**Structural analysis of L198A mutation on the internal UBA domain of DNA repair protein hHR23a using Molecular dynamics simulations**

*A*

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*By*

Vaibhav Anand

(18807843)

*to the*

Department of Biological Sciences and Bioengineering

Indian Institute of Technology, Kanpur

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# CERTIFICATE

# ACKNOWLEDGEMENTS

# ABSTRACT

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# CHAPTER 1: INTRODUCTION

## Importance of Proteins

Proteins serve as essential macromolecules in living organisms, comprising one or more extended chains of amino acid residues known as polypeptides. These molecular entities play a crucial role in a myriad of biological functions, ranging from pivotal tasks like DNA replication and molecule transportation to catalyzing intricate metabolic reactions and providing structural integrity to cells.

In addition to their structural roles and involvement in fundamental cellular processes, proteins contribute significantly to the regulation and coordination of various physiological activities within an organism. Enzymes, a class of proteins, act as catalysts in metabolic pathways, accelerating chemical reactions that are vital for energy production, nutrient breakdown, and waste elimination. Furthermore, proteins are integral components of signaling pathways, facilitating communication between cells and orchestrating responses to external stimuli.

The diverse functionalities of proteins are intricately linked to their multi-tiered structural organization.

## Protein Structural Hierarchy

## Protein Three-Dimensional Structure

## Protein Structure Prediction and CASP experiments

## AlphaFold

## Deficiencies of AlphaFold

## Human Rad23 Protein

### Ubiquitin Associated Domain

# CHAPTER 2: METHODOLOGY

# CHAPTER 3: RESULTS