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# COMPUTATIONAL STUDIES ON THE ROLE OF CARBON IN PROTEINS

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**ABSTRACT**

Hydrophobic contacts largely determine the strength of the biomolecular interactions. Carbon content and distribution throughout protein sequences, especially in enzymes, are crucial yet underutilized elements. We've developed a computational approach for determining the distribution of carbon atoms inside a protein sequence, which should allow us to capture these events. This cutting-edge strategy has already been applied to several proteins. In this case, it is broadened to include several enzymes critical to creating chemicals with roles in the nervous system. Tyrosine hydroxylase, tryptophan hydroxylase, and aromatic amino acid decarboxylase are among the enzymes considered. Presented below is research on the carbon distribution along these enzymes. The function of carbon is investigated via computational simulations. Hydropathy plots are compared to carbon distribution plots. To better comprehend the carbon distribution in certain enzymes, several applications are carried out and explained.



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## 1. INTRODUCTION

Proteins have undergone extensive research to understand their nature better. In all living things, the primary force that causes proteins to carry out metabolic activities is hydrophobic contact. Carbon is the most important ingredient in hydrophobic interaction. The carbon distribution along the protein sequence was estimated in this work by treating the protein sequence as a series of atoms rather than amino acids. Given any length, the highest frequency occurs at 31.44% carbon. All globular proteins prefer 31.44% carbon[1-2]. This is true not just globally but also locally. It is hoped that this newly discovered carbon distribution profile will aid in the identification and development of active sites, the study of protein stability, the evolutionary understanding of proteins, gene identification, and the resolution of the long-standing problem of protein-protein and protein-DNA specific and non-specific interactions. This may also identify toxic, infectious, and pathogenic proteins.

## 2. CARBON DISTRIBUTION PLOT AND HYDROPATHY PLOT

The biomolecular association is mostly governed by hydrophobic interactions[3–4]. The sole component that affects the hydrophobic interactions is carbon. The carbon distribution along proteins is investigated, and the hydropathy plot is contrasted. The human erythrocyte glucose transporter protein is the subject of the investigation. The carbon distribution profile shows where the maximal hydrophilicity or hydrophobicity is with great clarity. The carbon distribution profile may replace hydropathy plot.

## 3. CARBON DISTRIBUTION IN ENZYMES

The sole ingredient that helps hydrophobic interactions in proteins is carbon. Hydrophobic interactions mostly govern the biomolecular association. Carbon content and distribution throughout protein sequences, especially in enzymes, are significant determinants that have not yet been fully utilized [5–7]. To capture these events, we have created a computer technique to determine the carbon distribution in a protein sequence. This newly created technique has already been used on various proteins. Here, it is expanded to include a wide range of enzymes involved in manufacturing key chemicals for the nervous system. Considerable consideration is given to human and animal enzymes such as tyrosine hydroxylase, tryptophan hydroxylase, and aromatic amino acid decarboxylase. This article studies and presents the carbon distribution along these enzymes. The technique can identify active regions (the carbon-rich area) that are the same across species but varied in the amino acid sequence. These three enzymes' carbon distribution profiles in humans and other animals are shown and explained.

Proteins are substantial chemical molecules consisting of linearly ordered amino acids. [1-4] These amino acids' side chains, which are chemically distinct from one another in several respects, may be roughly divided into hydrophobic and hydrophilic substances. These side chains' carbon concentration distinguishes the amino acid. Large hydrophobic residues in the protein folding and disorder area have been referred to and thought to be a substantial contribution by carbon. This research compares the variance in carbon content between homosapiens and pan troglodytes and concludes that proteins like to have 27% of big hydrophobic residues in their structural makeup for stability.

## 4. CONCLUSION

This article examined and compared the carbon content of phenylalanine hydroxylase in humans, mice, fruit flies, bovine, rats, and worms. Generally, the carbon content is more significant in all species examined here than the predicted amount (31.44%)[1-6]. Between 100 to 400 residues include this. The carbon content of this enzyme may be decreased by substituting polar residues with non-polar residues.


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The authors declare no conflict of interest.

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