

### Introduction =

Proteins are complex biomolecules that play essential roles in almost all the cellular processes. They are necessary for the cell's functioning, signaling, regulation, and structure. All the chemical reactions in the body are catalyzed by proteins. Furthermore, proteins, perform various functions within the organism like DNA replication, providing structure to cells, messenger, transporting molecules, and antibody to fight against pathogens.

The basic building blocks of proteins are amino acids. These amino acids are attached in long linear chains to form the protein biomolecules. Proteins transform from linear chains into unique 3D (tertiary) structures via a process called protein folding, which makes them biologically functional. Sequence of amino acids is key to protein folding and so, not all the linear chain of amino acids forms a stable 3D structure. Few of them remain unfolded and few misfolded. If the protein fails to acquire its native structure, it might be inactive. There are exceptions where misfolded proteins may possess modified or toxic properties. Hence it is vital to understand protein sequence-structure and sequence-function.

The sequence of amino acids in proteins dictate unique shapes/structures and functions of protein. Therefore, protein's properties can be changed by altering the position of their amino acids. Similarly, substituting a naturally occurring amino acid with a different amino acid, known as mutation, can change the properties of proteins. Changing a particular protein sequence to derive the desired property is protein engineering. It is essential to understand the structure of the protein, and its folding & unfolding capabilities as these are the only ways that will help to determine the usefulness or harmfulness of a particular protein. Protein engineering can also make a protein more thermos-stable, change the substrate specificity, tolerance to extremes of pH and organic solvents.

## How Calpion Helps -

Calpion has helped many clients enhance the property of proteins using cutting-edge technologies. We operate on amino acid sequences to predict a protein's functionality. We automatically extract all the information on proteins using our algorithm rather than depending on the manual entry.

Calpion is using state of the art deep learning algorithms to be at the forefront of technology used for screening large number of mutations for any protein function. By integrating multiple teams globally for AI, Computational Chemistry and Protein Synthesis, we can translate the predictions of our algorithms into a reality.

We design and build state-of-the-art Machine Learning models using concepts of image processing, sequence learning, graph neural networks, GANs, which has helped Calpion to develop the strategies to predict active proteins that are not yet discovered in nature. We focus on Al-based technology to build and get insight into protein engineering, understand the protein's sequence-function and structure-function relationships, and solve the problems that occur on the client's end.



# Difficulties in Restructuring Specific Properties of a Protein

Proteins typically contain few hundreds to thousands of amino acids, it is practically impossible to synthesize and characterize every possible sequence of a small protein of even 100 amino acids due to astronomically large number of mutations for the same protein sequence. So, if we want to change a property of the protein, rounds of high-throughput screening need to be tried to achieve the desired results. Furthermore, total number of mutations in a given protein can be very large to synthesize and characterize in the laboratory.

#### AI/ML in Protein Evolution

Machine learning (ML) can drastically reduce the time, cost, and effort needed to derive the desired value of the proteins. It can aid in gaining a better understanding of structure and function of proteins. ML models can determine which mutations are essential for a targeted function. ML model can learn the sequence-function relationship of proteins and locks the best performing variant for the next round of optimization cycle. To enhance a particular property of a protein, ML can help to reduce the number of protein variants to be synthesized and the number of experiments that need to be performed in the laboratory, hence cutting the time and cost of the research.

# **Conclusion**

Calpion is a leading tech company that delivers exceptional results using modern cutting-edge technologies to its clients. With our expertise and optimum use of AI, ML, RPA, and deep learning, we have excelled in the field of biotechnology. We have optimized the performance of the production industry and have worked on complex technologies like protein engineering. Our capability to bring data scientists, industry experts, subject matter experts, and deep learning professionals into the same room helped us succeed and excel in this esoteric field. Are you having business problems? Do you believe in working on the frontiers of technology? Do you wish to take your business to new heights using protein engineering? In that case, we have a dedicated team for you who can work on your problem statements and give you the results you always wanted. Contact Calpion for more details

- Dr. Manish & Dr. Som

Calpion is a Dallas, Texas based technology consulting company with offices across US and India. We have been working with organizations that have been striving for digital excellence. We provide technology solutions for various industries like, Healthcare, Biotechnology,

Logistics and Supply Chain, Manufacturing and Retail, etc.

