

VISVESVARAYA TECHNOLOGICAL UNIVERSITY
Jnana Sangama, Belagavi - 590018



Project Report

on

**“LEVERAGING ANN FOR TARGETED DRUG
SENSITIVITY PREDICTION ON GDSC DATA”**

Submitted in partial fulfillment of the requirements for the award of the degree of

BACHELOR OF ENGINEERING

in

COMPUTER SCIENCE & ENGINEERING

by

DHANUSH S SHETTY

4MT21CS047

**Under the Guidance of
Mrs. Suma K
Assistant Professor**



DEPARTMENT OF COMPUTER SCIENCE & ENGINEERING

MANGALORE INSTITUTE OF TECHNOLOGY & ENGINEERING

(A Unit of Rajalaxmi Education Trust ®, Mangalore)

Autonomous Institute Affiliated to V.T.U, Belagavi, Approved by AICTE, New Delhi

Accredited by NAAC with A+ Grade & ISO 9001:2015 Certified Institution

2024-25

MANGALORE INSTITUTE OF TECHNOLOGY & ENGINEERING

(A Unit of Rajalaxmi Education Trust ®, Mangalore)

Autonomous Institute Affiliated to V.T.U, Belagavi, Approved by AICTE, New Delhi

Accredited by NAAC with A+ Grade & ISO 9001:2015 Certified Institution

DEPARTMENT OF COMPUTER SCIENCE & ENGINEERING



CERTIFICATE

Certified that the project work entitled **Leveraging ANN for Targeted Drug Sensitivity Prediction on GDSC Data** carried out by **Mr. DHANUSH S SHETTY (USN: 4MT21CS047)** a bonafide student of **Mangalore Institute of Technology & Engineering** in partial fulfillment for the award of **Bachelor of Engineering in Computer Science & Engineering** of the **Visvesvaraya Technological University, Belagavi**, during the year **2024-25**. It is certified that all corrections/suggestions indicated for Internal Assessment have been incorporated in the Report deposited in the departmental library. The project report has been approved as it satisfies the academic requirements in respect of Project Work prescribed for the said Degree.

Signature of the Guide

Mrs. Suma K

Signature of the HOD

Dr. Ravinarayana B

Signature of the Principal

Dr. Prashanth C M

External Viva

Name of the Examiners

Signature with Date

1.

2.

MANGALORE INSTITUTE OF TECHNOLOGY & ENGINEERING

(A Unit of Rajalaxmi Education Trust ®, Mangalore)

Autonomous Institute Affiliated to V.T.U, Belagavi, Approved by AICTE, New Delhi

Accredited by NAAC with A+ Grade & ISO 9001:2015 Certified Institution

DEPARTMENT OF COMPUTER SCIENCE & ENGINEERING



DECLARATION

I, **DHANUSH S SHETTY** (4MT21CS047) student of 7th semester BE in Computer Science & Engineering, **Mangalore Institute of Technology and Engineering, Moodabidri**, hereby declare that the project work entitled “**Leveraging ANN for Targeted Drug Sensitivity Prediction on GDSC Data**”, submitted to the **Visvesvaraya Technological University, Belagavi** during the academic year **2024-25**, is a record of an original work done by us under the guidance of **Mrs. Suma K**, Assistant Professor, Department of Computer Science & Engineering, Mangalore Institute of Technology and Engineering Moodabidri. This project work is submitted in partial fulfillment of the requirements for the award of the degree of Bachelor of Engineering in Computer Science & Engineering. The results embodied in this report have not been submitted to any other University or Institute for the award of any degree.

Date:

Place: MOODABIDRI

DHANUSH S SHETTY

ABSTRACT

Personalized medicine is transforming cancer treatment by tailoring therapies to the genetic variations found in cancer cells, significantly improving patient responses to specific drugs. This project, titled "Leveraging ANN for Targeted Drug Sensitivity Prediction on GDSC Data", utilizes a machine learning approach with Artificial Neural Networks (ANN) to predict drug sensitivity in cancer cell lines using data from the Genomics of Drug Sensitivity in Cancer (GDSC) dataset. The model focuses on predicting IC50 values, a key measure of drug effectiveness, by integrating genomic features such as gene mutations, gene expression profiles, and copy number alterations (CNAs) to identify potential biomarkers for personalized therapies. The system employs an ANN architecture that captures complex nonlinear relationships within the genomic data, optimizing predictions with techniques like normalization, feature selection, and hyperparameter tuning. The approach uses a Flask-based web interface that enables users to easily input genomic data through labeled form fields, ensuring accessibility without the need for file uploads. The interface displays IC50 predictions in real-time, making it suitable for both clinical and research use. Model performance is evaluated using key metrics like Mean Squared Error (MSE), Mean Absolute Error (MAE) and R-squared (R^2). Visualization tools further enhance interpretability, displaying the comparison between predicted and actual IC50 values. This project highlights the potential of ANN models in advancing personalized oncology treatment by providing actionable drug response insights based on genomic data. Future work will focus on integrating additional datasets, enhancing multi-omics data integration, and conducting clinical validation to ensure broader applicability in real-world cancer therapies.

ACKNOWLEDGEMENTS

The satisfaction and the successful completion of this project would be incomplete without the mention of the people who made it possible, whose constant guidance encouragement crowned our efforts with success.

This project is made under the guidance of **Mrs. Suma K, Assistant Professor**, in the Department of Computer Science and Engineering. I would like to express my sincere gratitude to my guide for all the helping hand and guidance in this project.

I would like to thank my project coordinator **Mr. Shivaraj B G, Assistant Professor** in the Department of Computer Science and Engineering, for his cordial support, valuable information and guidance, which helped me in completing this project through the various stages.

I would like to express appreciation to **Dr. Ravinarayana B, Professor and Head**, Department of Computer Science and Engineering, for his support and guidance.

I would like to thank our Principal **Dr. Prashanth C M**, for encouraging me and giving me an opportunity to accomplish the project.

I also thank our management who helped me directly or indirectly in the completion of this project.

My special thanks to faculty members and others for their constant help and support.

Above all, I extend my sincere gratitude to my parents and friends for their constant encouragement with moral support.

DHANUSH S SHETTY

TABLE OF CONTENTS

Contents	Page No
ABSTRACT	i
ACKNOWLEDGEMENT	ii
TABLE OF CONTENTS	iii
LIST OF FIGURES	Vi
LIST OF TABLES	vii

Chapter no	TITLE	
1.	INTRODUCTION	1-4
1.1	Introduction	1
1.2	Problem Statement	2
1.3	Objectives	3
1.4	Scope of the project	3
1.5	Organization of the report	4
2	LITERATURE SURVEY	5-8
2.1	Existing System	5
2.2	Limitations of existing systems	7
2.3	Proposed System	8
3	SYSTEM REQUIREMENTS SPECIFICATION	9-13
3.1	Overall description	9
	3.1.1 Product Perspective	9
	3.1.2 Product Functions	10
	3.1.3 User classes and Characteristics	10
	3.1.4 Design and Implementation constraints	10
	3.1.5 Assumptions and Dependencies	10
3.2	Specific Requirements	11
	3.2.1 Hardware Requirements	11
	3.2.1 Software Requirements	11
3.3	Functional Requirements	12
	3.3.1 Model Development and Prediction	12
	3.3.1 User Interface and Accessibility	12
	3.3.3 Model Validation and Evaluation	12

	3.3.4 Data Security	13
3.4	Non-Functional Requirements	13
	3.4.1 Usability	11
	3.4.1 Reliability	11
	3.4.3 Performance	13
	3.4.4 Maintainability	13
4	GANTT CHART	15-16
5	SYSTEM DESIGN	17-22
5.1	Architecture Diagram	17
5.2	Use Case Diagram and Description	19
5.3	Sequence Diagram	20
5.4	Activity Diagram	21
5.5	Data flow Diagram	22
6	IMPLEMENTATION	23-28
6.1	Module Implementation	23
6.2	Data Preprocessing	23
6.3	Model Development	24
6.4	Web Interface Development	27
6.5	Deployment	28
7	TESTING	29-32
7.1	System Testing	29
7.2	Testing Methodology	29
7.3	Test cases	29
7.4	Evaluation Metrics	31
7.5	Test Results and Analysis	31
7.6	Challenges and Resolutions	32
8	RESULTS AND SNAPSHOTS	33-39
8.1	Introduction	33
8.2	Model Performance Metrics	33
8.3	Visualizations of Model Predictions	34
8.4	Snapshots of Web Interface	36
8.5	User Feedback	38
8.6	Observations and Insights	39

9	CONCLUSION AND FUTURE WORK	40
9.1	Conclusion	40
9.2	Future Work	41
	REFERENCES	43
	PAPERS PRESENTED	44

LIST OF FIGURES

Figure No.	Figure Name	Page No.
Figure 4.1	Gantt Chart	16
Figure 5.1	Architectural Diagram	18
Figure 5.2	Use Case Diagram	19
Figure 5.3	Sequence Diagram	20
Figure 5.4	Activity Diagram	21
Figure 5.5	Data Flow Diagram	22
Figure 8.1	Error Metrics for Model Evaluation	34
Figure 8.2	Actual vs Predicted LN_IC50 Values	34
Figure 8.3	Training vs Testing Loss	35
Figure 8.4	Drug Response Prediction	35
Figure 8.5	Home Page	36
Figure 8.6	Predicted IC50 Page	37
Figure 8.7	Drug Lookup Page	38
Figure 8.8	Drug Response Prediction	38

LIST OF TABLES

Table No.	Table Name	Page No.
Table 4.1	Gantt Chart of Planning and Scheduling of Project	15
Table 7.1	Test Cases	30