud computing in IoT data storage, processing, and analytics.
- Explore cloud computing platforms and services for deploying and managing IoT solutions.

Fog Computing, Smart Cities, and Smart Homes

- Explain the concept of fog computing and its role in extending cloud capabilities to the edge of the network.
- Discuss the applications of IoT in smart cities and smart homes, including urban planning, energy management, and home automation.
- Identify IoT-enabled solutions for improving efficiency, sustainability, and quality of life in urban environments.

Industrial IoT and Case Studies

- Explore the applications of IoT in industrial automation, predictive maintenance, and supply chain management.
- Analyze case studies in agriculture, healthcare, and activity monitoring to understand real-world implementations of IoT solutions.

- Discuss the challenges and considerations for deploying and scaling IoT projects in different industries.

3.4 CONCLUSION:

Completing the NPTEL course on the Internet of Things (IoT) has been a rewarding experience, offering valuable insights into the vast potential of connected technology. Throughout the course, we have explored the foundational concepts, practical applications, and real-world implications of IoT, gaining a deeper understanding of its role in shaping the future.

From understanding the basics of IoT architecture and networking protocols to working on hands-on projects with Arduino and Raspberry Pi, each module has provided a comprehensive overview of IoT technology. We have learned how sensor networks collect valuable data and how communication protocols facilitate seamless interaction between devices.

Moreover, the exploration of real-world applications has highlighted the transformative impact of IoT across various sectors, from agriculture to healthcare and beyond. Witnessing how IoT is revolutionizing processes and improving efficiency has been both inspiring and eye-opening.

3.5 COURSE DURATION: 7 WEEKS

4. REVIEW ARTICLE

Demystifying Metabolomics: Understanding Metabolites and Beyond

Metabolomics and the Human Microbiome: Impact on Health and Disease

Metabolomics provides a comprehensive tool for examining the pathophysiology of complex illnesses, such as depression, because it considers both hereditary and environmental influences. It is becoming increasingly clear that the microorganisms that reside peacefully within people play an important role in both health and disease. The gastrointestinal system has the highest concentration of these microorganisms. Microbial mix reflects the host's lifestyle and genetic background. This microbiota has both immediate and long-term effects on the host in a dynamic equilibrium. Dysbiosis, or microbial disruption, can raise the risk of health problems. Numerous bacterial genes that create enzymes that degrade estrogen have been discovered. Thus, the gut flora can alter blood estrogen levels.

On the other hand, chemicals that resemble estrogen may promote the growth of certain bacterial species. Thus, a synergistic interplay of endogenous hormones, estrogen-like compounds, and microbiota may protect against disease while increasing the risk of hormone-related disorders. Without a question, the microbiome is the human body's second genome, serving a range of functions in both health and disease. However, the microbiome's breadth, which contains approximately 3.3 million genes with unknown roles, hinders translation progress. Over the last ten years, a slew of research have revealed how the microbiome influences various types of cancer that are particular to specific organs. These impacts include altered energy balance, increased body fat, the production of genotoxins and tiny signaling molecules, immune response priming and modulation, and the metabolism of indigestible food items, xenobiotics, and pharmaceuticals.

Globally, diabetes is becoming more common, yet it still has serious side effects including cardiovascular and kidney problems. More focused prevention and treatment may result from a deeper comprehension of the molecular mechanisms

underlying the genesis and course of diabetes as well as the discovery of biomarkers for disease screening, diagnosis, and prognosis. Thanks to developments in analytical methods, metabolomics can now identify and quantify many biomarkers simultaneously in a high-throughput way. Because metabolomics provides information on underlying metabolic pathways, it can help find novel variables that contribute to diabetes and its development.

New biomarkers for type 2 diabetes (T2D) and its implications have been found through the application of metabolomics in epidemiological research. These biomarkers include branched-chain amino acids, phenylalanine metabolites, metabolites involved in energy metabolism, and lipid metabolism. Possible drug-modulated pathways have also been investigated using metabolomics. A thorough metabolic network may be produced by addressing diabetes research from a systems biology viewpoint and integrating metabolomics with other omics data, such as genetics, transcriptomics, proteomics, and clinical data. This makes causal inference easier.

Metabolomics has great promise for improving our understanding of molecular processes, identifying targets for potential therapies, and preventing and controlling type 2 diabetes and its effects.

Insulin resistance is the underlying pathophysiology of type 2 diabetes and metabolic syndrome. It has been proposed that commensals' carbohydrate metabolism accounts for up to 10% of the host's total energy extraction, potentially impacting the etiology of obesity and prediabetes. However, the underlying process remains unknown.

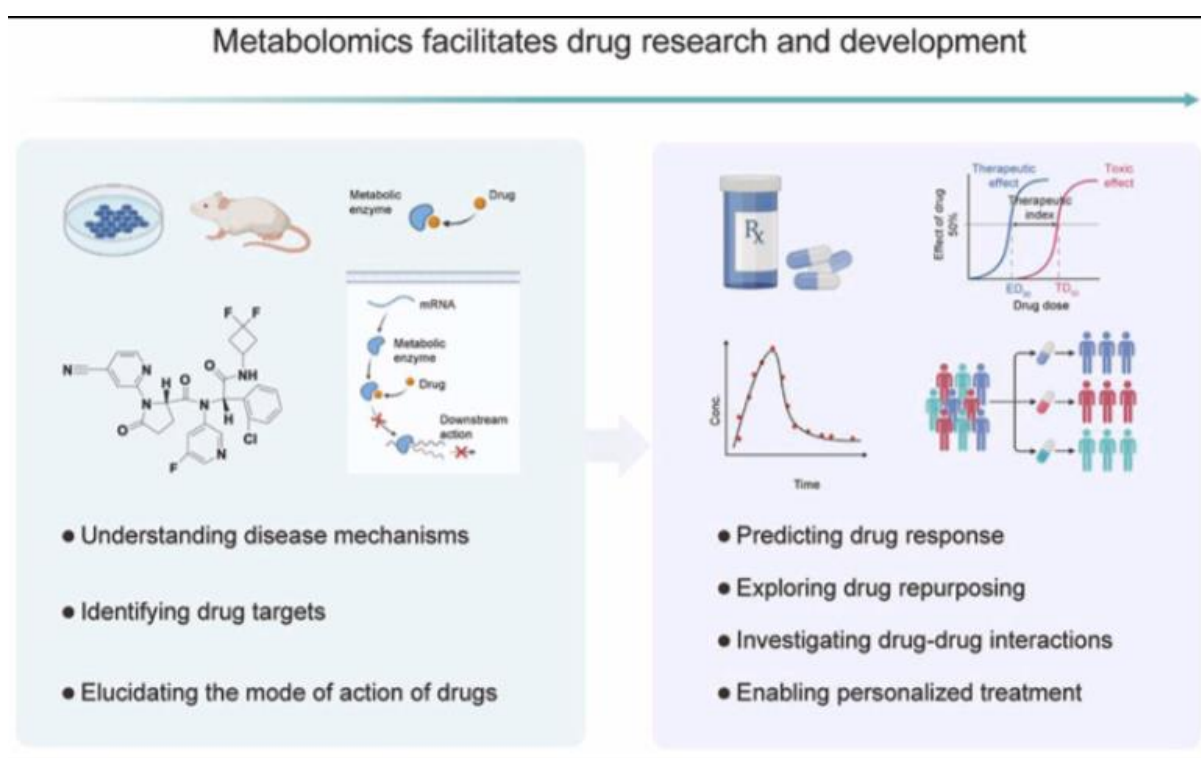
Metabolomics in Pharmacology: Advancing Drug Development

Metabolomics simplifies pharmaceutical development and research, assisting with anything from predicting medication response and enabling personalized treatment to understanding illness mechanisms and discovering therapeutic targets.

Proteomics and other 'omics technologies were early adopters in the pharmaceutical industry, where they were employed for drug development. Even though metabolomics has lagged behind in this advancement, it is now a widely known and

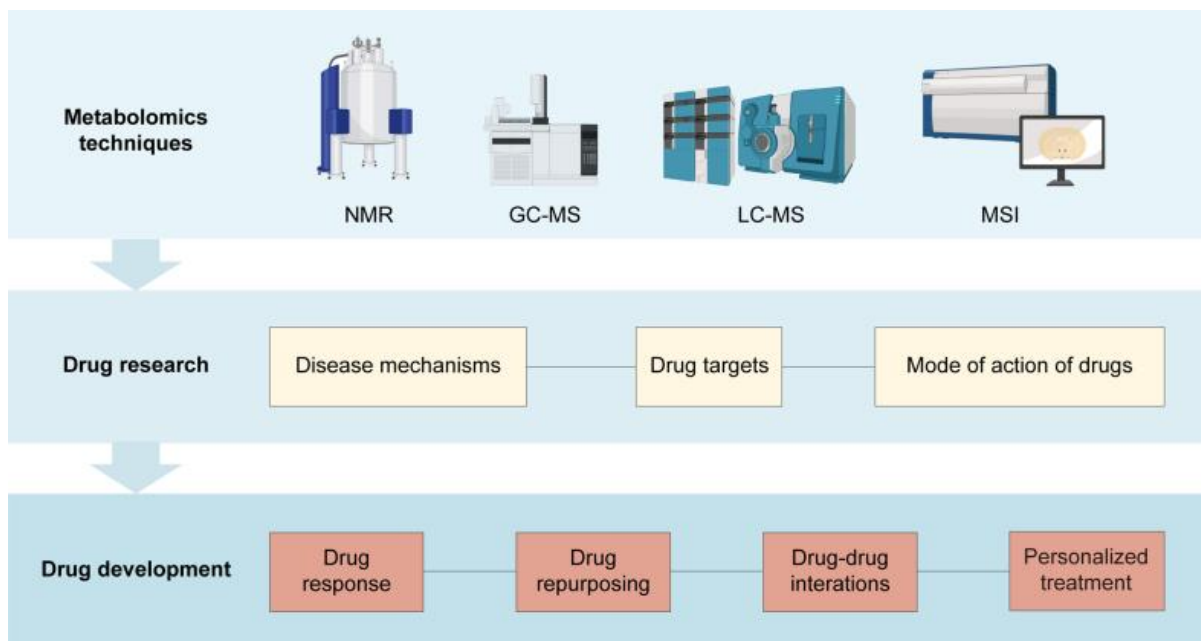
often utilized technology in the early stages of drug development. Metabolomics has evolved over the previous few decades from a simply exploratory tool to a more sophisticated and quantitative biochemical technique. Many metabolomics-based technologies are now being used in the early stages of drug discovery. Metabolomics study can help define physiological response and target engagement (TE) markers, as well as clarify the mode of action (MoA) of investigational medication candidates.

A thorough knowledge of the metabolic processes involved in biological systems may be obtained through metabolomics. Metabolomics provides unprecedented benefits in fundamental drug research by utilizing cutting-edge analytical tools, assisting in the clarification of therapeutic targets, understanding illness mechanisms, and explaining how pharmaceuticals operate. More importantly, by anticipating pharmacokinetics, pharmacodynamics, and therapeutic response, metabolomics greatly accelerates drug development. Furthermore, metabolomics facilitates investigations into pharmaceutical repurposing, drug-drug interactions, and the development of personalized treatment strategies.



In addition to more traditional procedures such as spectroscopy, electrophoresis,

and enzymatic testing, mass spectrometry (MS) has emerged as an incredibly strong and versatile instrument that is critical to many aspects of modern drug research. Target identification, MoA elucidation, TE marker discovery, and physiological response (PR) indicators, such as therapy monitoring, are all key areas where metabolomics can be used during drug development.



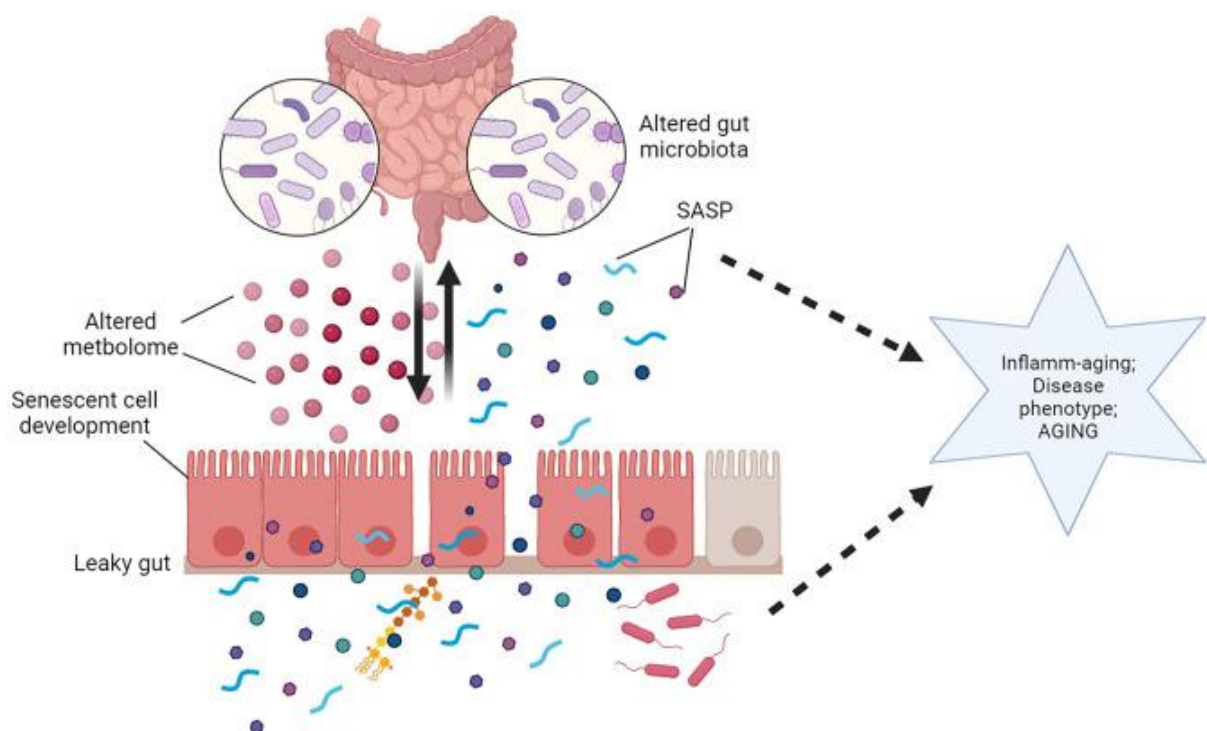
Metabolomics and Aging: Exploring Metabolomic Changes with Age

Age-related changes in gut microbiota and metabolites happen simultaneously. It is commonly known that the gut microbiota's variety, makeup, and functional characteristics are key factors in determining an individual's health. Studies have demonstrated a substantial correlation between human aging and gut microbiota, with alterations in the microbiome having the capacity to forecast human longevity. Moreover, there is growing evidence that gut microbial dysbiosis is associated with chronic age-related diseases. A perspective focusing on cellular senescence has emerged on the aging process, thanks to recent developments in our understanding of the cellular and molecular aspects of biological aging.

Because the microbiome directly affects the digestive system, it plays a significant role in human aging. It's unclear exactly how microbes affect skin, though. For

instance, cellular senescence, an inherent aging process, has been connected in recent times to microbial imbalance. Senescence is the term for the process by which aging cells react to stress by going into permanent growth arrest yet continuing to have a high metabolic activity. Numerous chronic illnesses and aging have been associated with an excess of the senescence-associated secretory phenotype (SASP), which is composed of proinflammatory cytokines, chemokines, growth factors, proteases, lipids, and extracellular matrix components.

Given that the skin is a typical place for accumulation, senescence may be especially harmful to dermatological conditions. Through the release of microbial metabolites and the gut-skin axis, the gut microbiota affects cellular senescence and skin disruption in two different ways. The identification and measurement of substances linked to senescence is made possible by metabolomics. In addition, new anti-senescent therapies are needed because of the poor safety records of the drugs that are currently on the market. Probiotics and prebiotics may be useful substitutes because of the connection between a healthy microbiota and aging. However, more investigation into the senescence-associated changes in the gut flora is required to create immunomodulatory treatments.



Maintaining gut-skin homeostasis requires the presence of distinct microbial

populations, which are present in the human gut. Deviations from the normal interaction between the gut microbiota and immune system might have a direct impact on the skin and hasten the development of skin diseases. The way in which the gut bacteria affects skin health remains unclear.

Metabolomics in Forensic Science: Unraveling Mysteries in Criminal Investigations

If no matching fingerprints or DNA profiles are discovered, crimes may remain unsolved. In this case, forensic investigators face a significant lack of evidence and data on the unidentified criminal and/or victim, as well as any individuals who may be absent. However, human hair is a biological trace that is regularly found at crime scenes. Hair, which serves as a biochemical storage medium, can provide crucial information about a person's characteristics and behaviors.

To discover important, distinctive molecules in hair, an untargeted metabolomics technique has been successfully developed and used to a cohort of 68 hair samples taken from people in the Netherlands. There was emphasis on the benefits of using hair as an analytical matrix. Because of its wide detection range, extended stability in ambient circumstances, non-invasive collecting method, ability to do intricate temporal pattern studies, potential for retrospective analysis, and accessibility, it is a crucial tool in forensic research.

Our study therefore successfully illustrates, despite certain drawbacks (methodology differences) and restrictions (use of open-source MS data platforms), how untargeted LC-HRMS analysis of biological trace material, such as human hair, may assist in the lifestyle profile of unknown donors. This is notably the case in forensics, where donor profiling plays a crucial role in producing leads and advancing a criminal investigation, especially in circumstances when potential suspects are linked to a certain crime scene and victims or perpetrators are unknown.

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REVIEW ARTICLE

PROTEIN-LIGAND DOCKING IN DRUG DISCOVERY: FINDING THE PERFECT FIT

AKULWAD SHALINI BAPURAO

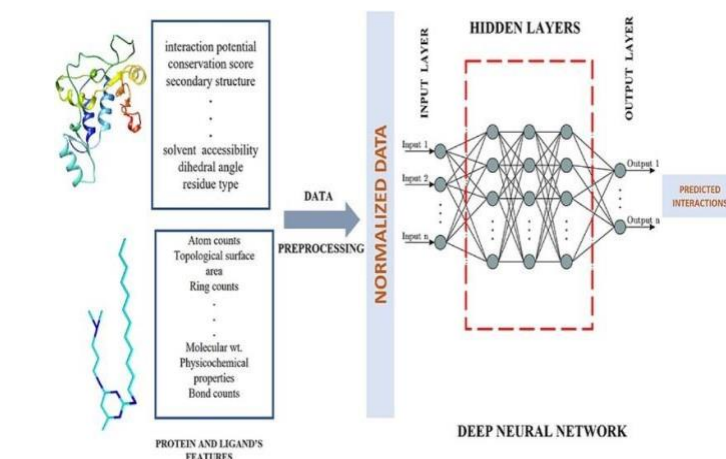
HIGH-THROUGHPUT SCREENING IN STRUCTURAL BIOLOGY

The latest updates

Exploring protein-ligand interactions is extremely interesting because it provides deeper insights into molecular recognition, interaction mechanisms, and subsequent functions. It is difficult to predict an exact model for a protein-ligand interaction.

Molecular docking is a computer method for predicting a ligand's preferred orientation, binding conformations, and binding affinity to a macromolecular target, particularly a protein.

Structure-based HTS (SBHTS) uses the structure of the target protein to compute the interaction energy of the drug under test. When high-resolution structural data for the target protein is available, this method is favored. This type of medication design is based on 3D structure knowledge derived from crystallographic, spectroscopic, or bioinformatics approaches. SBHTS entails locating a potential ligand-binding site on target molecules and docking ligands to a protein target. Following that, a scoring function is used to predict the likelihood that a ligand would bind to the protein with high affinity. It is the energy function that is used to calculate the free energy of binding between protein and ligand.



Picture Caption: To make your document look professionally produced, Word provides header, footer, cover page, and text box designs that complement each other.

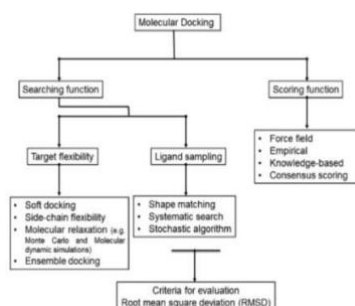
PRINCIPLES OF PROTEIN -LIGAND DOCKING

Protein-ligand docking entails several processes, including determining active sites, ligand flexibility, and interaction energy between ligand and protein. In the lack of target receptor 3D structures, homology modeling is utilized to create a 3D model of the receptor for virtual screening/docking.

Understanding the ruling principles whereby protein receptors recognize, interact, and associate with molecular substrates and inhibitors is of paramount importance in drug discovery efforts. Protein-ligand docking aims to predict and rank the structure(s) arising from the association between a given ligand and a target protein of known 3D structure.

Despite the breathtaking advances in the field over the last decades and the widespread application of docking methods, several downsides still exist. In particular, protein flexibility—a critical aspect for a thorough understanding of the principles that guide ligand binding in proteins—is a major hurdle in current protein-ligand docking efforts that needs to be more efficiently accounted for.

APPLICATIONS IN STRUCTURE-BASED DRUG DESIGN



In comparison to the developing and widespread bacterial resistance to commercial treatments and the pressing need for remedies for intractable diseases, the number of drugs hitting the market or clinical trials has decreased dramatically. As a result, it has become critical to develop more reasonable and efficient ways for designing and developing innovative medications. Structure-based drug design/discovery (SBDD) is a computer-aided method for designing or discovering new medications based on knowledge of the 3D structures of the relevant particular targets. SBDD has shown considerable promise and success in the field of drug discovery during the last few decades.

CHALLENGES IN PREDICTING BINDING AFFINITIES

scoring function is an important part of docking procedures. The scoring function in protein-ligand docking typically analyzes the overall favorability of a protein-ligand complex and is intended to be comparable to the free energy of binding of the protein and ligand. For practical reasons, alternative qualities such as toxicity and features associated to absorption, distribution, metabolism, and excretion may be preferred.

A generic scoring function cannot yet compute the binding affinities of protein-ligand complexes with high accuracy. Because of the combinatorial explosion of alternative conformational states of the flexible protein and ligand, as well as the surrounding water molecules and ions, the computation is exceptionally difficult. Furthermore, the binding process includes a balancing of many different physical interactions: a flexible ligand may gain advantageous interactions while suffering a significant entropic penalty as a result of binding. When charged polar groups join, they may acquire advantageous electrostatic interactions while losing favorable interactions with the solvent.

The contribution of each of these interactions can be significant, but they tend to cancel each other out; thus, the total binding free energy involves a delicate balance, and errors in the computation of any one type of interaction can lead to significant errors in the computation of total binding free energies.

ADVANCES IN DOCKING ALGORITHMS

The latest updates

Several popular traditional docking programs are taken into account. Their search for the optimal ligand posture is based on the global optimization problem, either explicitly or implicitly. Several algorithms are employed to handle this problem, with the heuristic genetic algorithm standing out due to its popularity and intricate design. For their acceleration, all traditional docking systems use preliminary estimated grids of protein-ligand interaction potentials or optimal locations of protein and ligand conjugation. The docking accuracy is severely limited by these methodologies and commonly used fitting parameters. In the course of global optimization and the search for the optimal ligand poses, solvent is considered in extremely simplistic techniques.

More precise techniques based on implicit solvent models are routinely utilized for more precise binding energy predictions after docking. A new generation of docking programs has recently been developed. They discover the spectrum of a protein-ligand complex's low energy minima, including the global minimum. Because they do not use a preliminary calculated grid of protein-ligand interaction potentials and other simplifications, the energy of any conformation of the molecular system is calculated in the frame of a given forcefield, and there are no fitting parameters, these programs should be more accurate. For the new docking programs, a new docking algorithm is created and implemented.

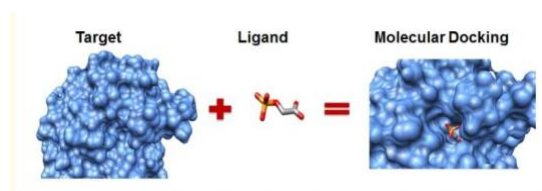
On the basis of the global energy minimum search, this approach allows docking a flexible ligand into a flexible protein with several dozen mobile atoms. This type of docking improves the accuracy of ligand location in the docking process. A good choice of molecular energy calculation method results in greater docking location accuracy. A breakthrough in the use of quantum chemistry approaches for docking and scoring is revealed.

VIRTUAL SCREENING APPROACHES

Recent improvements in high-throughput protein structure determination and computational chemistry have shifted focus back to virtual screening and quick automated docking approaches.

Virtual screening is classified into two types: ligand-based virtual screening and structure-based virtual screening. The properties of a selection of ligands known to bind to the therapeutic target of interest are used to develop a model for the common qualities thought to be relevant for a ligand's biological effects in ligand-based virtual screening. This model can then be used to locate novel ligands with similar properties. Ligands are modeled as physical entities in structure-based virtual screening, and scoring functions are employed to predict the ligand's affinity for the binding site of interest.

Docking software is commonly used in structure-based virtual screening to investigate the different binding modes of a ligand within a binding site of interest, as well as scoring methods to assess the ligand's affinity for the binding site of interest.



FUTURE TRENDS IN PROTEIN-LIGAND DOCKING

Several processes occur at hidden levels, and the expected decision is eventually output by the output layer. There has been a lot of interest in utilizing ML and particularly powerful deep learning approaches to forecast PLIs because it does not require explicit hard-coded rules curated by human specialists to make prediction and could give good prediction accuracy.

A considerable amount of training data is required to generate highly accurate predictions for new data. The accumulation of structural information for protein-ligand complexes, as well as its cataloging into databases, has enabled researchers to investigate artificial intelligence (AI) methodologies, primarily machine learning (ML) methods, for virtual screening.

Virtual screening is an essential component of drug development, and the innovative significance of machine learning approaches requires special attention. By introducing fresh scoring functions in protein-ligand docking, recent improvements in machine learning approaches have improved the performance of SBVS systems.

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6. MATLAB COURSES

- ✓ Signal Processing with MATLAB
- ✓ Image Processing with MATLAB
- ✓ MATLAB Programming Techniques
- ✓ MATLAB for Data Processing and Visualization
- ✓ Machine Learning with MATLAB
- ✓ Image Processing Onramp
- ✓ Solving Nonlinear Equations with MATLAB
- ✓ Deep Learning with MATLAB
- ✓ Statistics Onramp
- ✓ Wireless Communications Onramp
- ✓ MATLAB Fundamentals
- ✓ Reinforcement Learning Onramp
- ✓ Computer Vision Onramp
- ✓ Deep Learning Onramp
- ✓ Object-Oriented Programming Onramp
- ✓ Machine Learning Onramp
- ✓ Simulink Onramp
- ✓ MATLAB Onramp

1.MATLAB ONRAMP

DESCRIPTION:

MATLAB Onramp is an interactive tutorial designed to introduce beginners to MATLAB, a high-level programming language used in technical computing and data analysis. It covers fundamental concepts such as variables, arrays, plotting, and programming logic through hands-on exercises and quizzes. By completing MATLAB Onramp, I gain essential skills to start utilizing MATLAB for various scientific and engineering tasks.

2.REINFORCEMENT LEARNING ONRAMP

DESCRIPTION:

Reinforcement Learning Onramp offers a comprehensive introduction to reinforcement learning (RL), a subset of machine learning focused on decision making. Participants learn key RL concepts such as Markov decision processes, policy optimization, and Q-learning through practical examples and exercises. By completing the Onramp, I acquire the foundational knowledge needed to apply RL algorithms to solve complex decision-making problems in various domains.

3.OBJECT-ORINENTED PROGRAMMING ONRAMP

DESCRIPTION and LEARNING OUTCOMES:

The Object-Oriented Programming (OOP) Onramp provides a structured introduction to OOP concepts, such as classes, objects, inheritance, and polymorphism. Through interactive lessons and coding exercises, I learn how to design and implement robust software solutions using OOP principles. By mastering OOP fundamentals, I develop the skills necessary to build modular, maintainable, and scalable programs in languages like Java, Python, and C++.

4.MACHINE LEARNING ONRAMP

DESCRIPTION and LEARNING OUTCOMES:

The Machine Learning Onramp offers a beginner-friendly exploration of machine

learning techniques and algorithms. I learn essential concepts like supervised and unsupervised learning, model evaluation, and feature selection through hands-on exercises and real-world examples. By completing the Onramp, I gain the foundational knowledge needed to start building and deploying machine learning models for various applications.

5.COMPUTER VISION ONRAMP

DESCRIPTION and LEARNING OUTCOMES:

The Computer Vision Onramp provides a structured introduction to the field of computer vision, covering topics such as image processing, object detection, and deep learning for visual recognition. Through practical exercises and projects, I learn how to extract meaningful information from images and videos using state-of-the-art techniques. By completing the Onramp, I gain the foundational skills necessary to tackle real-world computer vision tasks across industries such as healthcare, automotive, and robotics.

6.MATLAB FUNDAMENTALS

DESCRIPTION and LEARNING OUTCOMES:

MATLAB Fundamentals offers a foundational understanding of MATLAB, focusing on its syntax, data types, and basic operations. I learn to write scripts and functions, manipulate matrices, and visualize data using built-in plotting functions. By mastering these fundamentals, I gain the proficiency needed to start programming in MATLAB for various scientific and engineering applications.

7.SIMULINK ONRAMP

DESCRIPTION and LEARNING OUTCOMES:

The Simulink Onramp introduces participants to Simulink, a graphical programming environment for modeling, simulating, and analyzing dynamic systems. Through interactive tutorials, I learn to build and simulate models using blocks representing system components. By completing the Onramp, I gain proficiency in using Simulink to design and simulate complex systems across industries such as automotive,

aerospace, and control systems.

8.MATLAB FOR DATA PROCESSING AND VISUALIZATION

DESCRIPTION and LEARNING OUTCOMES:

MATLAB for Data Processing and Visualization teaches how to leverage MATLAB for efficient data analysis and visualization tasks. I learn techniques for importing, cleaning, and analyzing data, as well as creating insightful visualizations using MATLAB's powerful plotting capabilities. By completing this course, I gain essential skills to extract valuable insights from data and present findings effectively.

9.MACHINE LEARNING WITH MATLAB

DESCRIPTION and LEARNING OUTCOMES:

Machine Learning with MATLAB provides a comprehensive introduction to machine learning techniques and algorithms using MATLAB's powerful toolbox. I learn to preprocess data, train and evaluate machine learning models, and deploy them for practical applications. By completing this course, I gain the skills necessary to tackle real-world machine learning challenges using MATLAB.

10.DEEP LEARNING WITH MATLAB

DESCRIPTION and LEARNING OUTCOMES:

"Deep Learning with MATLAB" offers an immersive journey into deep learning concepts and applications using MATLAB's Deep Learning Toolbox. I delve into neural network architectures, training strategies, and deployment techniques for tasks like image classification and object detection. By completing this course, I gain proficiency in leveraging MATLAB for building and deploying deep learning models in various domains.

11.DEEP LEARNING ONRAMP

DESCRIPTION and LEARNING OUTCOMES:

The Deep Learning Onramp provides a foundational understanding of deep learning principles and techniques using MATLAB. I learn to design, train, and deploy deep neural networks for tasks such as image classification and sequence prediction. By completing the Onramp, I gain essential skills to start applying deep learning to solve real-world problems efficiently.

12.IMAGE PROCESSING ONRAMP

DESCRIPTION and LEARNING OUTCOMES:

The Image Processing Onramp offers a structured introduction to image processing techniques using MATLAB. I learn to enhance, analyze, and manipulate digital images through hands-on exercises and projects. By completing the Onramp, I gain the foundational knowledge needed to process and analyze images for various applications in fields such as healthcare, remote sensing, and computer vision.

13.MATLAB PROGRAMMING TECHNIQUES

DESCRIPTION and LEARNING OUTCOMES:

"MATLAB Programming Techniques" explores advanced programming concepts and best practices for efficient MATLAB coding. I learn techniques for optimizing code performance, debugging, and modularizing code for maintainability. By completing this course, it enhance my proficiency in MATLAB programming and develop skills to tackle complex computational tasks effectively.

14.STATISTICS ONRAMP

DESCRIPTION and LEARNING OUTCOMES:

The Statistics Onramp provides a foundational understanding of statistical concepts and techniques using MATLAB. I learn to analyze data, perform hypothesis testing, and conduct various statistical tests through interactive tutorials. By completing the Onramp, I gain essential skills to interpret and draw meaningful insights from data using statistical methods.

15.SOLVING NONLINEAR EQUATION WITH MATLAB

DESCRIPTION and LEARNING OUTCOMES:

"Solving Nonlinear Equations with MATLAB" equips participants with techniques to find numerical solutions to nonlinear equations. Through practical examples and exercises, I learn methods like Newton-Raphson and secant methods for root finding. By completing this course, I gain proficiency in using MATLAB for solving a wide range of nonlinear equations efficiently.

16.SIGNAL PROCESSING WITH MATLAB

DESCRIPTION and LEARNING OUTCOMES:

"Signal Processing with MATLAB" introduces fundamental concepts and techniques for analyzing and manipulating signals. I learn to apply digital filters, perform spectral analysis, and implement signal processing algorithms using MATLAB's toolbox. By completing this course, I develop the skills needed to process and analyze various types of signals encountered in fields such as telecommunications, audio processing, and biomedical engineering.

17.SIGNAL PROCESSING ONRAMP

DESCRIPTION and LEARNING OUTCOMES:

The Signal Processing Onramp provides a structured introduction to signal processing concepts and techniques using MATLAB. I learn to analyze, filter, and visualize signals through interactive tutorials and exercises. By completing the Onramp, I gain essential skills to process and interpret various types of signals encountered in fields such as communications, audio processing, and biomedical engineering.

18.IMAGE PROCESSING WITH MATLAB

DESCRIPTION and LEARNING OUTCOMES:

"Image Processing with MATLAB" offers a comprehensive exploration of techniques for analyzing and manipulating digital images. I learn to perform tasks like image

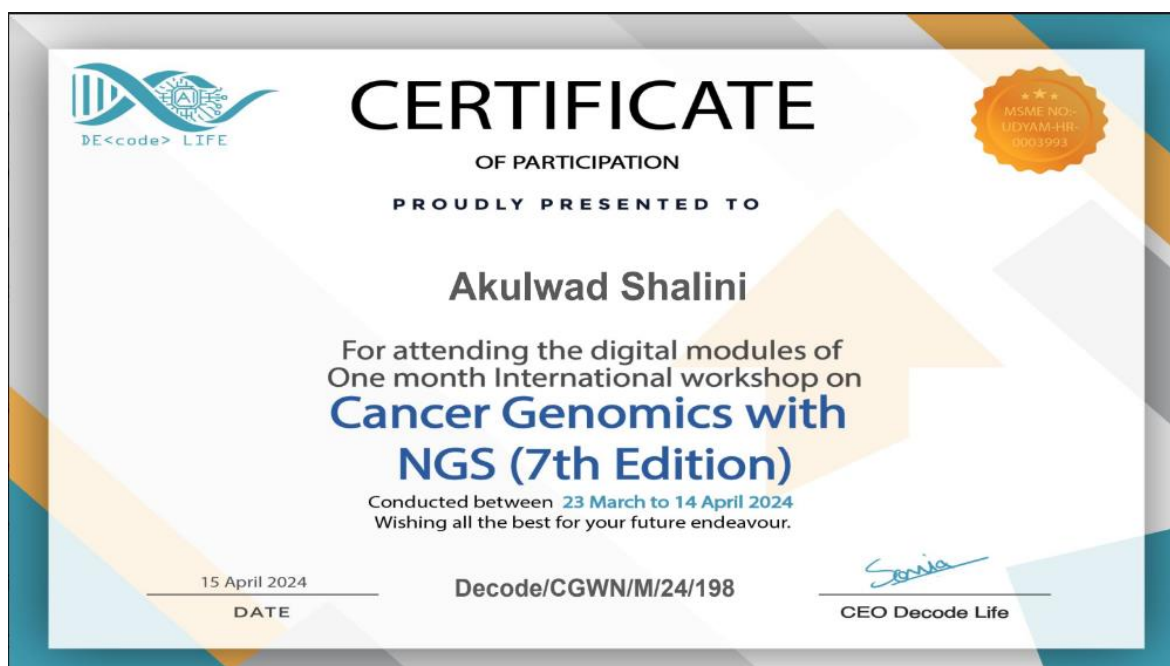
enhancement, segmentation, and feature extraction using MATLAB's toolbox. By completing this course, I gain proficiency in utilizing MATLAB for a wide range of image processing applications in fields such as medicine, surveillance, and remote sensing.

SKILLS THAT I GAINED FROM THE MATLAB COURSES:

- **Programming Proficiency:** I developed a strong understanding of MATLAB's syntax, data structures, and programming logic, enabled me to write efficient and effective code.
- **Data Analysis:** I learned various techniques for importing, cleaning, and analyzing data, allowed me to extract valuable insights and patterns from datasets.
- **Visualization:** I gained proficiency in creating insightful visualizations using MATLAB's plotting functions, enabled me to present data in a clear and understandable manner.
- **Problem Solving:** I honed problem-solving skills by tackling various challenges and projects in MATLAB, equipped me to tackle real-world problems in scientific and engineering domains.

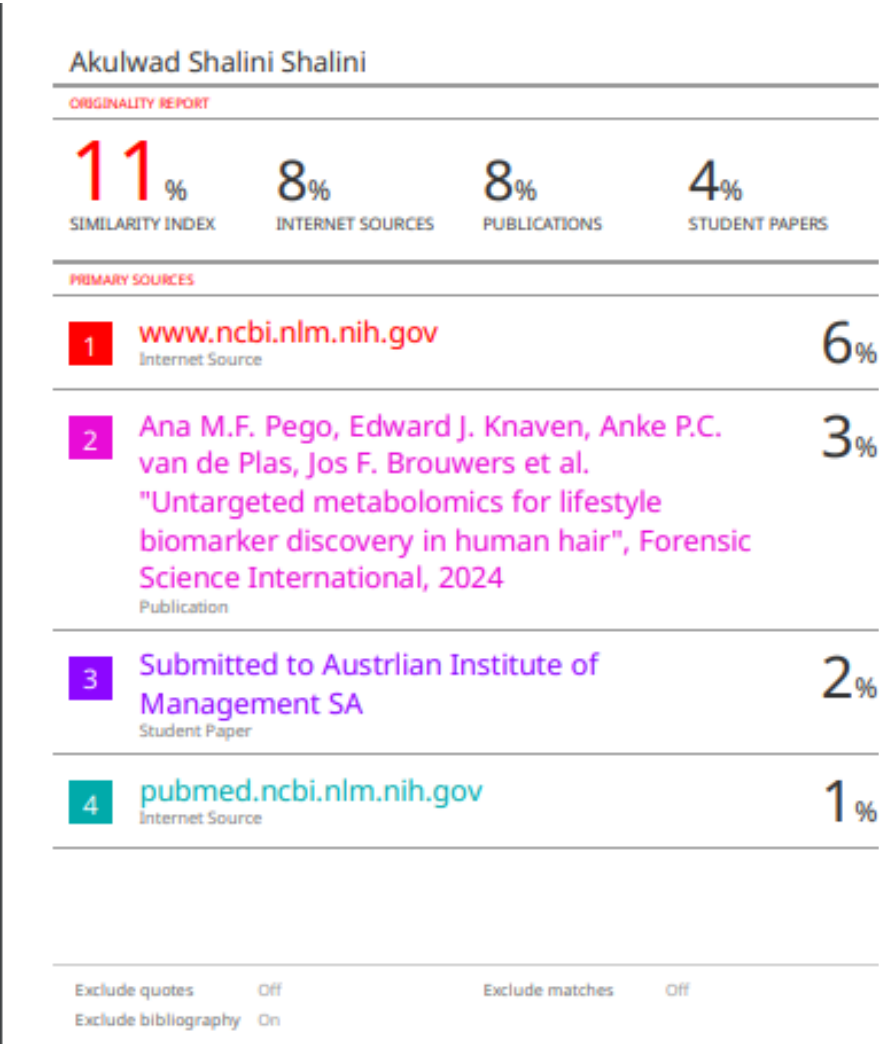
WORKSHOP CERTIFICATE:

CANCER GENOMICS WITH NGS



REVIEW ARTICLE PLAGIARISM REPORT :

Demystifying Metabolomics: Understanding Metabolites and Beyond



MATLAB CERTIFICATES



Course Completion Certificate

Akulwad Shalini Bapurao

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MATLAB Onramp

A handwritten signature in black ink, reading 'Raj L. Santos'.

DIRECTOR, TRAINING SERVICES

12 November 2023



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MATLAB Fundamentals

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12 December 2023



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MATLAB for Data Processing and Visualization

A handwritten signature in black ink, appearing to read "Rajesh Shetty".

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Object-Oriented Programming Onramp

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Image Processing with MATLAB

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Craig T. Santos
DIRECTOR, TRAINING SERVICES

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Signal Processing with MATLAB

Craig T. Santos
DIRECTOR, TRAINING SERVICES

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App Building Onramp

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