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Computational Studies on Role of Carbon Atom in Proteins - Phenylalanine Hydroxylase Protein

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Abstract

Proteins are large organic compounds made of amino acid arranged in a linear fashion. The side chain of these amino acids are chemically different from one another in some respect can be classified broadly in two ways hydrophobic and hydrophilic. Carbon is the only element contributes towards this, which is high in large hydrophobic residues. This paper analyzes and compares the carbon content in phenylalanine hydroxylase of human, mouse, and fruit fly, bovine, rat and worm. Generally in all species studied here the carbon content is higher than the expected value (31.44%). This is found in residues between 100 and 400. By reducing the carbon content (that is replacing non polar residues by polar residues) might improve the activity of this enzyme.

Keywords: Carbon distribution, sequence analysis, proteome, comparative analysis, C program

Introduction

All Proteins are constructed from linear sequences of smaller molecules called amino acids. Proteins also fold up to form particular three dimensional shapes, which give them their specific chemical functionality. Although it is easily demonstrable that the linear amino acid sequence completely specifies the three dimensional structure of most proteins. In addition a protein's three-dimensional is not fixed; many proteins move and flex in constrained ways, and that can have a significant role in their biochemical function. Also some proteins bind to other groups of atoms that are required for them to function. A widely accepted principle is that protein evolution is mainly determined by constraints on activity, specificity, folding and stability. The

lowest level of biological organization is that of atoms in biological macromolecules. Specifically, individual amino acids and whole proteins can vary greatly in their content of carbon [1, 2]. Hydrophobic and Hydrophilic Residues play a major role in protein folding and function. The distribution hydrophobic and hydrophilic residue along polypeptide chain is critical feature of the ability of biologically evolved amino acid sequence to direct the folding of proteins [3, 4]. Carbon is the only element contributes towards this, which is dominated by large hydrophobic residues. Protein prefers to have 27% of large hydrophobic residues in its structure for stability. This paper analyzes and compares variation of carbon content in phenylalanine hydroxylase of Human (Hs), Mouse (Mm), Fruit fly (Dm), Bovine (Bt), Rat (Rn) and Worm (Ce). This method is able to identify the active sites (carbon rich portion).

Methodology

To understand the carbon content in proteins, the phenylalanine hydroxylase protein of Homo sapiens and other species are selected here. The protein sequences of selected species are downloaded from the protein sequence database (SWISS PROT). The home made ATOMSCAN program written in C is used for identifying the carbon content along the protein sequences (http://rajasekaran.net.in/tools/carbana.html). This program simply read the protein sequence, converts into atomic sequence and then does a window analysis based on carbon content. The predicted carbon content variations are analysed and discussed.

Results and discussion

Distribution of Carbon usage in Phenylalanine hydroxylase enzyme of Homo sapiens, Mus musculus, Drosophila melanogaster, Bos taurus, Rattus norvegicus, and Caenorhabditis elegans, the averaged number of carbon atoms found in residue side chains for each protein was calculated, and the totality of all these frequencies was described by X Y scatter with smooth lines. The carbon content higher in the residues between 110 and 400. Reduction in carbon content that is replacing with polar residues might improve the activity as there will be enough electrophilicity.

Table (1): Number of amino acids and average deviation of carbon content of phenylalanine hydroxylase in different species

SPECIES	No of AMINO ACIDS	Average deviation of Carbon content
Homo sapiens (Human)	452	0.08529
Mus musculas (Mouse)	453	0.084214
Drosophila melanogaster (Fruit fly)	452	0.107026
Bos Taurus (Bovine)	451	0.084981
Rattus norvegicus (Rat)	453	0.087079
Caenorhabditis elegans (Worm)	457	0.103948

The number of amino acids and deviation in carbon content of phenylalanine hydroxylase in different species are given in the table [1]. The number of amino acid does not vary much among the species but the carbon content varies significantly. Given the average carbon content deviation the fruit fly and C.elegan are having greater carbon content. The deviation supposed to be zero for a normal functioning protein.

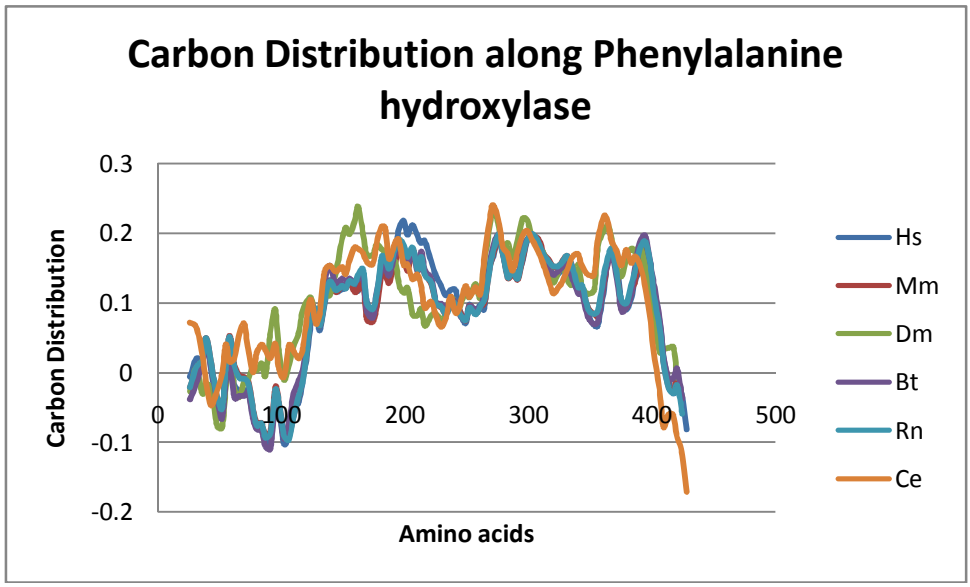

Fig (1): Distribution of carbon along the Phenylalanine hydroxylase in different species.

Comparative analyses of complete genome sequence were anticipated to reveal the molecular bases of biodiversity as well as to increase our comprehension of the constraints that shaped protein composition and structure. Protein carbon contents differ more between species than with each proteome, because the largest variations in protein atomic content were observed for carbon, which is the main architectural component of proteins, we focused our analysis on this atom. Fig. (**1**) Shows that the variations in protein carbon content. This indicates that although the residues are not much changes also at mRNA level but mean values of protein carbon contents largely differ between species.

Conclusion

This paper analyzes and compares the carbon content in phenylalanine hydroxylase of human, mouse, and fruit fly, bovine, rat and worm. The carbon content is higher than the expected value (31.44%). The higher carbon content is found in residues between 110 and 400. By reducing the carbon content (that is replacing non polar residues by polar residues) might improve the activity of this enzyme.

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