

DEEP LEARNING
AT
Sathyabama institute of science and technology

Submitted in partial fulfillment of the requirements for the award of a
Master of Science degree in Bioinformatics and Data Science

By

SNEHA SUNIL
REGISTER NO:
43739027



**DEPARTMENT OF BIOINFORMATICS AND
DATA SCIENCE**

SATHYABAMA

**INSTITUTE OF SCIENCE AND TECHNOLOGY (DEEMED TO
BE UNIVERSITY)**

**Accredited with Grade "A" by NAAC | 12B Status by UGC | Approved by AICTE
JEPPIAAR NAGAR, RAJIV GANDHI SALAI, CHENNAI - 600 119**

APRIL- 2024



SATHYABAMA

INSTITUTE OF SCIENCE AND TECHNOLOGY

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DEPARTMENT OF BIOINFORMATICS AND DATASCIENCE

BONAFAIDE CERTIFICATE

This is to certify that this Intern Report is the bonafide work of Sneha sunil (43739027) who carried out the internship entitled "Deep learning" from September 2023- November 2023.

Internal Guide

External Guide (if Applicable)

Head of the Department

Submitted for Viva-voce Examination held on:

Internal Examiner

External Examiner

DECLARATION

I, **SNEHA SUNIL** hereby declare that the Internship Report entitled Deep learning done by me under the guidance **Mrs. R.SUDHA** at Sathyabama institute of science and technology is submitted in partial fulfilment of the requirements for the award of **Master of Science degree in Bioinformatics and data science**.

DATE:

SNEHA SUNIL

PLACE:

SIGNATURE OF THE CANDIDATE

ACKNOWLEDGEMENT

I am pleased to acknowledge my sincere thanks to the **Board of Management of SATHYABAMA** for their kind encouragement in doing this Internship and for completing it successfully. I am grateful to them.

I convey my thanks to **Dr. REKHA CHAKRAVARTHI M.E., PH.D. DEAN OF ARTS ANDSCIENCE**, and **Dr. JEMMY CHRISYT HEAD OF THE DEPARTMENT** for providing me necessary support and details at the right time during the progressive reviews.

I wish to express my thanks to all Teaching and Non-teaching staff members of the Department of Bioinformatics and Data science who were helpful in many ways in the completion of the Internship.

(SNEHASUNIL)

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CERTIFICATE OF COMPLETION



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CERTIFICATE

This certificate is presented to Sneha sunil from MSc.Bioinformatics and DataScience, 1st year for successfully completing the three months Value Added Course (Internship) on Deep Learning held from September 2023 to November 2023 , organized by the Dept. of Computer Science & Engineering, Sathyabama Institute of Science & Technology.

Dr.T.Sasikala
Dean
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(Faculty Coordinator)

Mrs.R.Sudha
(Faculty Coordinator)

CHAPTER-1

1. Abstract

During my internship at Sathyabama Institute of Science and Technology, I had the opportunity to delve into the fascinating world of deep learning, which is a type of artificial intelligence. Deep learning is used in various fields, such as identifying objects in images, understanding languages, and making predictions based on data. Throughout the internship, we used programming tools like Tensor Flow and Keras to put our learning into practice.

The internship was focused on understanding how deep learning can be applied to solve real-world problems. We explored tasks like teaching computers to recognize different objects in images, which is crucial for applications like self-driving cars and medical imaging. Additionally, we worked on language-related tasks, such as teaching computers to understand human language and translate between different languages. These tasks involved using techniques like neural networks and recurrent neural networks.

One important aspect of our work was ensuring that the models we created were fair and unbiased. We discussed how biases can inadvertently creep into AI systems and learned techniques to mitigate these biases. This is crucial for creating AI systems that treat everyone fairly and without discrimination.

Overall, the internship provided me with a deeper understanding of how deep learning works and how it can be used to tackle a wide range of problems. It was a valuable experience that equipped me with practical skills and knowledge in the field of artificial intelligence.

CHAPTER-2

2.1 Introduction to deep learning

Deep learning is a branch of artificial intelligence (AI) that replicates how the human brain processes information and forms patterns to be used in decision-making. It has become a game-changing technology with applications in many different industries. I had a fantastic opportunity to delve into the depths of deep learning and examine its applications and ramifications in the contemporary world during my internship at SATHYABAMA INSTITUTE OF SCIENCE AND TECHNOLOGY.

During my tenure at Satyabhama institute of science and technology, I set out on a quest to comprehend and leverage the capabilities of deep learning algorithms. With the support of knowledgeable mentors and an exciting learning atmosphere, I explored the complexities of neural networks, including recurrent neural networks (RNNs), convolutional neural networks (CNNs), and other cutting-edge methods.

CHAPTER-3

3.1 Purpose of the Internship

The purpose of the internship was to provide hands-on experience and practical learning opportunities in the field of deep learning. It aimed to familiarize participants with advanced concepts and techniques in deep learning and to apply these skills to real-world problems. Additionally, the internship sought to develop a deeper understanding of how deep learning can be utilized across various domains, including image recognition, natural language processing, and computer vision.

Through the internship, participants were expected to gain practical skills, theoretical knowledge, and an understanding of the ethical considerations involved in deploying deep learning solutions. Overall, the internship aimed to prepare participants for future careers in artificial intelligence and related fields by providing them with valuable experience and expertise in deep learning.

CHAPTER-4

4. Objective

The objective of my internship at Satyabhama institute of science of technology was to gain practical experience and in-depth understanding of deep learning, a rapidly advancing field within artificial intelligence (AI).

The primary goal of the internship was to bridge the gap between theoretical knowledge acquired in academic settings and the practical application of deep learning techniques in real-world scenarios. By working on hands-on projects under the guidance of experienced mentors, I aimed to develop the skills and expertise necessary to tackle complex problems using deep learning algorithms.

Additionally, the internship aimed to explore the diverse applications of deep learning across different domains. From image recognition and natural language processing to computer vision and predictive analytics, I sought to gain exposure to a wide range of applications to understand the versatility of deep learning technology.

Furthermore, an important objective of the internship was to cultivate an understanding of the ethical considerations surrounding deep learning. Discussions and workshops focused on topics such as bias, fairness, and transparency in AI systems, aiming to instill a sense of responsibility and awareness in the development and deployment of deep learning solutions.

As I embarked on this internship journey, my objectives were clear: to gain practical experience in deep learning, explore its applications, and understand the ethical implications of AI technology.

CHAPTER-5

5. Internship Experience

I had a fantastic opportunity to fully immerse myself in the deep learning realm during my internship at Sathyabama institute of science and technology getting practical skills and insights into this innovative area of artificial intelligence (AI).

In addition, my internship gave me insightful knowledge about the team-based nature of AI research and development. Working in interdisciplinary teams taught me how to successfully exchange knowledge, convey ideas, and participate in group problem-solving. These conversations created a lively learning atmosphere where concepts were shared, difficulties were overcome, and creativity was encouraged.

Upon reflection on my internship, I am appreciative of the chances and encounters that have enhanced my comprehension of deep learning and equipped me for upcoming pursuits in this fascinating field. This introduction lays the groundwork for a thorough examination of the tasks, difficulties, and insights I gained from my internship.

CHAPTER-6

6. Learning Outcomes

I gained a wide range of learning outcomes from my internship that have improved my comprehension and competence in deep learning. Through experiential learning and guided instruction, I have met a number of important learning objectives.

First off, I've gotten good at using frameworks like Tensor Flow for deep learning problems and at programming languages like Python. This has given me the confidence to create, train, and assess recurrent neural networks (RNNs), convolutional neural networks (CNNs), and other sophisticated designs.

Secondly, the internship has improved my comprehension of the real-world uses for deep learning. By working on projects related to computer vision, natural language processing, and image recognition, I have learned about the adaptability of deep learning technology and its potential to address practical issues.

The internship has also improved my critical thinking and problem-solving capabilities. Through overcoming obstacles throughout project execution, I have developed my ability to identify issues, come up with workable solutions, and refine strategies in order to get the results I want.

6.1. Achievement: Received Internship completion certificate.

CHAPTER-7

7. Conclusion

To sum up, I can say that my deep learning internship has been incredibly fulfilling and has given me important knowledge, abilities, and insights that will help me in my future work in the artificial intelligence industry.

I got the chance to work on a range of projects throughout the internship, each with its own set of difficulties and potential for growth. I got practical experience implementing deep learning techniques and models, from image recognition to natural language processing, which improved my comprehension of neural networks, convolutional neural networks (CNNs), recurrent neural networks (RNNs), and other sophisticated structures.

The main thing I've learned from the internship is how to use deep learning frameworks like Tensor Flow and Keras and programming languages like Python in a practical way. This has made it possible for me to efficiently construct and train models, as well as to test various architectures and maximize performance for certain applications.

Furthermore, the internship has extended my comprehension of the multifaceted uses of deep learning in several fields. I have personally seen how deep learning has revolutionized the healthcare, financial, and automotive industries, demonstrating its capacity to spur creativity and provide solutions to challenging issues.

In addition, the internship has improved my critical thinking and problem-solving capabilities. I have developed my ability to approach problems methodically, analyze data effectively, and iterate on ideas to attain desired outcomes by working through the hurdles experienced throughout project implementation.

I now have a strong feeling of ethical responsibility for the design and implementation of deep learning systems thanks to the internship. The significance of ethical considerations

in AI has been emphasized by discussions on bias, fairness, and transparency. This has shaped my
Way of thinking.

Upon reflection of my internship experience, I am appreciative of my colleagues' support and mentors' advice, as their knowledge and encouragement have been priceless. I'm sure that the abilities and information I've acquired from this internship will be helpful to me as I continue to research and make contributions to the fascinating topic of deep learning.

Finally, I would want to thank Sathyabama institute of science and technology from the bottom of my heart for giving me this wonderful internship opportunity. I can't wait to apply the knowledge I've gained and contribute significantly to the future development of AI and deep learning approach to AI development with responsibility and integrity.

CHAPTER-8

8.1 MINI PROJECT

DRUG REPURPOSING

Drug repurposing is also called as drug repositioning or drug reprofiling is the process of giving medications that are currently on the market and have already received approval for various uses new uses. Compared to creating brand new medications, this method has a number of benefits including lower development costs, quicker development times and a recognized safety profile

8.1.1 Aim: Drug thioguanine target screening and analysis- To investigate the potential of thioguanine as a treatment for Acute Myeloid Leukemia (AML) patients with NUDT15 biomarker variations

8.1.2 Objective: An derivative of thiopurine, thioguanine, has potential as a repurposed treatment for patients with Acute Myeloid Leukemia (AML), especially those with mutations in the NUDT15 gene. Thioguanine was first used to treat inflammatory bowel disease (IBD) and acute lymphoblastic leukemia (ALL). However, it has gained notice for its possible effectiveness in treating acute myeloid leukemia (AML), a condition marked by unchecked myeloid cell growth in the bone marrow.

First, we will evaluate the impact of NUDT15 gene variants on AML patients' thioguanine response.

Second, we will assess thioguanine's safety, tolerability, and mechanisms in AML, as well as how it affects leukemic cells.

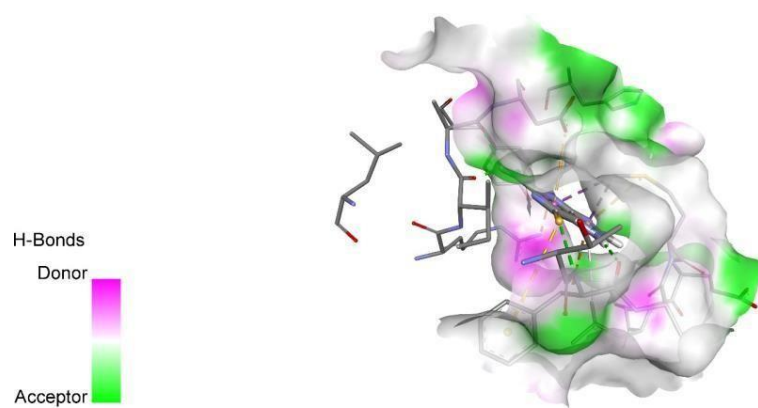
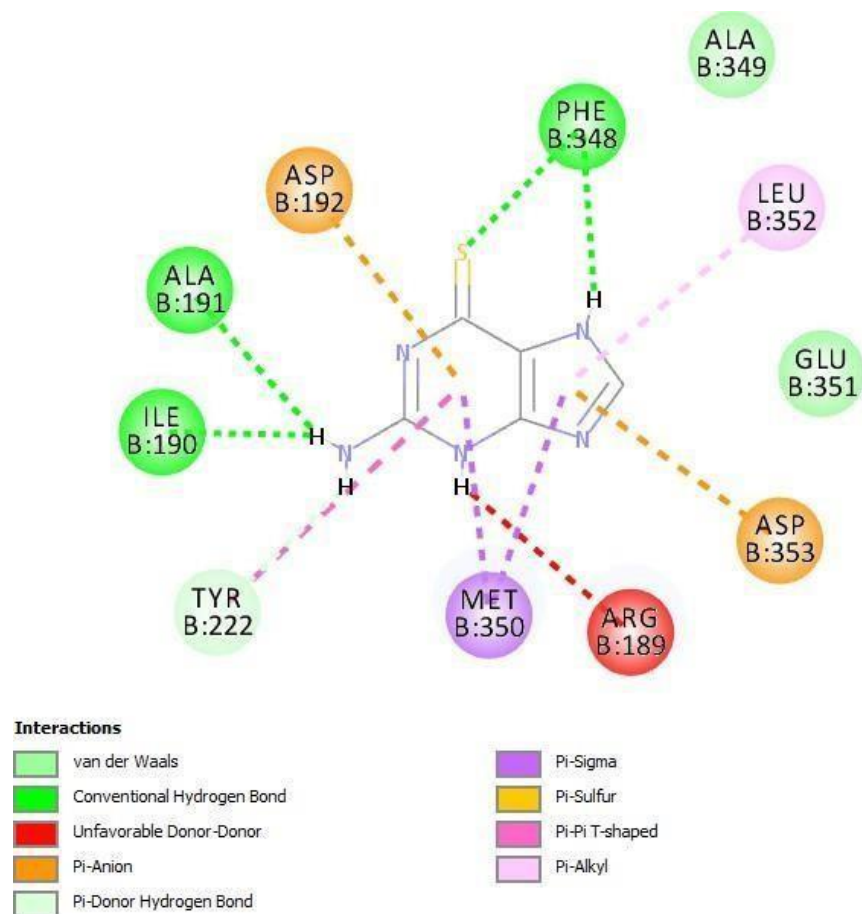
In addition, with the goal of optimizing treatment regimens, we will ascertain the optimal dosage and combination therapy for thioguanine in AML patients. We'll also find more biomarkers that predict responsiveness to thioguanine besides NUDT15.

Lastly, we will evaluate response rates, relapse-free survival, and overall survival in thioguanine-treated AML patients, with an emphasis on those with NUDT15 variants. The goal of this study is to progress thioguanine as a repurposed therapy for AML, with the potential to improve treatment outcomes and provide individualized care.

8.1.3 Methodology :

1. Thioguanine's molecular structure is downloaded in SDF format.
2. The drug's name is converted into its canonical SMILES notation.
3. The SMILES notation is entered into Swiss Target Prediction.
4. Over 20 potential targets are identified with high probability.
5. A network is created in Cytoscape, revealing hub genes.
6. Protein Data Bank (PDB) structures of hub genes are obtained, considering domain availability and resolution under 2.5.
7. The drug is docked with the protein structures in Discovery Studio.

8.1.4 Result



8.1.5 Interpretation

Drug name: Thioguanine

Approved for which disease: Acute myeloid leukemia

Suggested targets: PRKM3 ,HIST1H4A, CBP, RP11-109A6.1, GEMIN-5, APOL-II, MITOTIN, MN, ZNF294.

Chosen Target: PRKM3

NAME	PLP1	PLP2	JAIN	PMF	DOCK SCORE
2ZOQ					
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2723601	51.22	45.88	0.46	39.69	26.121
2723601	43.78	42.97	0.17	45.43	25.617
2723601	40.03	36.41	-0.51	53.54	24.998
2723601	43.01	36.69	0.08	32.14	24.389
2723601	48.87	40.04	0.2	56.22	24.092
2723601	40.47	37.56	0.15	20.79	24.038
2723601	48.79	39.85	0.01	52.12	23.964
2723601	26.4	25.34	-0.38	40.29	21.52
2723601	38.04	38.42	-0.05	32.34	15.14

NAME	DISTANCE	CATEGORY	TYPE	FROM	TO
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B:ASP192:OD2 - 2723601	4.12961	Electrostatic	Pi-Anion	B:ASP192:OD2	2723601
B:MET350:CE - 2723601	3.74674	Hydrophobic	Pi-Sigma	B:MET350:CE	2723601
2723601:S1 - B:PHE348	5.45789	Other	Pi-Sulfur	2723601:S1	B:PHE348
B:TYR222 - 2723601	5.7324	Hydrophobic	Pi-Pi T-shaped	B:TYR222	2723601

B:ARG189:NH 1 - B:ASP353:OD1	3.62674	Hydrogen Bond;Electrostatic	Salt Bridge	B:ARG189:NH 1	B:ASP353:OD1
B:ARG189:NH 2 - B:ASP353:OD2	4.2033	Electrostatic	Attractive Charge	B:ARG189:NH 2	B:ASP353:OD2
B:LEU163:N - B:ARG189:O	2.78656	Hydrogen Bond	Conventional Hydrogen Bond	B:LEU163:N	B:ARG189:O
B:HIS195:CD2 - B:ASP192:OD2	3.03847	Hydrogen Bond	Carbon Hydrogen Bond	B:HIS195:CD2	B:ASP192:OD2
B:ASP192:OD2 - 2723601	4.12961	Electrostatic	Pi-Anion	B:ASP192:OD2	2723601
2723601:H15 - B:TYR222	2.70055	Hydrogen Bond	Pi-Donor Hydrogen Bond	2723601:H15	B:TYR222

CHAPTER-9

9.1 Value added course:

9.1.1 NPTEL course: Mathematical modeling: analysis and application

Mathematical modelling is a powerful tool used to represent real-world phenomena mathematically. It involves creating mathematical equations that describe the behavior of systems, allowing us to understand and predict their behavior.

Through mathematical modelling, we can analyze complex systems, make predictions, and optimize processes, ultimately enhancing our understanding of the world around us and improving decision-making.



NPTEL Online Certification

(Funded by the MoE, Govt. of India)

This certificate is awarded to
SNEHA SUNIL
for successfully completing the course

Mathematical Modelling: Analysis and Applications

with a consolidated score of **51** %

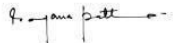
Online Assignments	20.83/25	Proctored Exam	30/75
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Total number of candidates certified in this course: **36**



Prof. Kaushik Ghosh,
Professor (Chemistry)
Coordinator CEC

Jan-Feb 2024
(4 week course)



Prof. Ranjana Pathania,
Professor (BSBE)
Coordinator (NPTEL)



Indian Institute of Technology Roorkee



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Roll No: NPTEL24MA32S544101326 To verify the certificate 

No. of credits recommended: 1 or 2

CHAPTER-10

10.1 MATLAB:

App Building Onramp

With its interactive, do-it-yourself design, App Building Onramp will provide quick video lessons and hands-on activities to help you learn how to use the MATLAB Application Designer to build interactive applications. After completing the application creation process, you can design, develop, and deploy MATLAB applications for a wide range of uses, from advanced computing to data visualization.

MATLAB Onramp

MATLAB Onramp, provided by Math Works, is a short, interactive course designed to introduce beginners to MATLAB programming. Through video tutorials and hands-on exercises, learners gain essential skills in variables, arrays, plotting, and basic programming concepts. It's a free resource accessible to anyone looking to start using MATLAB for academic, professional, or personal projects.

Signal Processing with MATLAB

Dive into the world of signal processing using MATLAB with the comprehensive Signal Processing Onramp. This interactive course combines theoretical concepts with hands-on exercises to help you understand and apply various signal processing techniques using MATLAB. From filtering and spectrum analysis to signal imaging, this Onramp gives you the capabilities to analyze and manipulate signals for a variety of applications.

Image Processing with MATLAB

Unleash the power of MATLAB for image manipulation with our Onramp image editor. This hands-on course is designed to introduce you to the basics of image processing and show you how MATLAB can be used to perform a variety of image analysis tasks. Through interactive tutorials and real-world examples, you will learn techniques such as image enhancement, segmentation and feature extraction that enable you to efficiently process and interpret images.

MATLAB Programming Techniques

Take your MATLAB skills to the next level with MATLAB Programming Techniques Onramp. This advanced course is designed for experienced MATLAB users who want to improve their programming skills. From optimization and debugging strategies to designing advanced data structures and algorithms, this Onramp covers a wide range of programming techniques to help you write powerful, robust, and maintainable MATLAB.

MATLAB for Data Processing and Visualization

It's a good idea to learn MATLAB for data processing and visualization, especially if you work with numerical data. Here are some things you might want to learn about processing and visualizing a data with MATLAB. These MATLAB capabilities enable you to handle a variety of data processing and visualization tasks, making it a powerful tool for data analysis and visualization.

Machine Learning with MATLAB

MATLAB is a versatile machine learning environment that contains rich built-in tools, functions, and documentation. Gaining knowledge of MATLAB machine learning will enable you to apply various machine learning techniques to real-world problems.

Image Processing Onramp

With an interactive, do-it-yourself approach, Image Processing Onramp offers short video courses and hands-on exercises to help you understand and use MATLAB image processing concepts. Complete the image processing onramp for a thorough understanding of image processing principles and methods. You will also gain hands-on experience using MATLAB to develop image processing algorithms.

Solving Nonlinear Equations with MATLAB

Unleash the power of MATLAB to solve complex nonlinear equations with Nonlinear Equation Solving Onramp. This self-paced course is designed to give you the skills you need to effectively handle nonlinear equations using the extensive computing capabilities of MATLAB. Through guided exercises, you will learn various numerical methods and

techniques for finding solutions to nonlinear equations in various scientific and engineering applications.

Deep Learning with MATLAB

Explore the advancement of deep learning with MATLAB with Deep Learning Onramp. This interactive course provides a thorough introduction to deep learning concepts and shows how to use MATLAB to build, train, and deploy deep neural networks. Whether you're new to deep learning or want to deepen your knowledge, this Onramp gives you the skills to tackle complex problems.

Statistics Onramp

Dive into the world of statistical analysis and data interpretation with MATLAB Statistics Onramp. This interactive learning experience provides a comprehensive overview of statistical concepts, from basic descriptive statistics to advanced data modeling techniques. By learning the statistical capabilities of MATLAB, you can analyze data, generate meaningful insights, and make informed decisions in a variety of fields.

MATLAB Fundamentals

Learn the basics of MATLAB programming from the ground up with MATLAB Fundamentals Onramp. Designed for beginners, this interactive course provides a structured learning path covering basic MATLAB syntax, data types, control flow, and function writing. Whether you're new to programming or transitioning from another language, this Onramp provides a solid foundation for your MATLAB journey.

Reinforcement Learning Onramp

Reinforcement Learning Onramp for MATLAB is a comprehensive introductory course that teaches you how to use MATLAB to build reinforcement learning algorithms and the principles of reinforcement learning.

Computer Vision Onramp

Computer vision is where knowledge from the real world meets digital data. Data from multiple cameras and sensors can be combined to create a digital reconstruction. In this course, you will use object recognition to find, track, and count turtles in a video.

Deep Learning Onramp

Deep Learning Onramp is an interactive, self-paced course that uses MATLAB to teach you how to apply and understand deep learning concepts through short video tutorials and hands-on activities. After completing the Deep Learning Onramp, you will have a thorough understanding of deep learning theories and methods and hands-on experience building and improving deep learning models in MATLAB.

Object-Oriented Programming Onramp

Journey through object-oriented programming (OOP) principles with the MATLAB object-oriented programming onramp. This interactive course combines concise video tutorials with hands-on exercises to teach you the basics of OOP in MATLAB. By the end of this Onramp, you will have a good understanding of how to use OOP concepts to create modular and reusable code in MATLAB.

Machine Learning Onramp

Journey through object-oriented programming (OOP) principles with the MATLAB object-oriented programming onramp. This interactive course combines concise video tutorials with hands-on exercises to teach you the basics of OOP in MATLAB. By the end of this Onramp, you will have a good understanding of how to use OOP concepts to create modular and reusable code in MATLAB.



Course Completion Certificate

Sneha Sunil

has successfully completed **100%** of the self-paced training course

MATLAB Fundamentals

DIRECTOR, TRAINING SERVICES

7 March 2024



Course Completion Certificate

Sneha Sunil

has successfully completed **100%** of the self-paced training course

MATLAB Programming Techniques

DIRECTOR, TRAINING SERVICES

22 March 2024



Course Completion Certificate

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Machine Learning Onramp



DIRECTOR, TRAINING SERVICES

4 February 2024



Course Completion Certificate

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Machine Learning with MATLAB



DIRECTOR, TRAINING SERVICES

13 March 2024



Course Completion Certificate

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Object-Oriented Programming Onramp



DIRECTOR, TRAINING SERVICES

21 December 2023



Course Completion Certificate

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has successfully completed **100%** of the self-paced training course

Reinforcement Learning Onramp



DIRECTOR, TRAINING SERVICES

5 March 2024



Course Completion Certificate

Sneha Sunil

has successfully completed **100%** of the self-paced training course

Signal Processing with MATLAB



DIRECTOR, TRAINING SERVICES

29 March 2024



Course Completion Certificate

Sneha Sunil

has successfully completed **100%** of the self-paced training course

Solving Nonlinear Equations with MATLAB



DIRECTOR, TRAINING SERVICES

26 March 2024



Course Completion Certificate

Sneha Sunil

has successfully completed **100%** of the self-paced training course

Statistics Onramp



Craig L. Santos

DIRECTOR, TRAINING SERVICES

29 February 2024



Course Completion Certificate

Sneha Sunil

has successfully completed **100%** of the self-paced training course

MATLAB Onramp



Craig L. Santos

DIRECTOR, TRAINING SERVICES

10 November 2023



Course Completion Certificate

Sneha Sunil

has successfully completed **100%** of the self-paced training course

Computer Vision Onramp



DIRECTOR, TRAINING SERVICES

4 February 2024



Course Completion Certificate

Sneha Sunil

has successfully completed **100%** of the self-paced training course

Deep Learning Onramp



DIRECTOR, TRAINING SERVICES

29 February 2024



Course Completion Certificate

Sneha Sunil

has successfully completed **100%** of the self-paced training course

Deep Learning with MATLAB

LEIGH HUNTER
DIRECTOR, TRAINING SERVICES

5 March 2024



Course Completion Certificate

Sneha Sunil

has successfully completed **100%** of the self-paced training course

Image Processing Onramp

LEIGH HUNTER
DIRECTOR, TRAINING SERVICES

21 March 2024



Course Completion Certificate

Sneha Sunil

has successfully completed **100%** of the self-paced training course

Image Processing with MATLAB

A handwritten signature in black ink, appearing to read "Ray L. Santos".

DIRECTOR, TRAINING SERVICES

26 March 2024

CHAPTER-11

11.1 Workshops

11.1.1) National Internal Property awareness mission



11.1.2) Microsoft using AI tools



Computational insight into drug discovery

System pharmacology approaches

INTRODUCTION TO SYSTEM PHARMACOLOGY

Systems pharmacology involves examining the impact of drugs on the human body as a complex biological system, utilizing principles from systems biology alongside high-throughput experiments. Additionally, it entails computational analysis of regulatory networks.

Analyzing networks that depict drug-target relationships can provide insights into the overall trends in approved drugs and the progress of drug discovery. With a rising number of targeted therapies both approved and in development, there emerges a fresh array of challenges concerning efficacy and adverse effects.

The expansively characterized domain of systems biology has amassed a significant volume of knowledge concerning the biological mechanisms underlying disease and the effects of drugs.

The majority of present drug discovery endeavors focus on intricate diseases, comprehending the pathophysiology at a systemic level. This could facilitate the formulation and advancement of drugs with enhanced success rates in clinical trials.

Considering the diverse mechanisms through which drugs can induce side effects, it's improbable for a singular approach to predict all potential adverse reactions across all medications. Systems biology approaches enable the integration of diverse datasets.

INSILICO SCREENING OF DRUG TARGETS

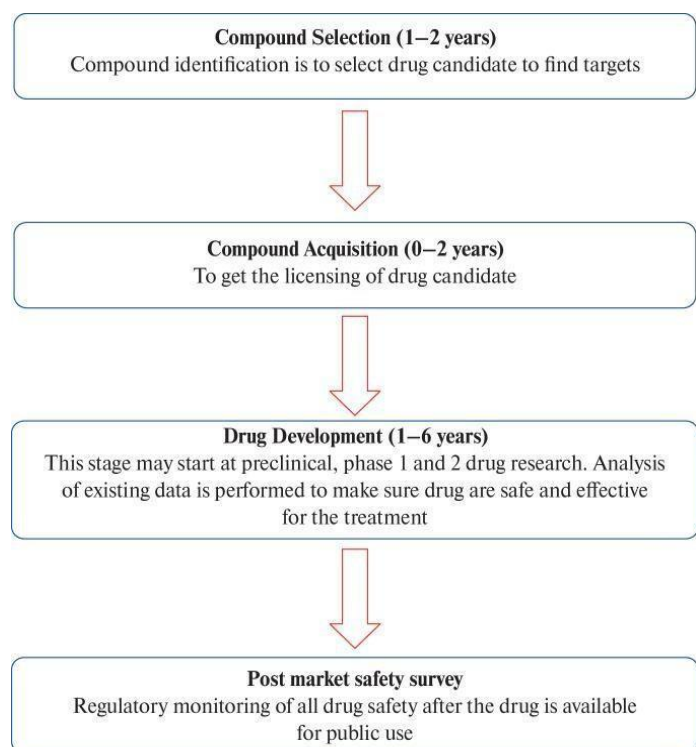
In Silico screening refers to a computer-based method utilizing virtual screening tools to anticipate the behavior of various compounds.

The introduction of computational approaches has greatly contributed to systematically guiding processes and reducing the time needed for drugs to reach the market. This is achievable under the premise that minimizing drug side effects is feasible when the drug candidate exhibits potency and high selectivity.

An in silico target prediction platform can serve for both structure-based target prediction and ligand-based target prediction. Graphic tools have been developed and integrated to aid in visualizing the targets. Numerous new tools and algorithms have emerged to assist in analyzing and visualizing the intricate data.

In silico screening finds applications in various domains reliant on biological research, encompassing drug development, food toxicology research, cosmetics development, and beyond.

Ligand-based and structure-based are the primary approaches utilized in in silico screening. When both the ligands and target have available structural data, these methods can also be merged.



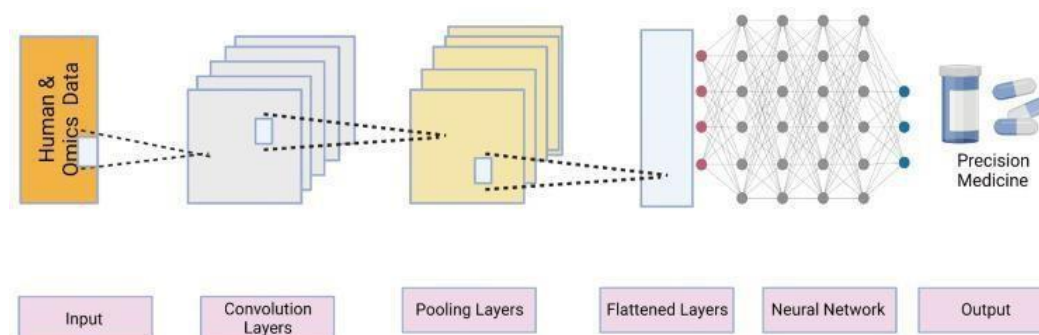
To achieve a shift towards personalized medicine, a comprehensive understanding of the pathogenesis of a drug events and side effects on a case-by-case basis will be essential. Systems pharmacology methodologies will aid in pinpointing off-target effects of drugs, thus elucidating unintended consequences.

NETWORK BASED DRUG REPURPOSING STRATEGIES

Drug repurposing involves utilizing an existing medication for a novel treatment that was not previously indicated. In the current healthcare landscape, drug repurposing has emerged as a necessity to accelerate the drug discovery process and provide expedited solutions to the overwhelming demands and needs within healthcare.

Repurposing involves identifying new compounds based on their phenotypic benefits, without requiring an explicit definition of their mechanism of action. These compounds can be directly evaluated in preclinical animal models, rendering the results more applicable to clinical research and real-world applications.

ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING IN PHARMACOLOGY



AI boosts efficiency and uniformity in handling individual case safety reports (ICSRs) by automating manual processes, eliminating bias, and furnishing valuable insights for data scientists and medical professionals.

CHALLENGES AND OPPORTUNITIES IN VIRTUAL DRUG DEVELOPMENT PIPELINES

AI offers numerous ways for assisting in the identification of the correct target. Initially, pinpointing the appropriate target fundamentally revolves around comprehending the underlying biology of the disease.

AI can aid in processing the vast array of information collected by scientists in extensive and diverse systems biology databases, facilitating the identification of promising targets. Furthermore, natural language processing systems have the capability to directly analyze scientific literature, serving the same purpose.

Although holding great promise, virtual drug development pipelines encounter obstacles concerning data quality, model accuracy, regulatory acceptance, ethical considerations, and interdisciplinary collaboration.



Overcoming these challenges involves ensuring the accessibility of high-quality and pertinent data for computational modeling, validating predictive models effectively, and meeting regulatory criteria for virtual drug development.

These hurdles represent significant barriers that necessitate careful navigation and innovative solutions within the field. Furthermore, addressing ethical and legal intricacies, including data privacy and intellectual property rights, demands meticulous attention and consideration.

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Systems pharmacology involves examining the impact of drugs on the human body as a complex biological system, utilizing principles from systems biology alongside high-throughput experiments. Additionally, it entails computational analysis of regulatory networks.

Analyzing networks that depict drug-target relationships can provide insights into the overall trends in approved drugs and the progress of drug discovery. With a rising number of targeted therapies both approved and in development, there emerges a fresh array of challenges concerning efficacy and adverse effects.

The expansively characterized domain of systems biology has amassed a significant volume of knowledge concerning the biological mechanisms underlying disease and the effects of drugs.

The majority of present drug discovery endeavors focus on intricate diseases, comprehending the pathophysiology at a systemic level. This could facilitate the formulation and advancement of drugs with enhanced success rates in clinical trials.

Considering the diverse mechanisms through which drugs can induce side effects, it's improbable for a singular approach to predict all potential adverse reactions across all medications. Systems biology approaches enable the integration of diverse datasets.

In Silico screening refers to a computer-based method utilizing virtual screening tools to anticipate the behavior of various compounds.

The introduction of computational approaches has greatly contributed to systematically guiding processes and reducing the time needed for drugs to reach the market. This is achievable under the premise that minimizing drug side effects is feasible when the drug candidate exhibits potency and high selectivity.

An in silico target prediction platform can serve for target prediction. Graphic tools have been developed and integrated to aid in visualizing the targets. Numerous new tools and algorithms have emerged to assist in analyzing and visualizing the intricate data.

In silico screening finds applications in various domains reliant on biological research, encompassing drug development, food toxicology research, cosmetics development, and beyond.

Ligand-based and structure-based are the primary approaches utilized in in silico screening. When both the ligands and target have available structural data, these methods can also be merged.

To achieve a shift towards personalized medicine, understanding of the pathogenesis of drug events and side effects on a case-by-case basis will be essential. Systems pharmacology methodologies will aid in pinpointing off-target effects of drugs, thus elucidating unintended consequences.

Drug repurposing involves utilizing an existing medication for a novel treatment that was not previously indicated. In the current healthcare landscape, drug repurposing has emerged as a necessity to accelerate the drug discovery process and provide expedited solutions to the overwhelming demands and needs within healthcare.

Repurposing involves identifying new compounds based on their phenotypic benefits, without requiring an explicit definition of their mechanism of action. These compounds can be directly evaluated in preclinical animal models, rendering the results more applicable to clinical research and real-world applications.

It further boosts efficiency and uniformity of handling individual case safety reports (ICSRs) by automating manual processes, eliminating bias, and furnishing valuable insights for data scientists and medical professionals.

It offers numerous ways for assisting in the identification of the correct target. Initially, pinpointing the appropriate target fundamentally revolves around comprehending the underlying biology of the disease.

It can aid in processing the vast array of information collected by scientists in extensive and diverse systems biology databases, facilitating the identification of promising targets. Furthermore, natural language processing systems have the capability to directly analyze scientific literature, serving the same purpose.

Although holding great promise, virtual drug development pipelines encounter obstacles concerning data quality, model accuracy, regulatory acceptance, ethical considerations, and interdisciplinary collaboration.

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