

**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

**ATCHAYA R
REGISTER NO:43739026**



**DEPARTMENT OF MECHANICAL
ENGINEERING SCHOOL OF MECHANICAL ENGINEERING**

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



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Jeppiaar Nagar, Rajiv Gandhi Salai, Chennai – 600 119

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DEPARTMENT OF BIOINFORMATICS AND DATASCIENCE

BONAFIDE CERTIFICATE

This is to certify Intern Report is the bonafide work of ATCHAYA R (43739026) who carried out an internship on “Deep Learning” from September 2023 to November 2023

—

Internal Guide

External Guide (if Applicable)

Head of the Department
(Name in Capital letters with Seal & Signature)

Submitted for Viva-voce Examination held on:

Internal Examiner

External Examiner

DECLARATION

I, Atchaya Ranjith hereby declare that the internship report entitles “deep learning” done by me under the guidance of Mrs. R Sudha at Sathyabama institute of science and technology is submitted in partial fulfilment of requirements for the award of master of science degree in bioinformatics and Data science

DATE:

(ATCHAYA RANJITH)

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 project 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 and science** and **Dr. Jemmy Christy 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.

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CHAPTER 1

INTERNSHIP

Deep Learning

1.1. DEEP LEARNING

Deep learning, at the forefront of the constantly evolving artificial intelligence landscape, is revolutionizing industries and expanding the capabilities of machines.

With a deep sense of enthusiasm and a commitment to continuous learning, I am excited to present this internship report, which chronicles my journey and insights into the world

Deep learning is a subset of artificial intelligence and machine learning(ML). Which can mimic the decision making skills by human.

CHAPTER 2

2.1. PURPOSE OF INTERNSHIP

My internship served a dual purpose: to acquire hands-on experience applying deep learning techniques and to actively engage in discussions about its evolving developments.

Deep learning, which draws inspiration from the brain's structure and operations, has become instrumental in addressing intricate problems across diverse fields. Throughout this internship, my objectives included immersing myself in the nuances of deep learning, grasping its fundamental principles, and investigating its capabilities in addressing practical challenges.

The internship encompassed topics ranging from introductions to networks, practical implementations, and other pertinent tools utilized in deep learning.

CHAPTER 3

3.1 OVERVIEW OF DEEP LEARNING

We'll start by building a comprehensive grasp of the foundational principles that underpin deep learning, encompassing neural networks, activation functions, and loss functions.

3.1.1 NEURAL NETWORK:

We'll delve into diverse neural network architectures, such as feedforward neural networks, convolutional neural networks (CNNs), and recurrent neural networks (RNNs), aiming to comprehend their designs and practical uses.

3.1.2 TRAINING AND OPTIMIZATION:

We'll explore the training procedures of neural networks, encompassing concepts such as gradient descent, backpropagation, and optimization algorithms crucial for achieving model convergence and improving performance.

3.1.3 APPLICATION AND ADVANCED TECHNIQUES:

Expanding on foundational knowledge, we'll delve into advanced methodologies within deep learning, such as transfer learning, generative adversarial networks (GANs), and reinforcement learning, unlocking their capabilities in addressing intricate tasks. Additionally, we'll investigate the extensive applications of deep learning across various domains, such as computer vision, natural language processing, healthcare, finance, and autonomous systems, demonstrating its adaptability and significance.

3.1.4 ETHICAL AND SOCIAL IMPACTS:

As we progress, we'll also discuss the ethical issues and societal impacts related to deep learning technologies. This involves talking about fairness, bias, privacy, and the responsible use of AI.

CHAPTER 5

4.1. BACKGROUND

My internship in Deep Learning was facilitated by Sathyabama Institute of Science and Technology, renowned for offering dynamic internship opportunities across various disciplines. Collaborating with top industries, the institute tailors structured programs to students' preferences, fostering hands-on learning and professional growth. Through mentorship from industry professionals and practical projects, students acquire invaluable insights and competencies, preparing them for successful careers. These internships prioritize not just technical skills but also soft skills like communication and teamwork, enhancing students' employability and networks. Sathyabama's internships bridge the gap between academia and industry, providing students with real-world experiences and ensuring their readiness for their chosen fields. Moreover, beyond technical expertise, the internships focus on holistic professional development, emphasizing essential soft skills such as problem-solving and leadership. By engaging in real world projects, students gain practical insights into industry practices and trends, earning academic credit along the way, which contributes to their overall academic advancement and career preparedness. In essence, Sathyabama Institute of Science and Technology's internship programs are instrumental in connecting academia with industry, empowering students to excel in their careers post-graduation.

CHAPTER 6

5.1. OBJECTIVES

5.1.1. PRACTICAL KNOWLEDGE:

Gain practical experience using deep learning frameworks like Tensor Flow and PyTorch, with the goal of implementing neural networks and improving their performance for targeted tasks.

5.1.2. APPLICABILITY:

Investigate the latest advancements in deep learning, examining their consequences and assessing their relevance across various fields such as computer vision, natural language processing, and robotics.

5.1.3. UNDERTAKING PROJECT WORK:

Embark on a hands-on project employing deep learning methods, utilizing academic understanding to address real-world challenges or improve current systems.

5.1.4. DOCUMENTATION:

document the learning process, experimental results, and project achievements, enabling the exchange of knowledge and enriching the collective comprehension of deep learning approaches.

CHAPTER 6

6.1. IMPORTANCE OF MY OBJECTIVES

6.1.1 SELF IMPROVEMENT:

These objectives were pivotal for my personal development, facilitating the acquisition of practical skills and knowledge vital for a career in deep learning.

Through hands-on experience and research, my aim was to enhance my understanding and expertise in this rapidly advancing field.

6.1.2. CAREER DEVELOPMENT:

Attaining these goals would elevate my professional growth, rendering me more competitive in the job market and unlocking avenues for elevated positions in deep learning and associated domains. Employers highly prize the capacity to execute projects and proficiently communicate findings through documentation and reporting.

6.1.3. CONTRIBUTION TO ORGANISATIONAL SUCCESS:

Achieving these goals would additionally serve the organization by arming me with the expertise necessary to contribute efficiently to ongoing projects and research endeavours. The practical skills and insights acquired during the internship would empower me to deliver significant contributions to the organization's goals within the realm of deep learning.

6.1.4. SHARING OF LEARNINGS:

Through documenting and reporting, my goal was to enhance the organization's and the wider research community's grasp of deep learning methodologies. By sharing insights and findings, I aimed to foster collaboration and innovation, ultimately driving the organization's progress in using deep learning for impactful solutions. In essence, the internship objectives were crucial for my personal growth and for

CHAPTER 7

7.1. INTERNSHIP EXPERIENCE:

During my Deep Learning internship, I acquired and honed a wide range of skills crucial for success in this field. Here's a breakdown of some key skills I developed:

7.1.1. PROGRAMMING SKILLS:

I got better at programming, especially in Python, and became proficient in using deep learning frameworks like Tensor Flow and PyTorch.

7.1.2. NEURAL NETWORK DESIGN:

I learned how to design and build different types of neural networks for tasks such as image classification and sequence prediction.

7.1.3. DATA HANDLING:

I mastered techniques for preparing and enhancing data to make models perform better.

7.1.4. OPTIMIZATION TECHNIQUE:

I learned how to fine-tune models for better performance using methods like grid search and adjusting parameters.

7.1.5. PERFORMANCE & EVALUATION:

I gained insight into assessing model performance and understanding metrics like accuracy and precision.

7.1.6. TRANSFER LEARNING:

I explored using pre-trained models for new tasks and adapting them to fit specific needs.

7.1.7. MANAGEMENT SKILLS:

I improved at organizing and documenting projects effectively.

7.1.8. CRITICAL THINKING:

I sharpened my ability to tackle problems and debug issues encountered during model development.

7.1.9. COMMUNICATION:

I learned how to communicate complex ideas clearly and present project findings effectively

CHAPTER 8

8.1. LEARNING OUTCOMES:

Reflecting on my experience during the Deep Learning internship, I've gained invaluable insights that have significantly broadened my understanding of this dynamic field. Here are some key reflections I'd like to share:

8.1.1. UNDERSTANDING COMPLEXITY:

Deep learning is incredibly intricate, from the inner workings of neural networks to the fine-tuning of algorithms. I've realized that mastering deep learning requires ongoing learning and exploration.

8.1.2. INTERDISCIPLINARY CONNECTION:

I've learned that deep learning connects with various fields like computer science, mathematics, and even neuroscience. This internship showed me how deep learning can be applied in diverse areas like healthcare and finance.

8.1.3. IMPORTANCE OF DATA:

The quality and quantity of data profoundly affect the performance of deep learning models. I've learned the significance of pre-processing and curating data for better model performance and the ethical considerations surrounding data usage.

8.1.4. ITERATIVE LEARNING:

Deep learning is all about continuous experimentation and refinement. Embracing failure as part of the learning process has been crucial, as each iteration brings valuable insights.

8.1.5. ETHICAL CONSIDERATION:

Deep learning technologies raise important ethical and social questions, such as bias and privacy issues. This internship has heightened my awareness of these concerns and the responsibility we have as practitioners to address them.

8.1.6. COMMUNITY ENGAGEMENT:

Engaging with the deep learning community has been enlightening. The openness to share knowledge and resources has expanded my network and exposed me to diverse perspectives.

8.1.7. ACTIVE LEARNING:

Deep learning is a field that's constantly evolving. This internship has instilled in me a commitment to continuous learning and staying updated on the latest developments.

CHAPTER 9

9.1. CONCLUSION:

The Deep Learning internship has been an enriching experience that has fuelled my passion for the field. It has equipped me with the skills and knowledge to pursue a rewarding career in artificial intelligence and machine learning.

ACHIEVEMENT:

Attached completed certificate.



ATCHAYA Ranjith

by OfficialTurnitin

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File name: 43749026.docx (14.59K)

Word count: 714

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Mathematical modelling Techniques in bioinformatics: Advancing Precision Medicine

Abstract

The concept of "precision medicine (systems medicine)" aims to bring about a change in healthcare systems in the future by emphasizing disease prevention over symptom treatment. This approach will be more proactive and predictive. The core of this strategy will be the individualization of care for every patient, with easy access to and computational integration of all patient medical data. Scientific funding programs in the USA and the EU, as well as biomedical researchers and trailblazing physicians³, are quickly adopting precision medicine. Both the White House Precision Medicine Initiative and [REDACTED], heavily rely on precision medicine. Treatment choices and patient care could be completely transformed by precision medicine.

Introduction

It is a relatively new idea to customize medical treatments to a patient's characteristics using contemporary tools. A few decades ago, a lot of scientists believed that this kind of idea was utopian. In the past, clinical judgment was based on pathophysiology knowledge and clinical experience, using a "one size fits all" methodology. This paradigm shift was accelerated by the Human Genome Project, which changed healthcare by enabling targeted therapies through the quick development of inexpensive DNA sequencing techniques.

Today's medicine combines a number of technologies for accurate diagnosis and treatment. The "five rights"—administering [REDACTED] to [REDACTED], and via the appropriate route of administration—form the basis of the framework for successful clinical outcomes.

Personalized genomics and disease risk assessment

It is a relatively new idea to customize medical treatments to a patient's characteristics using contemporary tools. A few decades ago, a lot of scientists believed that this kind of idea was utopian. In the past, clinical judgment was based on pathophysiology knowledge and clinical experience, using a "one size fits all" methodology. This paradigm shift was accelerated by the Human Genome Project, which changed healthcare by enabling targeted therapies through the quick development of inexpensive DNA sequencing techniques.

Today's medicine combines a number of technologies for accurate diagnosis and treatment. The "five rights"—administering [REDACTED] to [REDACTED], and via the appropriate route of administration—form the basis of the framework for successful clinical outcomes.

Modelling tumour evolution and heterogeneity

Agent-based models (ABMs) strive to capture complex and emergent behaviors of cell populations at the single-cell resolution using a set of straightforward rules. When specific cellular behavior mechanisms are unknown but the qualitative circumstances surrounding specific behaviors are understood, ABMs can be especially helpful. Cellular automata (CAs), which are arranged in a regular grid and have a limited number of discrete states that they can assume, are the most basic kind of ABM. Updates can be carried out synchronously or asynchronously, and rules are defined to modify the state of the cell based on its current value and the values of its neighbors.

Quantitative systems pharmacology

A new area of modelling technology called "quantitative systems pharmacology" (QSP) explains how medications and biological systems interact dynamically. Lately, QSP has been utilized more and more for different kinds of decision-making, including drug discovery and development in the pharmaceutical industry. Unlike empirical and statistical models, QSP integrates comprehensive biological information to represent complex systems of human physiology. As a result, it can be used for a variety of purposes, such as the identification of target and/or disease-related biomarkers, hypothesis testing, and clinical efficacy or toxicity prediction. Conversely, the enormous number of biological components in QSP models causes their structures to become extremely complex.

Conclusion

In order to ensure that bioinformatics can be applied in a clinical setting, predictive modelling approaches play a crucial role. [redacted] essential [redacted] appropriate [redacted] to integrate it [redacted] high-throughput technology [redacted] the bioinformatics pipeline. This will ensure that the results provided to clinicians are reliable and that there is a technological advantage over existing methodologies.

[redacted] early stages of development, [redacted] numerous [redacted] just [redacted] beginning to emerge [redacted] newly developed, cutting-edge academic technology. However, the transition [redacted] academic [redacted] to [redacted] is a lengthy learning and adaptation process.

ATCHAYA Ranjith

ORIGINALITY REPORT

SIMILARITY INDEX **10**%
INTERNET SOURCES%**6** PUBLICATIONS%**0** STUDENT PAPERS **4**%

PRIMARY SOURCES

1 www.ncbi.nlm.nih.gov Internet Source

5%

2 Submitted to University College London Student Paper

4%

3 www.law-right.com Internet Source

1%

Exclude quotes Off
Exclude bibliography On

Exclude matches Off

ATCHAYA Ranjith

GRADEMARK REPORT

GENERAL COMMENTS

FINAL GRADE **/0**

CHAPTER 10

REVIEW ARTICLE

I intend to write a review article on current growing research area in Bioinformatics
**“MATHEMATICAL MODELLING TECHNIQUES IN BIOINFORMATICS:
ADVANCING PRECISION MEDICINE”.**

ABSTRACT:

Precision medicine, also known as systems medicine, aims to revolutionize healthcare by shifting the focus from treating symptoms to preventing diseases. This proactive and predictive approach involves tailoring care to each patient and integrating all their medical data for easy access and analysis. In the USA and the EU, funding programs like the White House Precision Medicine Initiative and Horizon 2020 are driving the adoption of precision medicine by researchers and physicians. This approach has the potential to completely transform treatment decisions and patient care.

VIEW ON ADVANCING PRECISION MEDICINE:

Personalized genomics and disease risk assessment represent a ground breaking approach in modern medicine, leveraging contemporary tools to customize medical treatments based on individual patient characteristics. While this idea was once deemed utopian, the paradigm shift towards personalized medicine has been accelerated by advancements like the Human Genome Project. This initiative revolutionized healthcare by facilitating targeted therapies through the rapid development of cost-effective DNA sequencing techniques. Previously, clinical judgment relied on pathophysiology knowledge and experience, following a "one size fits all" methodology. However, the advent of personalized genomics has ushered in a new era where treatments are tailored to each patient's unique genetic makeup.

Today's medical landscape integrates a plethora of technologies to ensure accurate diagnosis and treatment. The "five rights" framework emphasizes administering medications correctly - to the right patient, at the right time, dose, and via the appropriate route of administration. This framework serves as the cornerstone for achieving successful clinical outcomes by prioritizing precision and efficacy in medical interventions.

In cancer research, modelling tumour evolution and heterogeneity is paramount for understanding disease progression and optimizing treatment strategies. Agent-based models (ABMs) are instrumental in capturing complex cell behaviours at the single-cell level. By employing straightforward rules, ABMs simulate emergent behaviours, making them invaluable tools when specific cellular mechanisms are not fully understood. Cellular automata (CAs), a fundamental type of ABM, are arranged in a regular grid and undergo state changes based on predefined rules, reflecting the dynamic nature of cellular interactions within tumours.

Another emerging area in medical modelling is quantitative systems pharmacology (QSP), which elucidates the dynamic interactions between medications and biological systems. QSP integrates comprehensive biological information to represent complex human physiology, offering insights into various aspects of drug discovery and development. Unlike empirical and statistical models, QSP accounts for the intricate network of biological components, enabling the identification of disease-related biomarkers, hypothesis testing, and prediction of clinical outcomes. However, the complexity of QSP models poses challenges due to the vast number of biological variables involved, necessitating sophisticated computational approaches for analysis and interpretation.

personalized genomics, ABMs, and QSP represent cutting-edge approaches transforming healthcare by enhancing treatment precision and efficacy. These innovative methodologies not only revolutionize disease management but also pave the way for more targeted and personalized medical interventions, ultimately improving patient outcomes and quality of life.

CONCLUSION:

Predictive modelling is vital for applying bioinformatics in clinical settings. It's important to choose the right modelling framework for each case and integrate it well with high-throughput technology and the bioinformatics pipeline. This ensures reliable results for clinicians and gives a technological edge over existing methods.

Clinical bioinformatics is still developing, and many start-ups are emerging from academic technology. However, transitioning to sustainable clinical bioinformatics services takes time and adaptation.

CHAPTER 11

MATLAB COURSES

MATLAB ONRAMP:

The objective of the MATLAB Onramp is to provide beginners with a comprehensive introduction to MATLAB, covering essential topics such as basic syntax, data types, plotting, and programming fundamentals. By the end of the Onramp, participants should have a solid understanding of how to use MATLAB for data analysis, visualization, and basic programming tasks. Additionally, it aims to equip learners with the skills and confidence to continue exploring MATLAB independently for their academic, research, or professional pursuits.

DEEP LEARNING:

Understand the fundamentals of deep learning and neural networks. Learn how to design, train, and evaluate deep learning models using MATLAB's Deep Learning Toolbox. Gain hands-on experience with building and deploying deep learning models for various tasks such as image classification and regression.

DEEP LEARNING WITH MATLAB:

Explore advanced deep learning concepts and techniques. Learn how to leverage MATLAB's capabilities for deep learning research and development. Dive deeper into topics such as convolutional neural networks (CNNs), recurrent neural networks (RNNs), and transfer learning.

STATISTIC ONRAMP:

Acquire a foundational understanding of statistical concepts and methods. Learn how to perform data analysis, hypothesis testing, and statistical modeling using MATLAB. Gain practical skills in exploring and visualizing data, fitting distributions, and conducting statistical inference.

INTRODUCTION TO SYMBOLIC MATH WITH MATLAB:

Familiarize yourself with symbolic math capabilities in MATLAB. Learn how to perform symbolic computations, solve algebraic equations, and manipulate symbolic expressions. Explore applications of symbolic math in calculus, linear algebra, and differential equations.

REINFORCEMENT LEARNING WITH MATLAB:

Understand the principles and algorithms of reinforcement learning. Learn how to implement and train reinforcement learning agents using MATLAB. Gain practical experience in solving reinforcement learning problems, such as control tasks and decision-making scenarios.

DATA PROCESSING AND VISUALISATION:

This Onramp equips participants with skills in importing, cleaning, and visualizing data using MATLAB. By mastering data manipulation and visualization techniques, learners can effectively communicate insights derived from datasets.

OBJECT ORIENTED PROGRAMMING:

In this Onramp, participants gain a solid understanding of object-oriented programming (OOP) principles within MATLAB. Through hands-on practice, they learn to design and implement classes, enhancing code organization and reusability in MATLAB projects.



Course Completion Certificate

Atchaya Ranjith

has successfully completed **100%** of the self-paced training course
MATLAB for Data Processing and Visualization

DIRECTOR, TRAINING SERVICES

27 March 2024



Course Completion Certificate

Atchaya Ranjith

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

DIRECTOR, TRAINING SERVICES

5 March 2024



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Deep Learning Onramp

A handwritten signature in black ink, reading "Ray L. Santos".

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5 March 2024



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Machine Learning Onramp

A handwritten signature in black ink, reading "Ray L. Santos".

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Deep Learning with MATLAB



DIRECTOR, TRAINING SERVICES

12 March 2024



Course Completion Certificate

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Introduction to Symbolic Math with MATLAB



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MATLAB Onramp



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Statistics Onramp



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Object-Oriented Programming Onramp

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

DIRECTOR, TRAINING SERVICES

9 February 2024



Course Completion Certificate

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

Machine Learning with MATLAB

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

DIRECTOR, TRAINING SERVICES

30 March 2024



Course Completion Certificate

Atchaya Ranjith

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

Reinforcement Learning Onramp



A handwritten signature in black ink, appearing to read "Craig Santos", written over a horizontal line.

DIRECTOR, TRAINING SERVICES

6 March 2024

CHAPTER 12

MINI Project:

MINI PROJECT:

DRUG REPURPOSING:

Drug repurposing, sometimes referred to 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 as lower development costs, quicker development times, and a recognized safety profile.

Aim:

Drug Nilotinib target screening and analysis- To investigate the potential of Nilotinib as a treatment for Chronic Myeloid Leukemia (CML) patients with BCR-ABL biomarker variations.

OBJECTIVE:

The objective for drug repurposing in nilotinib against Chronic Myeloid Leukemia (CML) can be multifaceted, but it generally revolves around optimizing treatment efficacy, overcoming drug resistance, and potentially expanding its therapeutic utility beyond its initial indication. Here are some specific objectives:

Enhancing Treatment Efficacy: Investigate whether nilotinib can achieve better outcomes in CML patients compared to existing therapies. This could involve conducting clinical trials to assess its efficacy in different patient populations, such as those with newly diagnosed CML or those who have developed resistance to other tyrosine kinase inhibitors (TKIs).

Overcoming Resistance: Explore whether nilotinib can

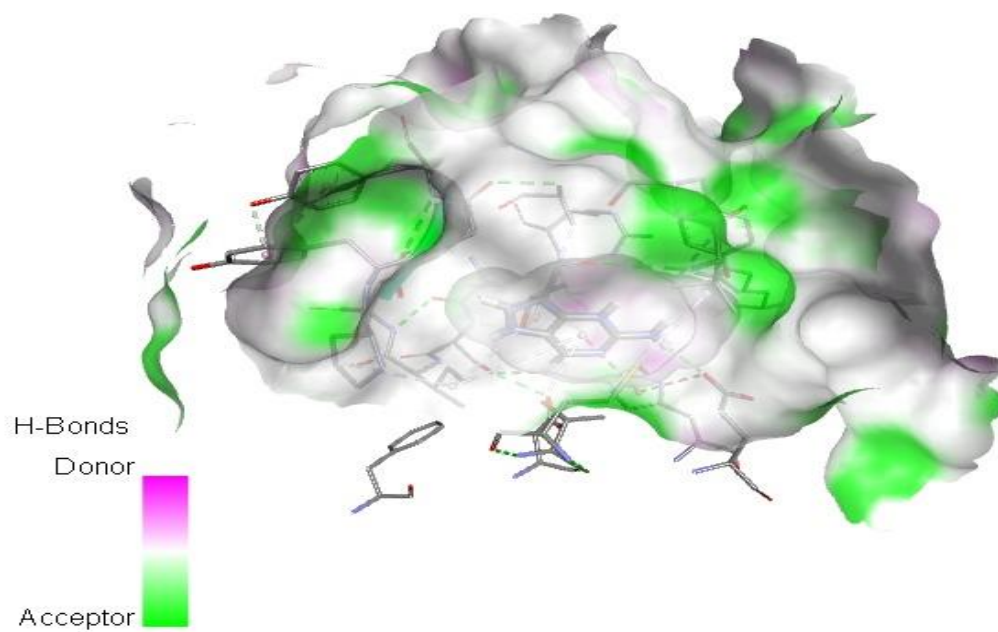
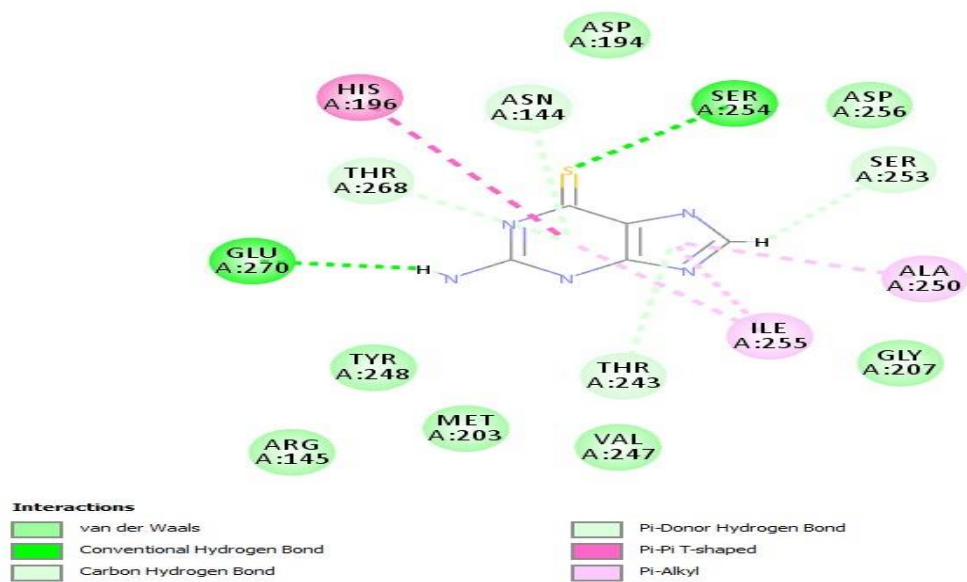
effectively overcome resistance mechanisms that develop in CML patients treated with other TKIs, such as imatinib. This may involve studying the molecular pathways involved in resistance and determining if nilotinib's distinct mechanism of action can circumvent these resistance mechanisms.

Combination Therapies: Investigate the potential synergistic effects of combining nilotinib with other drugs, either TKIs or non-TKI agents, to improve treatment outcomes. This approach could involve preclinical studies to identify promising drug combinations and subsequent clinical trials to evaluate their efficacy and safety in CML patients.

Methodology:

1. Nilotinib 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.

RESULT:



INTERPRETATION:

Drug name: Nilotinib

Approved for which disease: Chronic myeloid leukemia

Suggested targets: RPS, FYN, NSS, CSBP, SAPK, ABL, CLK1, HSP90N

Chosen Target: SAPK (Mitogen activated kinase)

MOLECULE TABLE:

NAME	PLP1	PLP2	Jain	PMF	Dock-score
6I5H					
31703	93.22	80.73	0.16	153.5	60.859
31703	39.6	53.01	-0.24	92.98	55.372
31703	57.92	63.17	1.09	163.44	54.856
31703	51.59	63.08	-0.91	102.1	54.206
31703	75.87	67.14	-0.77	99.44	53.536
31703	32.98	47.21	0.72	97.38	53.151
31703	87.27	74.56	-0.6	126.02	51.681
31703	80.81	69.18	-1.09	138.54	51.531
31703	97.91	92.04	2.24	122.41	50.631
31703	91.37	81.27	-0.21	146.95	50.406

NON – BOND TABLE:

Name	Distance	Category	Type	From	To
A:ARG160:NH2 - A:ASP180:OD2	2.81934	Hydrogen Bond;Electrostatic	Salt Bridge	A:ARG160:NH2	A:ASP180:OD2
A:ARG204:NH1 - A:GLU232:OE2	3.23237	Hydrogen Bond;Electrostatic	Salt Bridge	A:ARG204:NH1	A:GLU232:OE2
A:ARG266:NH1 - A:ASP263:OD1:B	2.71485	Hydrogen Bond;Electrostatic	Salt Bridge	A:ARG266:NH1	A:ASP263:OD1:B
A:ARG266:NH2 - A:GLU446:OE2	3.34316	Hydrogen Bond;Electrostatic	Salt Bridge	A:ARG266:NH2	A:GLU446:OE2
A:ARG449:NH1 - A:GLU446:OE1	3.00991	Hydrogen Bond;Electrostatic	Salt Bridge	A:ARG449:NH1	A:GLU446:OE1
A:LYS456:NZ - A:ASP452:OD2	3.08644	Hydrogen Bond;Electrostatic	Salt Bridge	A:LYS456:NZ	A:ASP452:OD2
A:ARG465:NH1 - A:GLU349:OE2	2.82962	Hydrogen Bond;Electrostatic	Salt Bridge	A:ARG465:NH1	A:GLU349:OE2
A:ARG465:NH2 - A:GLU349:OE1	2.88696	Hydrogen Bond;Electrostatic	Salt Bridge	A:ARG465:NH2	A:GLU349:OE1
A:ARG160:NH1 - A:ASP180:OD1	4.94277	Electrostatic	Attractive Charge	A:ARG160:NH1	A:ASP180:OD1
A:ARG223:NH1 - A:ASP320:OD2	4.66929	Electrostatic	Attractive Charge	A:ARG223:NH1	A:ASP320:OD2
A:ARG223:NH2 - A:ASP320:OD1	3.79091	Electrostatic	Attractive Charge	A:ARG223:NH2	A:ASP320:OD1
A:ARG223:NH2 - A:ASP320:OD1:B	4.27599	Electrostatic	Attractive Charge	A:ARG223:NH2	A:ASP320:OD1:B
A:LYS290:NZ - A:ASP288:OD1	3.9286	Electrostatic	Attractive Charge	A:LYS290:NZ	A:ASP288:OD1