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## DISTANCE DOMINATION ON BIOMOLECULES STRUCTURE

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### ABSTRACT

In this paper the distance, degree, domination of living basic elements like carbon (C), hydrogen (H), oxygen (O), nitrogen (N), phosphorus (P) and sulfur (S) of biomolecules such as carbohydrates, lipids and amino acids were discussed using mathematical approach. To classify the graphical structure into biomolecules component and biochemical component using distances domination concepts. If  $n$  is number of carbons in any biomolecules structure, then at least one carbon dominating all other living basic elements at  $n$  distance and this is need not true for acids. This present study deals with a brief account of relevant graphs and graph theoretic concepts. The structural and biological information derived from biomolecules structures using these methods is presented.

**Keywords: Biomolecules, Biochemical structures, Degree, Distance Domination**

### INTRODUCTION

There are several papers and books regarding domination in graph theory [2, 3, 4, 5]. In 1975, domination was extended to distance domination by Meir and Moon [1]. Many result showed on distance dominating set were extended by P.J.Slater in his paper R-domination in graphs in 1976 [6, 7, 8].

Graph theory is an area of discrete mathematics that deals with graphs. The study is characterized by its geometric approach. Despite the fact that the subject is over two centuries old, it is still relevant today and has long been employed in a variety of scientific and technical disciplines.

Graph theory has also been used to chemical molecules, which are made up of a set of atoms or groups of atoms (vertices) connected by covalent bonds (edges) [9].

The biomolecules deal with living basic elements. There are six elements of living matters like carbon, hydrogen, oxygen, nitrogen, phosphorus and sulfur, all this together constitute about 90% of the dry weights of the human body. The other elements Ca, K, Na, Cl, Mg, Fe, Cu, Co, I, Zn, F, Mo and Se are also available in human cells for functioning the human body. The Carbon is most important element of our body. It is approximately that about 90% of compounds found in living system always contain carbon and its length of the chain of carbon is infinity. The human life is composed of lifeless chemical molecules that is, a single cell of the bacterium, *Escherichia coli* contains about 6,000 different organic compounds. It is believed that human may contain about 1,00,000 different types of molecules, by the same time only a few of them have been characterized. The organic compounds such as amino acids, nucleotides and monosaccharides serve as the monomeric units or building blocks of complex biomolecules like proteins, nucleic acids (DNA and RNA) and polysaccharides respectively. The macromolecules (proteins,

lipids, nucleic acids and polysaccharides) form supramolecular assemblies (that is, membranes) which in turn organize into organelles, cells, tissues, organs and finally the whole organism. There are numerous books and articles available that cover the mathematics of graph theory, as well as its applications and computer algorithms. In the following section, a basic description of the graphs is given, along with properties of the graph that are relevant to the current article, and the formulation of biomolecules structure graphs and their applications are described in the following sections [10].

### **Structure of biomolecules**

The Carbon is a most important element of life because it is estimated that about 90% of components found in living system invariably contain carbon, it is to be form stable covalent bonds and C-C chains of unlimited length. In this paper let us consider  $n$  to be number of carbon in biomolecules structure [11, 12].

### **The chemical reaction for contracting a polymer from a set of monomers [13]**

The process for connecting two monomers together (forming a covalent bond) is called dehydration synthesis. Dehydration means “removal of water” and synthesis means “to join together”. So in this process, two monomers are covalently

bonded by the removal of a water molecule. Each organic monomer has a hydroxyl group (-OH) on one side and a hydrogen (H) on the other. When two monomers line up side by side, they will have these two functional groups facing one another (H & OH). The H and the OH will break off of their respective monomers and bond forming a water molecule. This is the dehydration part of the process. Each monomer now has a carbon atom that needs to covalently bond with something, so they bind to each other forming a polymer. That is the synthesis part of the process. Dehydration synthesis is an energy-requiring process. Every time a cell needs to build a protein or a starch, it has to expend some energy to form those chemical bonds. Dehydration synthesis is universal for building all organic polymers.

### Water Graphical Structure

The water component will be removed when two or more carbohydrates join together as single structure.



### Carbohydrates (CHO)[12]

The general formula for CHO is  $\text{C}_n\text{H}_{2n}\text{O}_n$  where n should be start with 3, 4, 5, ..... Now a day it has proved structure for n = 7 in biochemistry it is based on the number of carbon atoms, namely Trioses ( if n = 3), Tetroses ( if n = 4), Pentoses ( if n = 5),

Hexoses ( if n = 6), Heptoses ( if n = 7), There are two types of functional groups one is Aldoses and another one is Ketoses

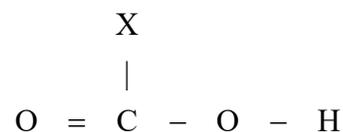
The condition of the CHO graphical structure described by degrees.



### Lipids (COOH) [12]

There is no general formula for COOH, but it has connected lot of carbon and hydrogen, most of COOH bond called fatty acids so it will be treated as biochemical not biomolecules.

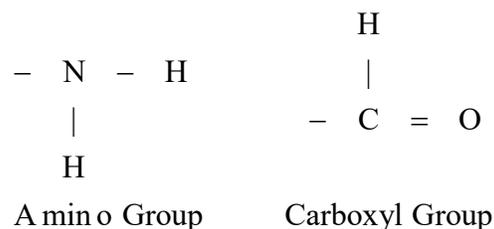
The general structure of lipids



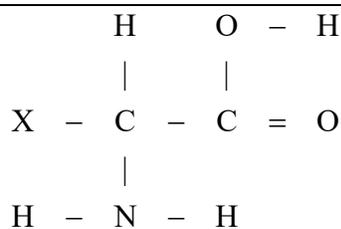
Where X is any element

### Amino Acids (COO<sup>-</sup>) [12]

This is a group of organic components containing two functional groups amino and carboxyl.



### The general structure of Amino Acids



Where X is any element

**Degree [9]:** The degree of the vertex is a number that how many edges incident with particular vertex and loop consider as twice.

**Maximum degree [9]:** In graph, let n be the degree of vertex is maximum, if any other vertices has degree less than n.

**Pendant Vertex [9]:** Any vertex has degree is one as known as pendant vertex.

**Degree Sequence [9]:** Let G be graph, if G has vertices  $v_1, v_2, \dots, v_n$ . The sequence  $d(v_1), d(v_2), \dots, d(v_n)$  is called degree sequence of G, for our convenience degrees are written by ascending orders.

**Dominating set [9]:** A dominating set is a subset D of V in G such that every vertex not in D is adjacent to at least one member of D.

**K-Distance Dominating Set [9]:** A graph G, a distance dominating set is a subset D of V such that every vertex u not in D, the distance  $d(u, v) \leq k$  for some v in D. Sometimes it is called as k-distance dominating set or kd-dominating set.

**The degrees of basic living element should be satisfied the following conditions:**

1. Degree of H is one that is  $d(\text{H}) = 1$
2. Degree of O is two that is  $d(\text{O}) = 2$

3. Degree of N is three that is  $d(\text{N}) = 3$
4. Degree of S is three that is  $d(\text{S}) = 3$
5. Degree of C is four that is  $d(\text{C}) = 4$
6. Degree of P is five that is  $d(\text{P}) = 5$

### The conditions of acids

Distance between any two oxygen is less than or equal to 2. That is  $d(\text{O}, \text{O}) \leq 2$

**The distance domination of CHO (single) should be satisfied the following conditions:**

1. The distance between any two carbons is less than n.
2. The distance between any two hydrogens is less than  $2n$ .
3. The distance between any two oxygens is less than or equal to  $n+1$

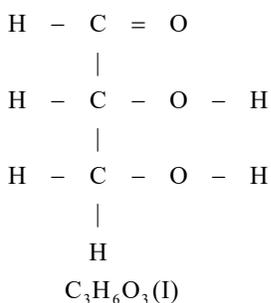
**The distance domination of CHO (double) should be satisfied the following conditions:**

1. The distance between any two carbons is less than  $n+2$ .
2. The distance between any two hydrogens is less than  $2n+2 = 2(n+1)$
3. The distance between any two oxygens is less than or equal to  $n+1+3 = n+4$

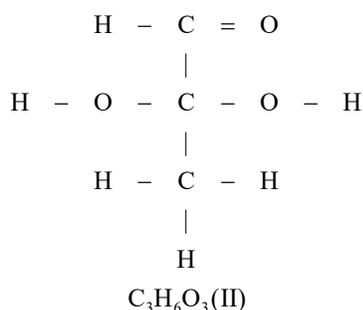
### The mathematical approach to carbohydrates

Let us consider the general form of the mono carbohydrate for  $n = 3$  that is the following graphical structure will appear. We

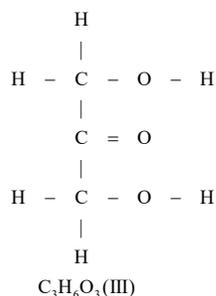
checked degree conditions are holds. The single carbohydrate distance domination conditions also hold. Therefore the following



Let us consider the general form of the mono carbohydrate for  $n = 3$  that is the following graphical structure will appear. We checked degree conditions are holds. The single carbohydrate distance domination



Let us consider the general form of the mono carbohydrate for  $n = 3$  that is the following graphical structure will appear. We checked degree conditions are holds. The

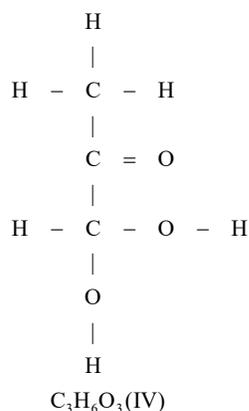


graph should be single carbohydrate ( $\text{C}_3\text{H}_6\text{O}_3(\text{I})$ )

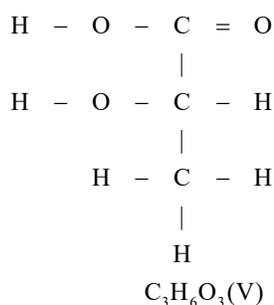
conditions not hold due to distance between any two oxygens less than  $n$ . Therefore the following graph should not be single carbohydrate ( $\text{C}_3\text{H}_6\text{O}_3(\text{II})$ )

single carbohydrate distance domination conditions also hold. Therefore the following graph should be single carbohydrate ( $\text{C}_3\text{H}_6\text{O}_3(\text{III})$ )

Let us consider the general form of the mono carbohydrate for  $n = 3$  that is the following graphical structure will appear. We checked degree conditions are holds. The single carbohydrate distance domination



Let us consider the general form of the mono carbohydrate for  $n = 3$  that is the following graphical structure will appear. We checked degree conditions are holds. The single carbohydrate distance domination

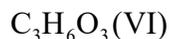
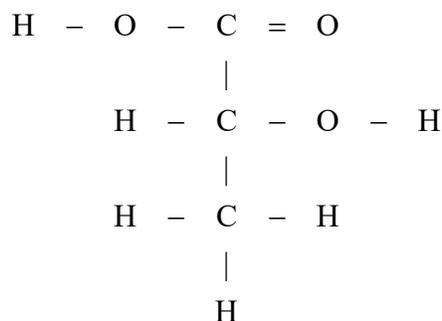


Let us consider the general form of the mono carbohydrate for  $n = 3$  that is the following graphical structure will appear. We checked degree conditions are holds. The single carbohydrate distance domination

conditions not hold due to distance between any two oxygens less than  $n$ . Therefore the following graph should not be single carbohydrate ( $\text{C}_3\text{H}_6\text{O}_3(\text{IV})$ )

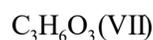
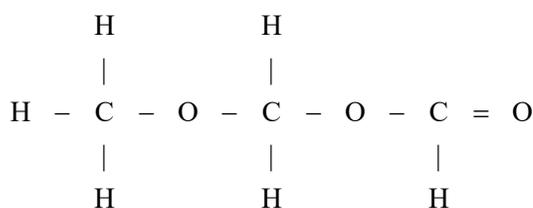
conditions not hold due to distance between any two oxygens less than  $n$ . Therefore the following graph should not be single carbohydrate ( $\text{C}_3\text{H}_6\text{O}_3(\text{V})$ )

conditions not hold due to distance between any two oxygens less than  $n$ . Therefore the following graph should not be single carbohydrate ( $\text{C}_3\text{H}_6\text{O}_3(\text{VI})$ )



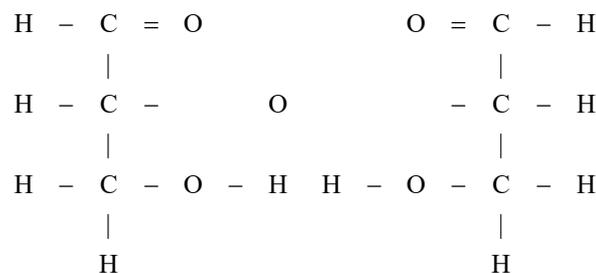
Let us consider the general form of the mono carbohydrate for  $n = 3$  that is the following graphical structure will appear. We checked degree conditions are holds. The single carbohydrate distance domination

conditions not hold due to distance between any two oxygens less than  $n$ . Therefore the following graph should not be single carbohydrate ( $\text{C}_3\text{H}_6\text{O}_3$ (VII))



Let us consider the general form of the di-carbohydrate for  $n = 3$  that is the following graphical structure will appear. Here water bond H-O-H will be removed while two carbohydrates join together. We checked degree conditions are holds. The

double carbohydrate distance domination conditions not hold due to distance between any two hydrogen less than  $2(n+1)$ . Therefore the following graph should not be carbohydrate ( $\text{C}_6\text{H}_{10}\text{O}_5$ (I))





## Properties

1. Sum of the degree of any CHO(single) is  $4n+2n+2n=8n$
2. Each carbon (C) adjacent with oxygen (O).
3. Each carbon (C) adjacent with at least one hydrogen (H).
4. Each carbon (C) having exactly one oxygen (O) at a distance one in CHO
5. Each carbon (C) having exactly one oxygen (O) with multiple edge in CHO
6. The carbon chain in biomolecules structure is satisfied middle distance dominating set [10].
7. The carbon chain in biomolecules structure is satisfied perfect distance dominating set [11].
8. All graphical structure of biomolecules is not simple graph.

## CONCLUSION

We discussed the distance, degree, domination of living basic elements carbon (C), hydrogen (H), oxygen (O), nitrogen (N), phosphorus (P) and sulfur (S), the mathematical approach to classified the graphical structure into biomolecules component and biochemical component using distances domination concepts, we showed that if  $n$  is number of carbon in any biomolecules structure then at least one carbon dominating all other living basic

elements at  $n$  distance and this is need not true for acids.

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