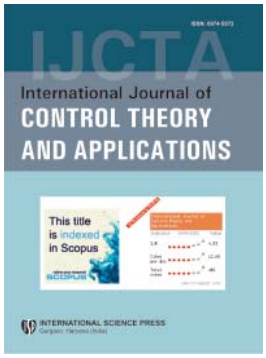

International Journal of Control Theory and Applications

ISSN : 0974–5572

Volume 9 • Number 42 • 2016

Atom Representation and Bonding of Sequenced Pathway

Anusree V.P[a] Divya Neupane B[a] and Pallavi M.S[a]

[a]*Department of Computer Science, Amrita School of Arts and Sciences, Amrita Vishwa Vidyapeetham, Amrita University, Mysuru Campus Karnataka, India*

E-mail: sumaanu.vp@gmail.com, divyaneupane.93@gmail.com, palls.ms@gmail.com

Abstract: The Bioinformatics and Medicinal Chemistry is one of the emerging technologies leading to the atom molecules conception through online specific tools. Creation of atom bonding and angle calculation of the Chemical structure for the visualization of protein in computational way is different from other technological growth. Complexity of finding the structure visualization of a molecular simulation in a computational way leads to explore. The stimulation of the project is to find the accurate pathway in the affected single cell in melanoma cancer and design the structure of a particular ligand and receptors. This method collects a BRAF protein sequence in the form of PDB and then it is converted into xml format. The list of the protein sequence that is fetched from PDB is taken as input in the simulation. It represents different types of atoms and bonding of the protein molecule. The proposed system will be implemented based on the particular conversion of the PDB file, visualize the structure in computational way and calculate the distinct atomic bonding of the sequence.

Keywords: *PDB; BRAF protein sequence; ligand; receptors; Topological Indices; informatics techniques; proteomics maps.*

1. INTRODUCTION

One of the key goals in the computer-aided drug design and discovery strategies is the identification of pathways for the specific diseases. The recognition of the pathway of melanoma is one among them. This can be achieved by adding informatics techniques. To treat melanoma the drug is to be designed. For this, the efficient pathways are to be identified for the cure of melanoma. In the melanoma pathway the ligand gets attached to the receptor. So, the protein molecules present in the receptor are analysed using the structure visualization of a particular protein molecule, atom and their bonding. The analysis process includes various processes like collecting the data sequences from the PDB and converting the PDB data into XML format. The PDB file contains the collection of the BRAF protein sequence of data of the protein molecules of a particular pathway in the form of list of ligand and receptors having different types of atoms and bonding. The collected sample of data in the form of PDB files is converted into XML format. This data converted into the XML format acts as an input in this method. The data is visualized in Chimera first by adding and removing the water molecule present in it and the ligand attaches to the receptor. In this, the Particular ligand and receptors are attached by the water molecules and the formation of the structure of water molecules using computational way and treated with the

PCR method before calculating the bond angles between H = O. Then a visualized form of data is represented in the 3D visualization form in the Chimera simulation tool. Then various types of bond visualization of the atoms in the molecule and their bonds are represented by the simulation tool. The simulation includes various methods of adding and removing the atom present in the molecule and its visualization by using different visualization format to be added. Computes the number of atoms to be represented as a result is taken as input and is visualized. Then the bonds of the atoms are structurally represented. Then the calculation of the bond angles is made. The drawing package is used to inherit the class used for inheriting an object, create line and to add graphics. The system uses various different representations and their distance and bond calculations using the system in parallel and computing the values between the atoms present. It directly builds the structural format and simulators. This method includes various processes for the structural representation of the atom, their bonding representation and then calculating the bond angle value between the atoms. The varied methods help to visualize the structure of the atom bonding calculation computationally present. This helps to find the drug for passing in the molecular signalling pathway for melanoma. The molecular signalling pathway is the pathway which is used to pass the signals. It is a sequence of undertaking among the particular molecule in the cells that guide to particular molecule or change in a cell. It assigns to the transduction of molecular signal in the form of an alteration by enlistment of the protein sequence along the protein complexes that triggers a biochemical events in a cell. The computational part of the molecular signalling pathway is to build a particular protein binding. The steps involve collecting the samples and passing that to the ligand and the ligand are received by the receptor for which the Polymerase chain reaction method is added that involve denaturation, annealing and elongation process. Molecules are indicated as a combination of atoms, bonds, angles etc. The atoms are themselves made of several parallel components. This kind of parallelism, that we call logical parallelism. The simulation is actually visualized at each step of resolution method. The binding of atoms builds the molecules. Different kind of molecules can be used to find the particular path. To relate the melanoma skin cancer dataset included in different kinds of binding molecules to detect the different kinds of binding molecules and find out the particular pathway that is accurate. The above steps are implemented in the methods to visualize the atom's structural way and to represent the bonding with angle calculation. The objective of the method is visualizing the atom of a particular molecule, bonding, calculation of angle between the atoms and the complete protein structural visualization.

2. LITERATURE REVIEW

González-Díaz et al [1] has proposed a system at work on the chemical structure encoding and biological activity. It involves numerical encoding of chemical structure and biological activity that encodes the information on the surface of the protein and their interaction. This perspective permits several procedures like instant gathering, explanation, improvement and withdrawal of chemical structure inside large databases. It can link to a method for connecting the chemical configuration with the true action of a protein. The Topological Indices encode the information of the protein surface and protein interaction networks.

Szafran et al [2] has proposed a system to represent the chemical structure of an atom present in a chemical system processed by a wave function by parallelization process and to get accurate outcome. It requires the computation at the essential level by the utilization of the parallelization of the process through accelerated outcome. This depicts the step by step procedure of calculating the structure of Piperidinecarboxylicacid, the structure is made by the groups of COOH and creates the electron and bonding each and other. The step by step bonding of the atom is visualized by the calculation of the distance of bonding between each atom. The result of this system is the representation of 4-piperidinecarboxylic acid hydrochloride in different structural form.

M S Pallavi et.al [3] has proposed a work on spam detection using support vector machine algorithm. The support vector machine algorithm determines the results fast and provide exact results for the problem. This algorithm can be used to find a quick and optimal solution for any kind of related works of optimization.

Sabitha Mangalathillam et.al [4] has proposed a work on curcumin loaded chitin nanogels to cure melanoma. The drug scatters in water and is less toxic. There is active transdermal penetration where occurs a vigorous elements transported through the skin for complete dissemination.

Flaherty et al [5] has proposed a work for treating melanoma with the metastatic condition by the usage of PLX4032 in Melanoma patients having V600E mutation lead to a condition of partial or complete regression in patients. It resulted in total or limited tumor degeneration in the majority of patients.

Frouin et al [6] has proposed a work on the method of comparison in the improvement of the detection of BRAF V600 mutations in highly pigmented Melanoma Specimens. In this study there is an application of three of the strategies for the improvement pigmented DNA refractory to PCR amplification detection improvements. The strategies used in it includes: BSA, the dilution of DNA, purification using NucleoSpingDNA Clean-up XS kit.

Meier et al [7] has proposed an approach on signalling pathways that shows the target of the molecules for the efficient treatment of advanced Melanoma. There are many molecules that play a key role in melanoma development and progression. Like a molecule of adhesion E-/N-cadhein,MelCAM and alphavbeta3 integration that is regulated by the pathway or can activate them. This MAPK and AKT signalling pathways that assure the therapeutic targets to melanoma.

Mourah et al [8] has proposed work on Cobas 4800 BRAF V600 mutation test and home brew method, by collecting the tumor samples and performed in routine in national laboratories and funded by the French National Cancer Institute. The result was founded by the laboratory is most tumour samples were surgical specimens 79% and 66% samples of metastases. The rate of discordance ranged from 0% to 31%. The highest discordance rates are 13.6% and 31.0%.

Poulikos et al [9] has a work on evaluating BRAF inhibition effects on patients affected by metastatic Melanoma Skin Cancer. Data was collected by 35 biopsies from 16 patients affected by metastatic melanoma by inhibiting BRAF inhibitor and analysing the melanoma antigens, T-cell makers and immune-modulator cytokines. It also reveals that the mechanism of sensitivity of ERK signalling to RAF inhibitors, that causes the activation of other pathways through ERK signalling and reduce the dependence on the tumour. Resistance develops with clinical activity in melanomas in BRAF V600 mutations.

Villanueva et al [10] have developed a model on defiance to BRAF inhibitors evolved by persistent therapy of BRAF V600. In the presence of the 1GF-1R/P13K improved the survivalist developing the resistance. It has given the future suggestion on strategies to treat to Melanoma.

R I Ramachandran et.al [11] explains the basics of computational chemistry and molecular modelling which is the fast evolving zone used for modelling and simulation to determine the behaviour of biological systems at molecular level.

3. METHODOLOGIES USED

The methodology of the current work that is in progress is carried out computationally as well as in simulation. The various methods are performed for the structural visualization to visualize the particular protein structure. Consider the particular protein structure in different kinds of molecule and interconnecting them by bonding. The dataset of BRAF protein sequence is collected in the form of the PDB from online. The obtained PDB contains a set of ligand and receptors. Many modifications are made to the PDB file like change of atom name PSO to PYS, deletion of the line of OD and HD, deleting the Hydrogen molecule in the water. A copy of PDB file is made by renaming it after the modification. Using the chimera tool with modified file the addition or removal of charges is done in the ligand file. Thus, the creation of the ligand and receptor is done by this and stored in the PDB format. In this method the simulation tool is used to represent a protein from PDB file and visualize the particular protein molecular structure. One of the most popular tools used in the visualization for the structure of protein is Chimera. Another method used is computational way is to visualize the particular atom. Using

the specific programming language, around will be included the graphic form and using the graphic format and by adding codes can create the structure of atoms and bonding. This method involves the procedure of converting the data from PDB to XML format, representing the number of atoms and bonding of atoms. For the computational way, we have to use drawing packages and graphics. The my.pen object is the drawing package used to store value of the atom needed. After the creation of graphics the value is stored in the array. Then the atoms to be displayed are coloured using the brush tool. These methods are used to represent the atoms, bonding of atoms and calculation of the bond angle between the atoms. The computational way can also visualize the particular atom. Using the specific programming language, there will be included the graphic form and using the graphic format and by adding codes can create the structure of atoms and bonding. The programming language can be used in drawing and graphic form. These two packages will create the visualization of graphical structure using particular coding and visualizing the atoms and bonding.

4. EXPERIMENTAL ANALYSIS

The experimental analysis of the proposed system visualizes the structure of atoms and bonds using simulation tool and computational way. The PDB file of a particular protein sequence can be visualized by adding and removing the ligand of water molecules. The PDB file can be converted to XML format. Based on the XML format to filter the water molecules and using the extracted file to create water molecules atoms in a simulation tool. On computational way, the number of atoms to be represented is taken as input. The output is in the form of visualization of the atom bonding that occurs between the atoms of a protein structure.

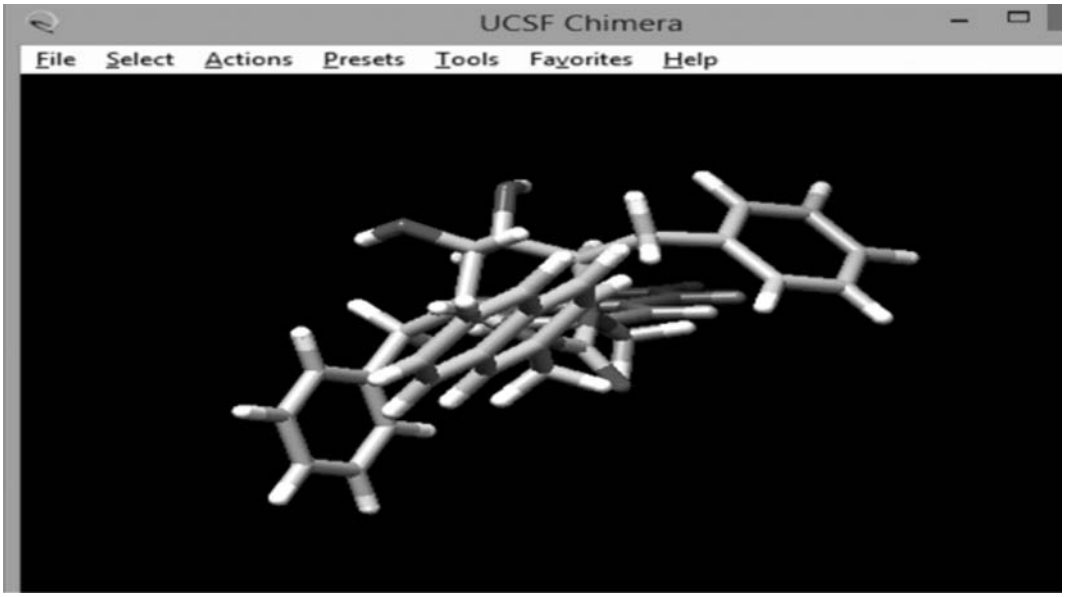

Figure 1: Simulation of the ligand in Chimera simulation tool

The Chimera simulation tool is the tool used to represent the molecular structure of protein molecules. The visualization of the receptor that attach to the ligand molecules with the addition and removal of atoms to it is represented in the Fig. 1.

The computational method includes number of atoms to be represented is taken as input. The output is in the form of visualization of the atom bonding that occurs between the atoms of a protein structure.

The Fig. 2 depicts the illustration of a atom. The number of atoms of a molecule is set as input by means of this the atom will be displayed as per the definite digit. The atom is visualized and the result is represented whereas The Fig. 3 is the representation of the bonding of the atoms of a protein molecule of the represented atoms in the structural way.

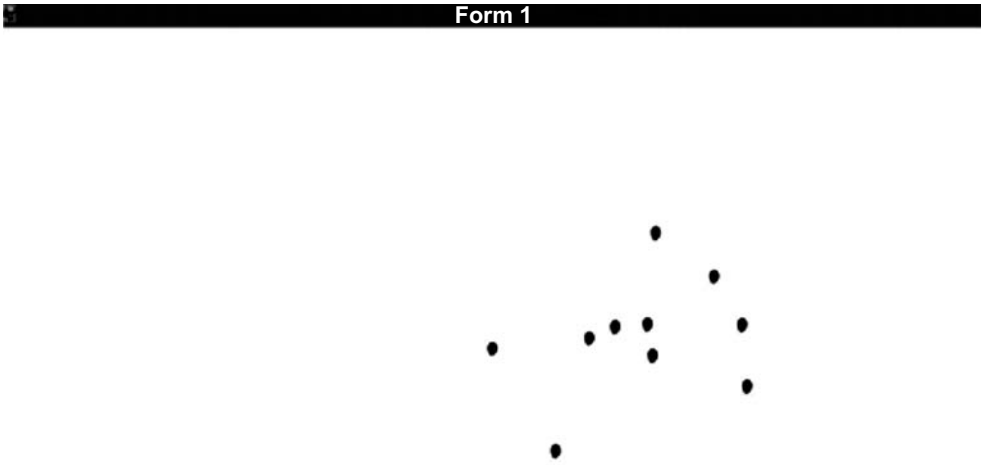

Figure 2: Atom representation

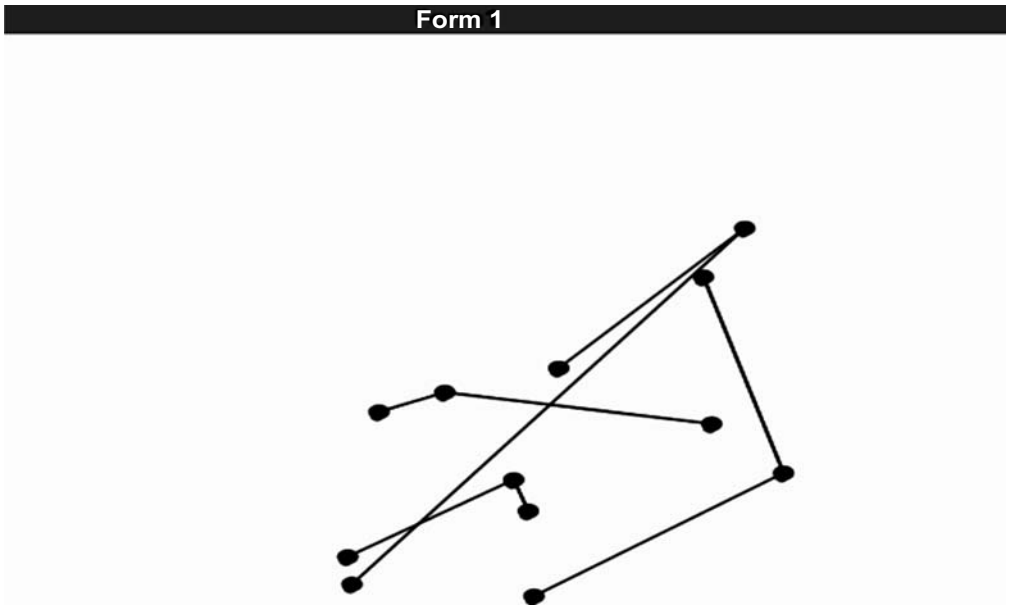

Fig. 3. Bonding of atoms

5. CONCLUSION

The progress and application is incredibly active field of research for the study of the atom bonding and their angle calculation. The method is concluded by the representation of structure of particular protein molecule and finding the bond angles between the atoms. The atoms formed with all its features to its binding and unbinding possibilities. This atom can be visualized graphically. It includes the steps like training data by collecting the tissue samples from PDB data and visualization of the variation of the data. These are the computational way for the representation of particular proteins and the calculation of the bond angle between the atoms. The protein sequence and dynamic protein molecular structural are being surveyed within each section. The atom bonding represents the atom bonding of each protein cells for cellular based activities. This method examines methods to improve the computational exploration of molecular dynamics of protein, bonding and its complete protein structure visualization.

6. ACKNOWLEDGMENT

First and foremost, we feel deeply indebted to Her Holiness Most Revered **MataAmritanandamayi Devi (Amma)** for her inspiration and guidance both in unseen and unconcealed ways.

Wholeheartedly, we thank our college, **Amrita School of Arts and Sciences, Amrita University, Mysore campus, Karnataka, India,** for providing the necessary environment, infrastructure, encouragement and for extending the support possible at each stage of this project.

We express our sincere gratitude and indebtedness to our parents who have bestowed their great guidance at appropriate times by providing encouragement in planning and carrying out the project.

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