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AN APPROACH OF INSILICO ANALYSIS: MOLECULAR DOCKING OF PHYTOCHEMICALS BELONG TO SELECTED *ALLIUM* SPECIES

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Abstract: In-silico analysis refers to experiments performed using computers or computer simulation. In-silico approaches gives feasible solution to the experimental methods which are used to characterize the proteins of different organisms which involves too much time, high cost and the certainty that these methods are not acquiescent to high throughputs of techniques. It is a process to analyze and study the interaction between a ligand and a protein molecule at a target specific region of the receptor protein. It is useful in the analysis of non-covalent bonds that form a stable complex of potential efficacy and more specificity. The primary objective of molecular docking is to hypothesize a ligand receptor complex with optimal conformations along with a valid binding free energy. Molecular docking of two selected ligands (gallic acid and quercetin) with target proteins attributed to antibacterial, antifungal and antioxidant activities belongs to selected *allium* species was carried out. This study presented the positive results by binding of ligands to target proteins.

Keywords: Molecular docking, Protein, Ligand, antioxidant, antibacterial, antifungal

I. Introduction:

In molecular docking, three-dimensional structures are used to represent various views of the structures. One can superimpose one structure on another by using complex molecular mechanics program. The same mechanism is applied to superimpose the three dimensional structure of a potential drug on the target site. This process is known as molecular docking. The prediction can be carried out for the structure of the intermolecular complex using two molecules in molecular docking. The ligand (small molecule) interacts generally with protein's binding sites. During the time of the production of compounds binding sites are known to be active. The mechanism of binding may occur in so many possible confirmations, which are known as binding modes. Along with that the energy of the complex, the strength of the binding and the types of signal produced are also predicted using this mechanism. In addition to that the calculation of the binding affinity is also done by using scoring functions between two molecules. The most favourable type of molecular docking is protein-ligand interaction, which is most applied in the pharmaceutical industries (Sahay A. and Shakya M., 2010; Ayaz Mahmood Dar and Shafia Mir, 2017).

There are two sections of molecular docking described as :- (I) Search algorithm and (II) Scoring function.

(I) Search algorithm: First of all, several numbers of configurations can be created by algorithm. These configurations include the experimentally determined binding modes. For docking analysis so many algorithms are used including genetic algorithms, molecular dynamics, fragment based methods, Monte Carlo methods, systemic searches and distance geometry methods.

(II) Scoring function: Binding affinity of two molecules after molecular docking is predicted using this. The strength of the non-covalent interaction is known as binding affinity. Along with that to predict the strength of the other types of intermolecular interactions, scoring functions have also been developed like between two proteins or between protein and drug or between protein and DNA. These scoring functions are used to evaluate these configurations and for the separation of the experimental binding mode from the others.

II. Material and Methodology:

The basic steps included in the molecular docking are given below:-

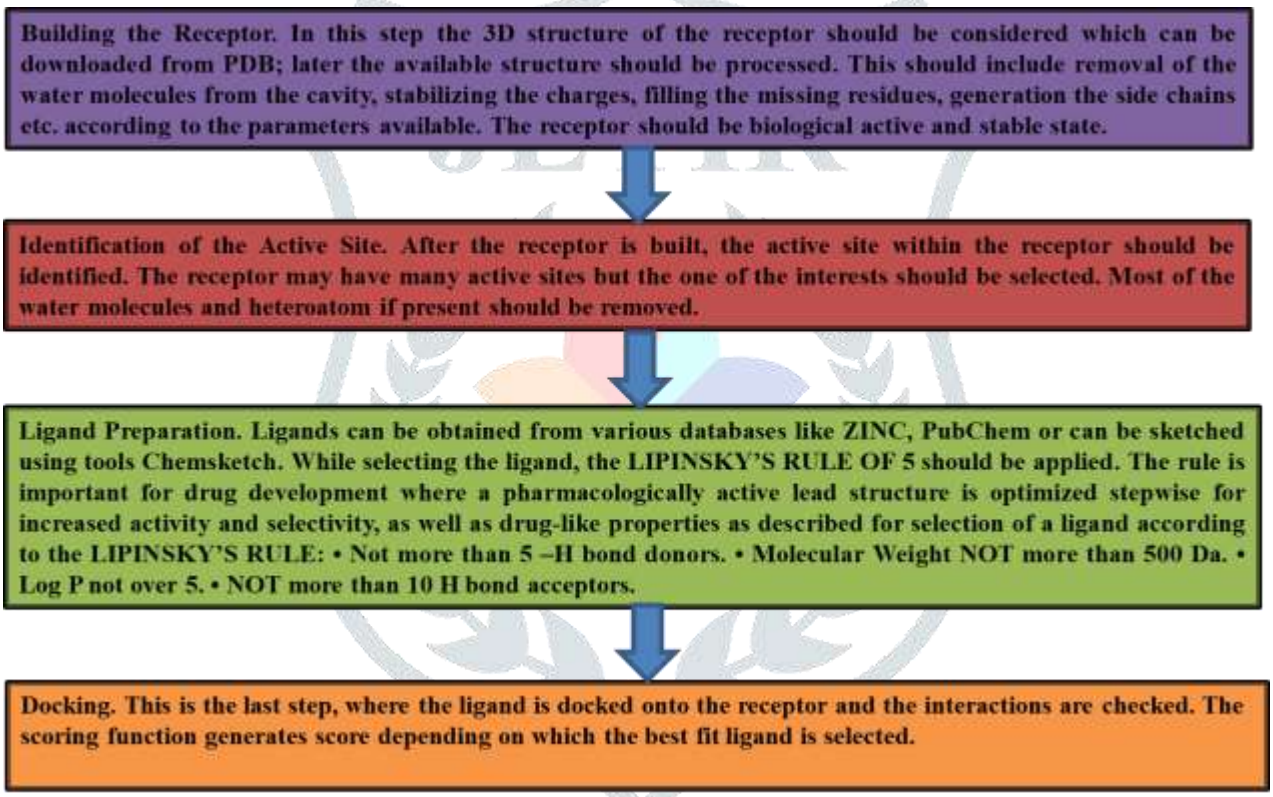

Figure 1: Flowchart Showing the Procedure of Molecular Docking

(I) Ligand Selection and Preparation

Three dimensional ligand structures of Gallic Acid and Quercetin were retrieved with the help of PubChem Database in the structure data format (SDF). The cleaning of polar hydrogen molecules and minimization of energy was carried out using Amber 03 force field and steepest descent method. For the minimization of energy Yasara software was used. Total two ligands were analyzed by following this method and kept it in the .sdf format as per the requirement of the software.

(II) Protein Preparation

Two ligands were selected and proteins from two plants *Allium cepa* L. and *Allium sativum* L. were selected for investigating binding affinity of plant proteins with two selected ligands. PDB structures of *Allium cepa* L. and *Allium sativum* L. were retrieved from PDB

(Protein Data Bank). There were certain parameters like removal of water molecule, selection of chain and minimization of energy carried out by Amber 03 force field for further molecular docking process.

(III) Molecular Docking

Molecular docking was carried out between two selected ligands (Gallic Acid and Quercetin) and proteins presented in two selected plants to understand the binding mechanism and their response to antibacterial, antifungal and antioxidant activities. Then molecular docking was performed. After that for further analysis protein-ligand interaction profile server was used.

3. Result:

Molecular docking of two selected ligands (gallic acid and quercetin) with the protein of different activities like antibacterial, antifungal and antioxidant was carried out. The result obtained here presented the positive result.

3.1 Molecular Docking

The result of molecular docking represented the binding energy and contacting receptor residues. Which was obtained as given below:- **(Table-1)**.

Table 1: Binding Energy and Analysis of Docked Complex

Name of the Activity	Name of Ligand	Binding Energy[kcal/mol]	Contacting Receptor Residues
Antibacterial Activity	Quercetin	6.318	HIS 54, SER 55, PRO 56, TYR 57, PHE 58, ILE 59, ASP 60, ASN 79, HIS 80, THR 124, ARG 125, ASP 126, ILE 130
	Gallic Acid	4.938	LYS 187, GLU 190, ALA 191, ALA 192, LEU 196, LEU 197, ALA 199, PHE 200, GLU 203
Antifungal Activity	Quercetin	8.124	VAL 10, ALA 11, ILE 19, GLY 20, TYR 21, LYS 22, GLY 23, LYS 24, MET 25, THR 58, SER 61, GLY 114, ALA 115, TYR 118, ASP 146, THR 147
	Gallic Acid	5.628	ILE 9, VAL 10, ALA 11, MET 25, GLU 32, ILE 33, PHE 36, ILE 62, LEU 69, ILE 112, TYR 118
Antioxidant Activity	Quercetin	8.226	MET 113, VAL 116, ARG 120, ILE 345, VAL 349, LEU 352, SER 353, TYR 355, LEU 359, PHE 381, LEU 384, TYR 385, TRP 387, PHE 518, MET 522, VAL 523, GLY 526, ALA 527, SER 530, LEU 531, LEU 534
	Gallic Acid	6.109	TYR 348, VAL 349, LEU 352, SER 353, PHE 381, LEU 384, TYR 385, TRP 387, PHE 518, MET 522, VAL 523, GLY 526, ALA 527, SER 530

3.2 Antibacterial Activity

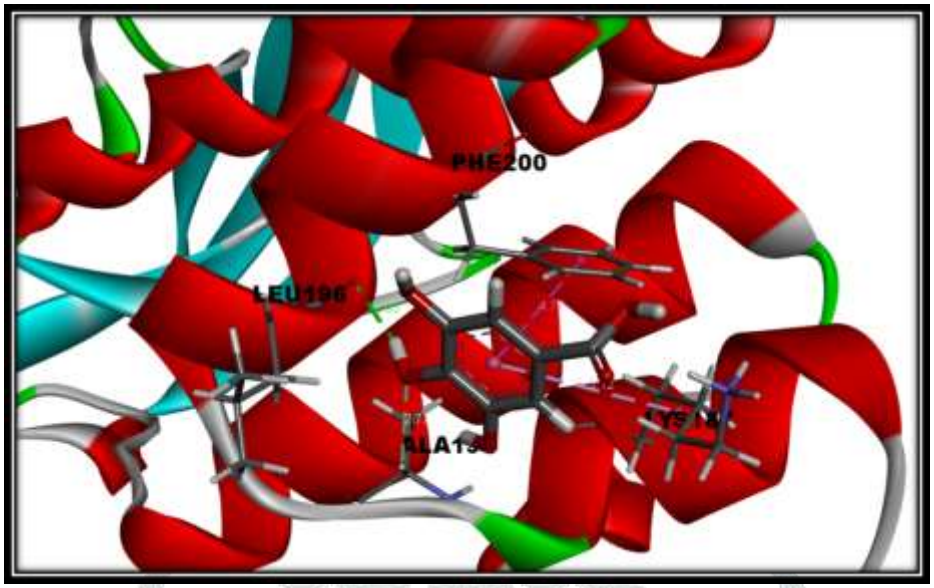

Figure 2: Protein–ligand interaction maps developed from protein-ligand interaction profiler server (Ligand Gallic Acid with Protein of Antibacterial Activity)

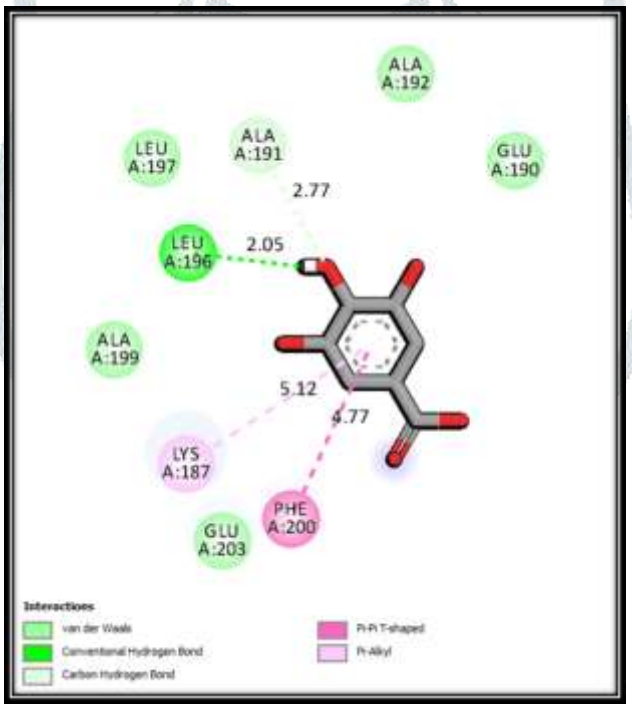

Figure 3: Bond Formation Between ligand Gallic Acid and Protein of Antibacterial Activity

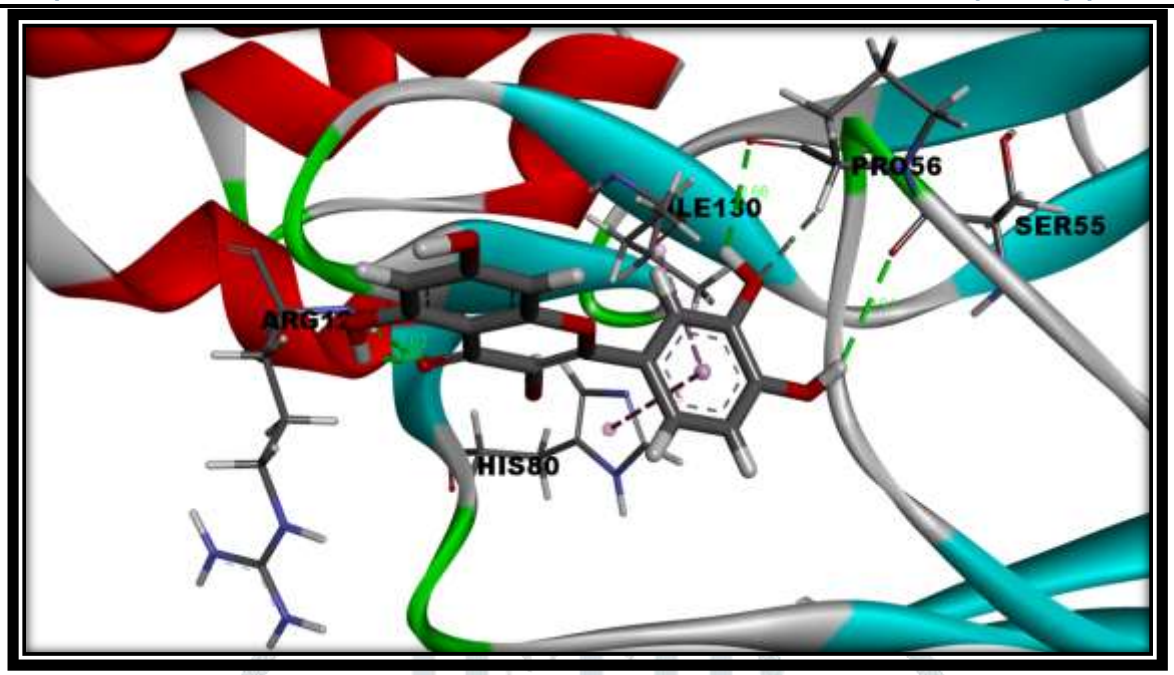

Figure 4: Protein–ligand interaction maps developed from protein-ligand interaction profiler server (Ligand Quercetin with Protein of Antibacterial Activity)

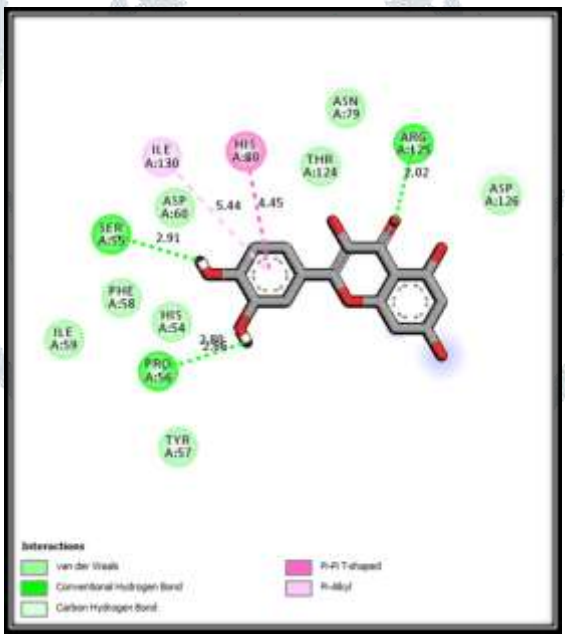

Figure 5: Bond Formation Between ligand Quercetin and Protein of Antibacterial Activity

3.3 Antifungal Activity

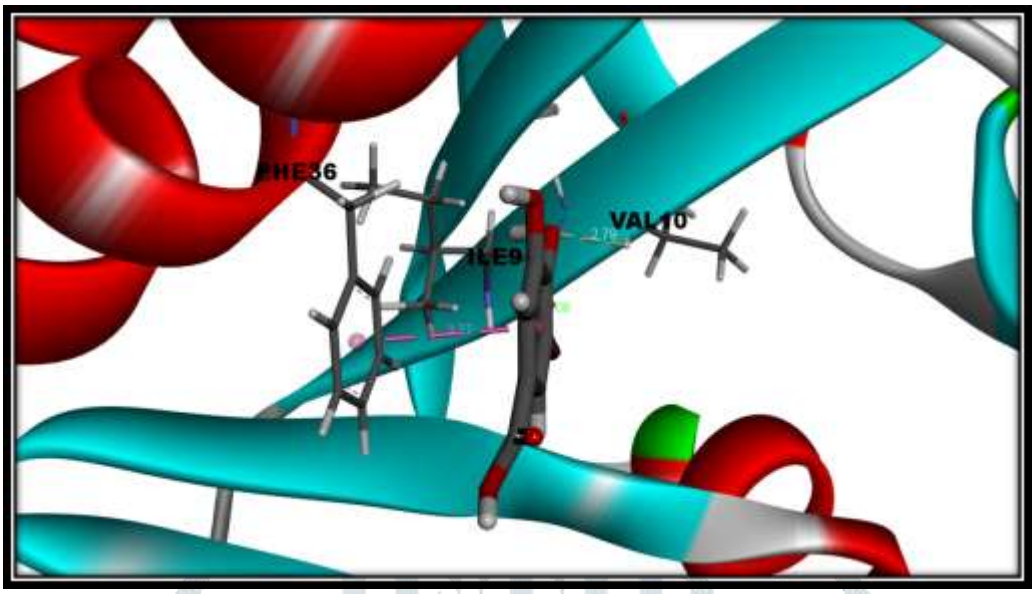

Figure 6: Protein–ligand interaction maps developed from protein-ligand interaction profiler server

(Ligand Gallic Acid with Protein of Antifungal Activity)

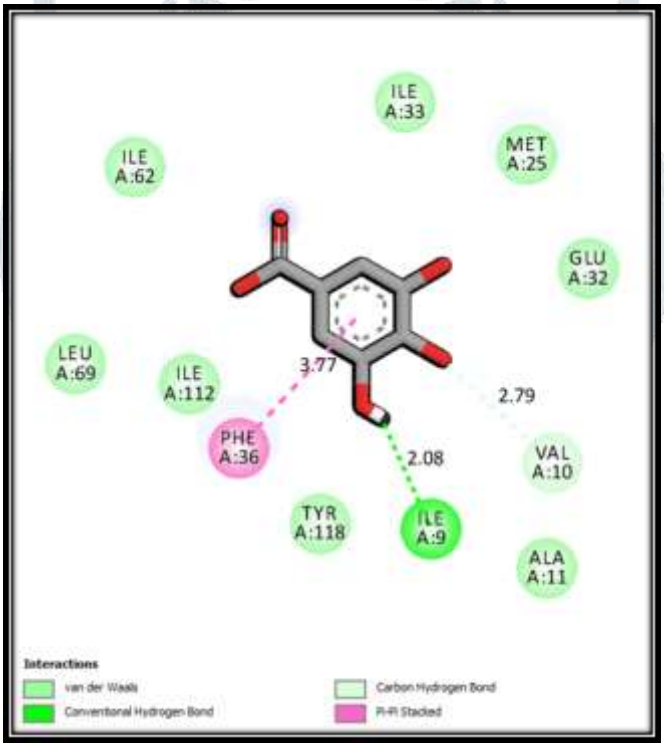

Figure 7: Bond Formation Between ligand Gallic Acid and Protein of Antifungal Activity

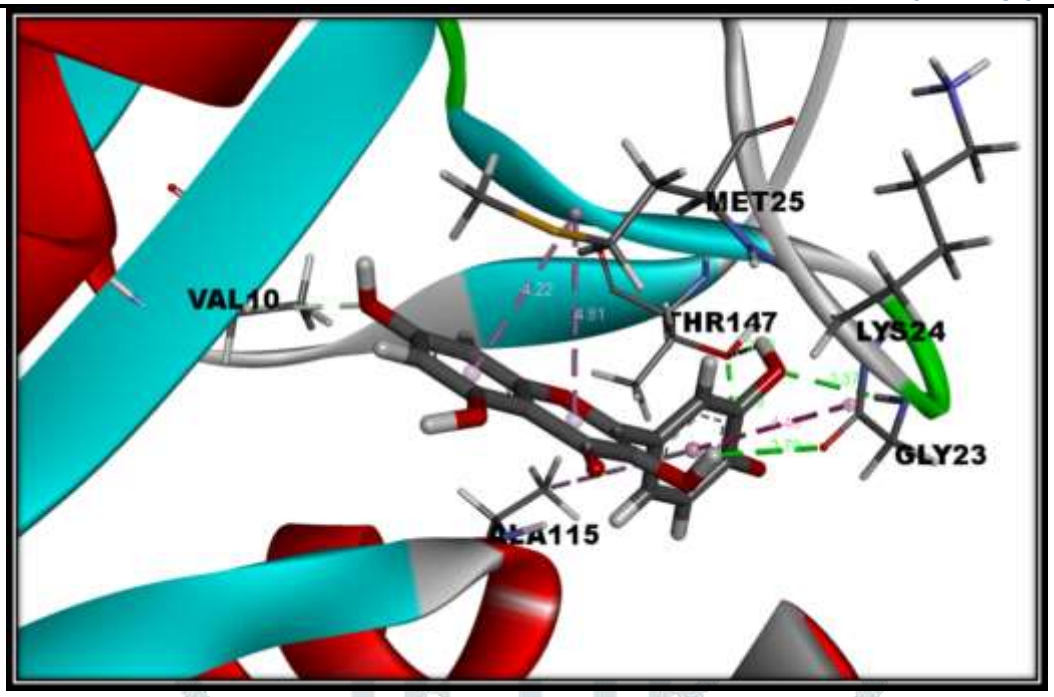

Figure 8: Protein–ligand interaction maps developed from protein-ligand interaction profiler server (Ligand Quercetin with Protein of Antifungal Activity)

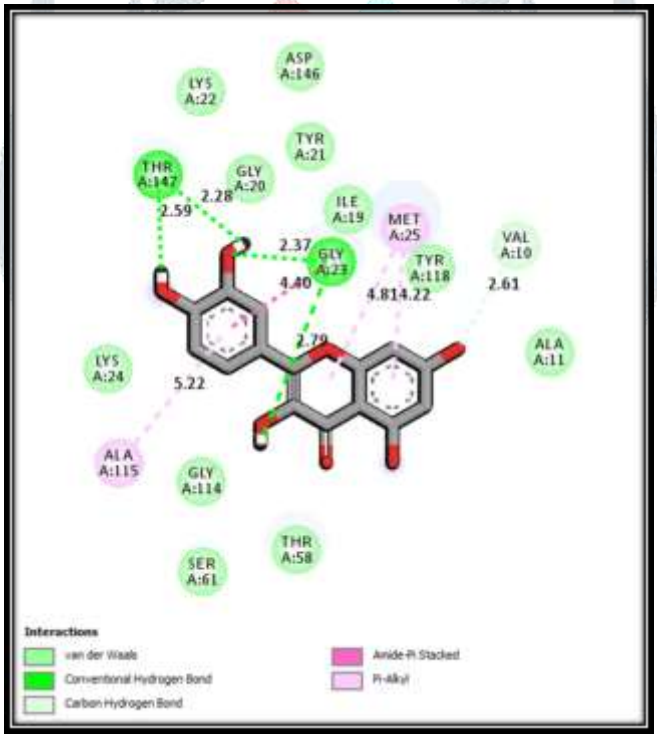

Figure 9: Bond Formation Between ligand Quercetin and Protein of Antifungal Activity

3.4 Antioxidant Activity

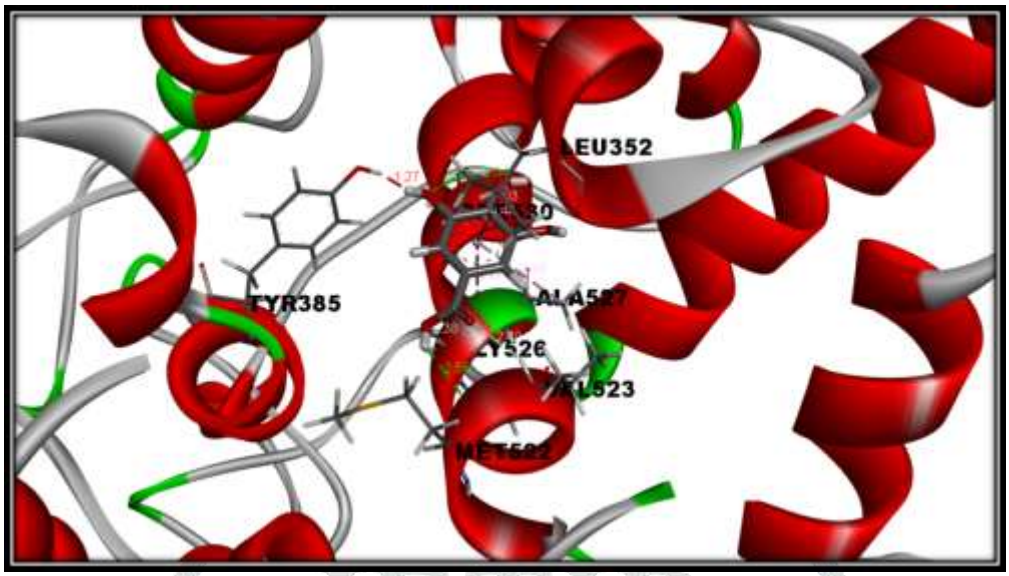

Figure 10: Protein–ligand interaction maps developed from protein-ligand interaction profiler server (Ligand Gallic Acid with Protein of Antioxidant Activity)

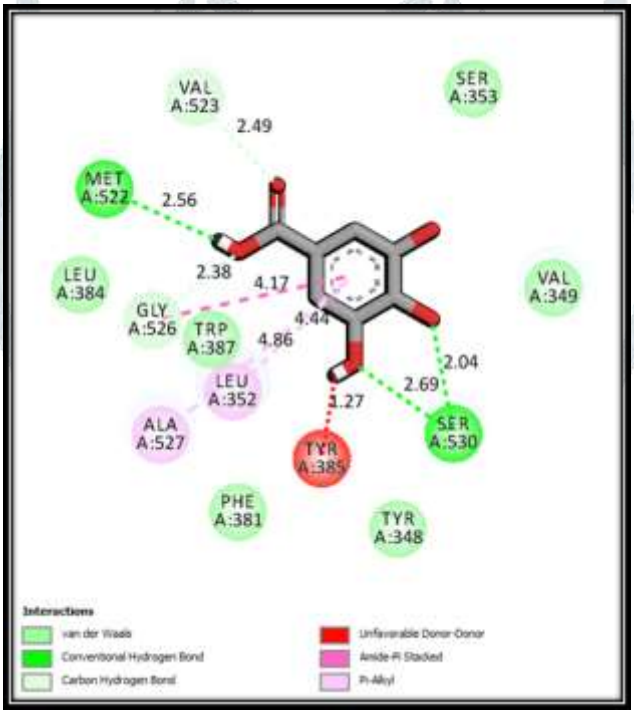

Figure 11: Bond Formation Between ligand Gallic Acid and Protein of Antioxidant Activity

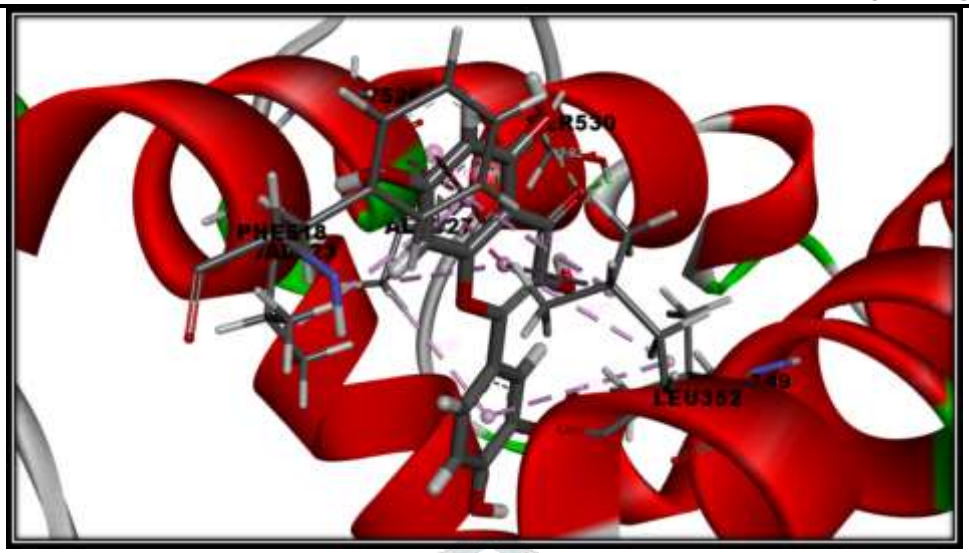

Figure 12: Protein–ligand interaction maps developed from protein-ligand interaction profiler server

(Ligand Quercetin with Protein of Antioxidant Activity)

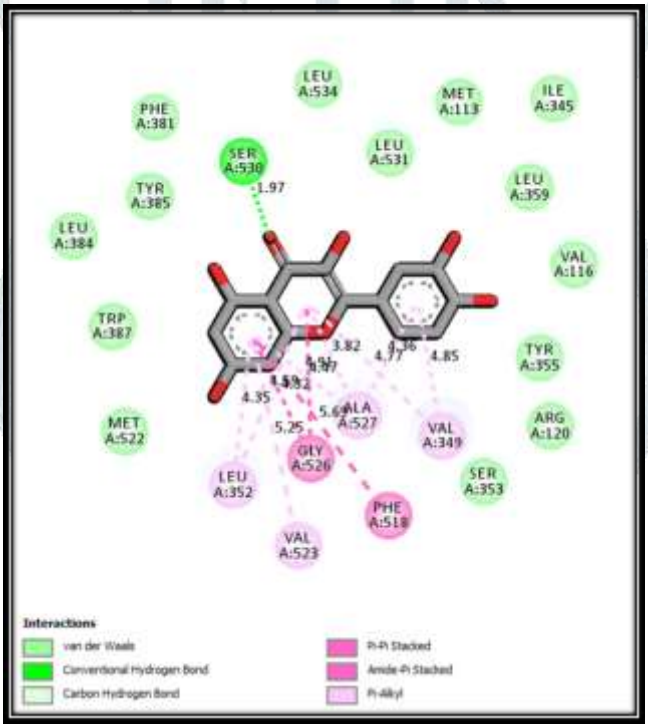

Figure 13: Bond Formation Between ligand Quercetin and Protein of Antioxidant Activity

4.10.5 Discussion:

The result obtained here was exhibited positive relation between the ligands and the protein of different activities. No similar experiment was observed related to this work. This work proved the potential of phenolic and flavonoid compounds to have antibacterial, antifungal and antioxidant activities.

5. Conclusion:

Molecular docking of two selected ligands (gallic acid and quercetin) with target proteins attributed to antibacterial, antifungal and antioxidant activities was carried out. This study presented the positive results by binding of ligands to target proteins. Thus, it can be concluded that this study of Bioefficacy of selected *Allium cepa* L. and *Allium sativum* L. extracts is supported by in-silico (molecular docking) study.

6. References:

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II. Sahay, Archna, and Madhvi Shakya. "In silico analysis and homology modelling of antioxidant proteins of spinach." *J Proteomics Bioinform* 3, no. 5 (2010): 148-154.