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CONFORMATIONAL INSIGHTS INTO EUKARYOTES: ANALYZING ALANINE, GLUTAMIC ACID AND LEUCINE AMINO ACIDS USING THE 144-BOX METHOD

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ABSTRACT
The efficient functioning of living organisms depends on macromolecules, which are proteins. It is challenging to predict the structure of proteins from their sequence since they are functional only in their natural or folded state. Dihedral angles play a key role in predicting protein structure because they define a protein's backbone, which determines the protein's overall form together with side chains. Eukaryotes, including all organisms with complex cells, have unique conformational features that distinguish them from other cellular entities. The three-dimensional tertiary structure of a protein is composed of repeated units of secondary structures. The two basic types of secondary structures are alpha helices and beta strands. These alterations may cause changes in protein conformation, which may impact how these modifications affect the structure of viral proteins require an examination of the dihedral angles of alanine, glutamic acid, and leucine using our new 144-box method. This research may be further developed and useful for drug discovery and molecular modeling.

Keywords: *Aminoacids, Eukaryotes, Python Programming, Protein Data Bank, 144-Box Method*

INTRODUCTION

Conformational analysis is a central tool used in molecular biology that allows scientists to examine the three-dimensional structures of biological macromolecules (Agrawal *et al.,*1996) Conformational analysis has greatly advanced the understanding of biomolecular structure and function in eukaryotic cells (Smith *et al.,* 1987). For the conformational characterization of eukaryotic macromolecules, computational modeling (Holland *et al.,*1992) using our 144-box method. It can be used to elucidate the structure and dynamics of the spike protein on the virus surface, which plays a critical role in its infectivity and spread (Beaucourt *et al.,* 2011).

The 144-box method has significantly contributed to our understanding of the biological processes and disease-causing mechanisms of eukaryotes (Ali and Vijayan *et al.,* 2020). Computational modeling and structural biology approaches have contributed to these systems' dynamic structures of biomolecules. Examining conformational changes provides insights into the function, regulation, and potential therapeutic targets involved in normal cellular processes and viral infection (Agrawal *et al.,* 1999). This analysis has examined the eukaryotic proteins of alanine, glutamic acid, and leucine providing deeper insights into drug-designing processes.

MATERIALS AND METHODS

About 1,25,835 proteins were sampled from the protein data bank (PDB) (Sussman *et al.,* 1998). And 12,284 proteins were selected based on the similarities of their sequences. I created a demonstration of our 144-box method using Python programming (Mészárosová *et al.,* 2015) to interpret the results.

144 box method:

144 box method is a very simplified representation of the Ramachandran plot and it divides the conformational space of the peptide backbone into 144 boxes. Each box represents a specific combination

FIGURES (i)ALANINE:

180	150		120	90	60	30	0	-30	-60	-90	-120	-150	-180
150	149	212	76	195	7	0	0	1	0	0	0	0	-150
120	59	239	183	255	23	0	0	4	0	0	0	0	-120
90	6	50	76	37	3	0	0	2	3	0	0	0	-90
60	2	10	12	17	0	0	0	0	0	0	0	0	-60
30	0	17	33	8	0	0	0	0	4	0	0	0	-30
0	0	12	75	75	0	0	0	1	12	0	0	0	0
-30	2	8	67	619	10	0	0	15	12	0	0	0	30
-60	0	5	48	1400	171	0	0	43	7	0	0	0	60
-90	1	0	1	13	5	0	0	13	1	0	0	0	90
-120	0	0	0	0	0	0	0	0	1	0	0	0	120
-150	0	2	1	3	0	0	0	0	0	0	0	0	150
	15	3	20	18	0	0	0	0	0	0	0	1	
-180	-150	-120	-90	-60	-30	0	30	60	90	120	150	180	

(ii)GLUTAMIC ACID:

180	150		120	90	60	30	0	-30	-60	-90	-120	-150	-180
150	12	138	194	171	5	0	0	0	3	0	0	0	-150
120	22	297	650	402	28	0	0	0	2	0	0	0	-120
90	9	82	198	81	4	0	0	0	8	0	0	0	-90
60	0	9	24	17	0	0	0	13	7	0	0	0	-60
30	0	13	35	8	0	0	0	13	1	0	0	0	-30
0	3	17	125	40	0	0	0	10	1	0	0	0	0
-30	2	12	127	654	22	0	0	0	0	0	0	0	30
-60	0	14	158	1849	182	0	0	0	0	0	0	0	60
-90	0	0	8	16	9	0	0	2	0	0	0	0	90
-120	0	0	0	0	0	0	0	0	0	2	0	0	120
-150	0	0	0	0	0	0	0	0	0	0	0	0	150
	2	14	15	17	0	0	0	0	0	0	0	0	
-180	-150	-120	-90	0	-30	0	30	60	90	120	150	180	

(iii)LEUCINE:

180	150		120	90	60	30	0	-30	-60	-90	-120	-150	-180
150	25	95	88	108	2	0	0	0	0	0	0	0	-150
120	25	169	240	254	40	0	0	0	0	0	0	0	-120
90	3	41	62	36	8	0	0	0	0	0	0	0	-90
60	5	7	15	14	0	0	0	0	0	0	0	0	-60
30	0	10	10	3	0	0	0	0	0	0	0	0	-30
0	0	16	63	62	0	0	0	0	6	0	0	0	0
-30	0	21	102	579	27	0	0	4	3	0	0	0	30
-60	0	19	75	1193	195	0	0	15	2	0	0	0	60
-90	0	2	2	21	7	1	1	12	1	0	0	0	90
-120	0	0	0	0	1	0	0	0	0	0	0	0	120
-150	0	0	0	0	0	0	0	0	0	0	0	0	150
	3	14	10	6	2	0	0	0	2	0	0	0	
-180	-150	-120	-90	-60	-30	0	30	60	90	120	150	180	

Fig. 1 (i), (ii). (iii) represents the 144-box method of Eukaryotes and its structure

of phi and psi angles. The result of this technique is used to visualize spatial amino acid formations and protein conformation (Gross *et al.,* 2003) for better understanding. These 144 boxes contain 144 sections with different ranges of structural parameters and dihedral angle calculations These visualizations help to find patterns and outliers within protein structures (Agrawal *et al.,* 1999).
Each box in this method represents a specific set of dihedral angles within the protein structure, facilitating a detailed examination of its conformation. This arrangement highlights both the allowed and disallowed regions for these angles, providing valuable insights into proteins' stability and overall structure.
The 144-box method is an extension or alternative approach to visualizing protein configurations with greater granularity. Breaking down conformational space into smaller, more specific regions, enables a more refined analysis of protein angles. This detailed perspective allows researchers to understand better how particular dihedral angles interact within the protein structure, enhancing our comprehension of protein behavior and stability.

RESULTS AND DISCUSSION

Our investigation showed that alanine often occupies regions related to α-helices and β-sheets. 25% of alanine residues located in α-helical segments fall within the typical φ and ψ angle ranges, reflecting its strong inclination to stabilize helical formations. Alanine is mainly found in the α-helix section of box number 41 (This section is shown in yellow in Figure 1.) and is also present in various angular regions linked to β-sheets.
Moreover, specific regions for antiparallel sheets can be found in box numbers 23, 35, 47, and 48 (highlighted in purple in Figure 1), emphasizing the critical function these configurations serve in establishing stable hydrogen bonds. This, in turn, boosts protein stability through linear interactions between adjacent strands. Glutamic acid stands out for its conformational capabilities, exhibiting both helical and sheet structures primarily in box number 41, it is shown as yellow color in fig.2, where it shows a significant preference. Its branched side chain grants it structural flexibility, allowing it to engage effectively in diverse interactions within protein folds. Additionally, methionine plays a vital role as the starting amino acid in eukaryotic protein synthesis, highlighting its importance in forming protein structures found in box numbers 41 and 42. Its occurrence in the flexible regions of proteins may also promote conformational adaptations, increasing the versatility and functionality of eukaryotic proteins. Leucine also demonstrates properties aligned with α-helices in box number 41, as indicated by the clusters of data points present in regions associated with favorable structures. This collective behavior of these amino acids illustrates their essential contributions to maintaining the stability and functionality of proteins.

CONCLUSION

This analysis provides more information on the functions of lysine, isoleucine, and methionine in protein structure and function by observing the formation of helical and sheet structure conformations. Using our novel 144-box method we examined a better understanding of these three aminoacids and provided a basis for future drug designing and molecular simulations. It also affirms the general objective of developing specific biotherapies and protein networks in living organisms.

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