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Antioxidant Activity Properties of Extract of Turmeric (Curcuma longa L.) Plant

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Abstract: In this study, it was aimed to determine the chemical components in the ethanol extract of the turmeric (Curcuma longa L.) plant rhizomes sold as powder in spice-sellers and to determine its antioxidant activity properties. For this purpose, turmeric rhizomes powder was extracted by maceration method using ethanol solvent and its chemical content was determined by Gas chromatography-Mass spectrometry (GC-MS) analysis. After chemical components were determinate for the turmeric ethanol extract, the inhibitory activities of these chemicals against the Crystal structure of Human peroxiredoxin 5 (HP5) (PDB ID: 1HD2) and Bovine Xanthine Oxidase (BXO) (PDB ID: 3NRZ) downloaded from the Protein Data Bank site were compared. The highest activity of the molecule was investigated by Gaussian calculations.

Keywords: Turmeric (*Curcuma longa* L.), Molecular docking, Extract, Antioxidant activity

1. Introduction

Turmeric (*Curcuma longa* L.) is a perennial and rhizomatous plant belonging to the Zingiberaceae family, which can grow up to 1 m in height and spreads in tropical and subtropical regions. Due to its economic importance and variety of usage areas, it is widely cultivated in Asian countries, especially in China and India [1,2]. Although it is commonly known as turmeric among the people, it is also called saffron root, yellow dye, curcuma and Indian saffron [2]. Especially the rhizomes and oils of the plant are of great importance. The most common uses include the food, textiles, cosmetics, pharmaceutical and paint industry [3]. Powdered rhizomes are mostly used as spices in a variety of dishes [1-3]. It tastes bitter and is a polyphenolic compound [2]. It preserves the freshness of the product to which it is added, gives a characteristic aroma and color [4]. Turmeric has an important place in Indian medicine especially because of its medicinal effects as well as its use as a spice [2]. Among the diseases in which the plant is traditionally used for treatment, there are colds, cough, sinusitis, anorexia, various eye diseases, stomach and digestive problems, rheumatic diseases, diabetic wounds, liver and skin diseases [1-3]. It is also used as a tonic and blood purifier [2-4]. Scientific studies have revealed that turmeric plants have a wide range of biological activities [5,6]. The main biological activities determined in turmeric rhizomes are antimicrobial, anticancer, antitumor, anti-inflammatory, antifungal, antiviral and antioxidant activities [4]. It is known that the main compound responsible for these biological activities is curcumin (yellow color pigment) [1,2,6]. It has been reported that curcumin has preventive properties against leukemia-lymphoma, gastrointestinal system cancers, genitourinary system cancers, breast cancer, ovarian cancer, head and neck cancer, lung cancer, melanoma, and neurological cancers [2].

In this study, it was aimed to determine the general chemical content by GC-MS analysis of the ethanol extract of turmeric rhizomes supplied in powder form and activity against antioxidant proteins [7].

2. Computational Method

2.1. Plant Material

In this study, turmeric (*C. longa* L.) plant, which was purchased in powder form from a spice-seller in Sivas province, was used as plant material. There

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are many methods for preparing plants extract [8-13]

Figure. 1 Turmeric (*C. longa* L.) rhizome powder used in the study

2.2. Extraction Method

Ethanol extraction was made by maceration method from turmeric purchased in powder form. Accordingly, 20 g of powdered turmeric was weighed, and 200 mL of ethanol was added on top. It was kept at room temperature on a magnetic stirrer at 150 rpm for 16 hours. At the end of the maceration, it was filtered with Whatman No:1 filter paper. The solvent was removed in a rotary evaporator to obtain the crude extract. The obtained crude extract was stored at +4ºC until analysis.

2.3. GC-MS Analysis

GC-MS analysis of ethanol extract from turmeric plant was performed by the Giresun University Central Research Laboratory Application and Research Centre. In the analysis, HP-5 MS IU capillary column (30 m; 0.25 mm; 0.25 µm) apparatus, 7890A (Agilent) model device and Helium as carrier gas (1.5 mL/min) were used.

2.4. Molecular Docking

Molecular docking calculations were performed to compare the activities of molecules against antioxidant proteins and to discover new and effective molecules for antioxidant. The program developed by Maestro Molecular modeling platform (version 12.8) by Schrödinger was used for molecular docking calculations. There are many modules in calculations. In the first step, the protein preparation module was used in the preparation of proteins. In this module, the active sites of the proteins were determined. In the next step, the studied molecules are prepared. First, the molecules are optimized in the gaussian software program, then the LigPrep module is prepared for calculations using optimized structures. The Glide ligand docking module [14-16] was used to examine the interactions between the molecules and the antioxidant protein after preparation. Calculations were made using the OPLS4 method in all calculations.

2.5. Gaussian calculation

The highest activity of the molecule was investigated by Gaussian calculations in hf/6-31++g(d,p) basis set.

3. Results and discussion

In this study, the activities of chemical molecules in turmeric (C. longa L.) extract against antioxidant proteins were compared. The chemicals in the ethanol extract were determined using the GC-MS analysis.

Chemicals according to their percentages are given in Table 1.

Table 1. Chemical compositions of turmeric ethanol extract

1	Alfa-Pinene	1.20
2	Camphene	5.47
3	Cubebene	2.00
4	P-Cymene	1.03
5	Citronellal	3.97
6	Menthofuran	2.11
7	Caryophyllane	1.87
8	Alfa-Bergamotene	1.34
9	Borneol	1.27
10	Ar-Turmerone	47.28
11	Turmerone	15.78
12	Alfa-Terpineol	0.63
13	Carvone	2.74
14	Linalool	1.06

15	Germacrene D	1.09
16	Beta-Sesquiphellandrene	3.18
17	Curcumene	3.78
18	Nerol	1.78
19	Phellandrol	1.34
20	Citronellyl Pentanoate	2.78
21	Xanthorrhizol	1.52

According to the results obtained from GC-MS analysis of the ethanol extract of turmeric (C. longa L.), it is seen that there are 21 different components in Table 1. It was determined that the substance with the highest amount of these components was Ar-Turmerone (47.28%). Some other substances defined according to the amounts of their presence are; It can be listed as Turmerone, Camphene and Curcumene.

A comparison of the activities of the chemicals in the extract of turmeric (C. longa L.) against antioxidant proteins was made. As a result of molecular docking calculations, many parameters are calculated. These parameters allow predicting the active sites of molecules. However, it is a common method used to synthesize more effective and more active molecules [17,18]. The most important parameters calculated are given in Table 2.

The most important parameter among these parameters is the docking score. The molecule with the most negative numerical value of this parameter is considered to have higher activity than the other molecular. The most important factor determining the numerical value of the molecular docking score parameter is the chemical interaction [19]. The interactions between antioxidant proteins, which are composed of many proteins, and molecules, determine the numerical value of the docking score parameter [20,21]. As the interactions between molecules and proteins increase, the numerical value of the docking score parameter becomes more negative. Therefore, the biological activity of the molecule is higher than other molecules.

These interactions have many interactions such as hydrogen bonds, polar and hydrophobic interactions, pi-pi and halogen [22-24]. These interactions are shown in Figure 2-5.

Table 2. Numerical values of the docking parameters of molecule against proteins

HP5	**Borneol**	**Terpineol**	**Cubebene**	**Camphene**
Docking Score	-5.30	-4.81	-4.08	-4.05
Glide ligand efficiency	-0.48	-0.44	-0.27	-0.41
Glide hbond	-0.61	-0.61	0.00	0.00
Glide evdw	-13.98	-9.92	-16.58	-16.30
Glide ecoul	-6.62	-5.98	0.55	0.19
Glide emodel	-26.03	-18.06	-19.62	-19.96
Glide energy	-20.59	-15.90	-16.03	-16.11
Glide einternal	1.63	5.40	0.45	0.00
Glide posenum	348	231	255	9
BXO	**Ar-turmerone**	**Carvone**	**Turmerone**	**Caryophyllane**
Docking Score	-7.36	-7.14	-7.14	-7.11
Glide ligand efficiency	-0.46	-0.65	-0.45	-0.47
Glide hbond	-0.34	-0.66	-0.11	0.00
Glide evdw	-33.79	-19.17	-30.92	-32.29
Glide ecoul	-6.04	-8.29	-5.71	0.49
Glide emodel	-54.63	-38.46	-48.84	-43.00
Glide energy	-39.83	-27.46	-36.63	-31.80
Glide einternal	4.79	0.02	5.68	0.00
Glide posenum	252	254	306	192

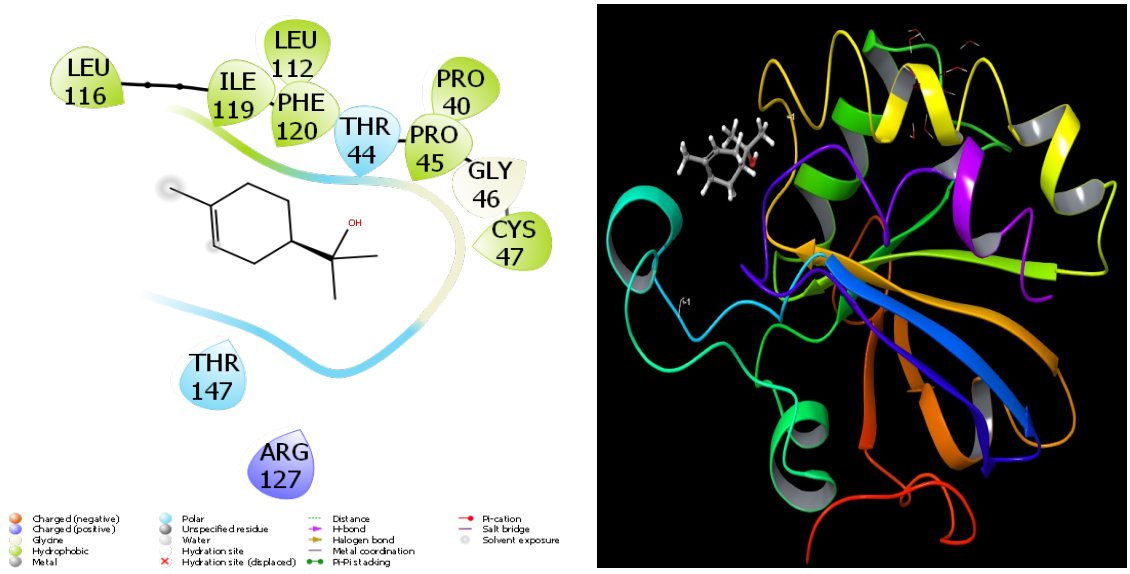

Fig. 2 Presentation interactions of Borneol with HP5 protein

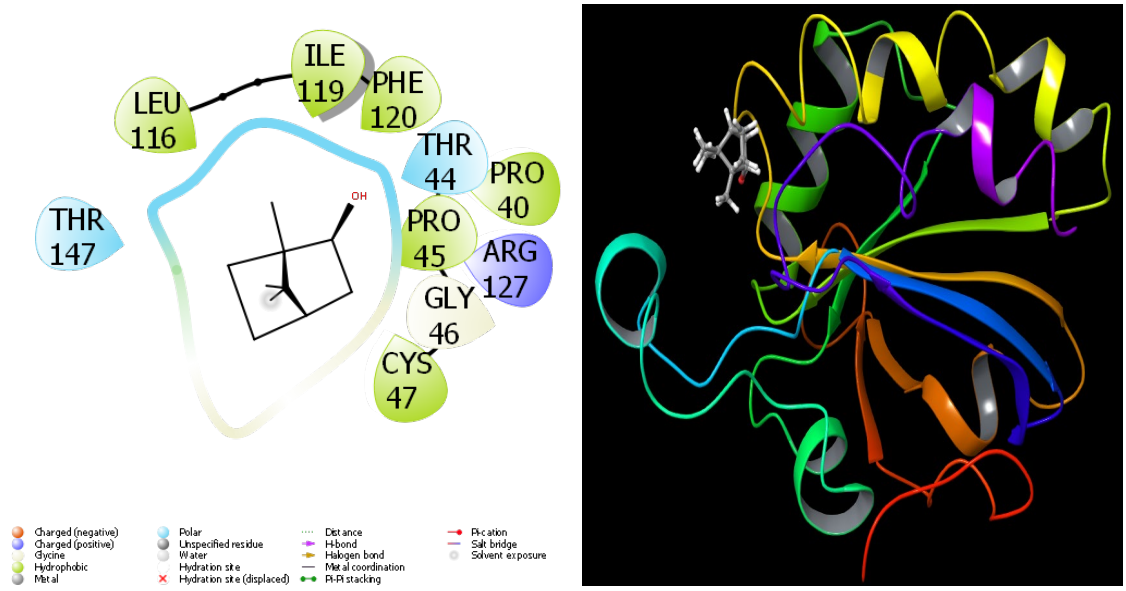

Fig. 3 Presentation interactions of Terpineol with HP5 protein

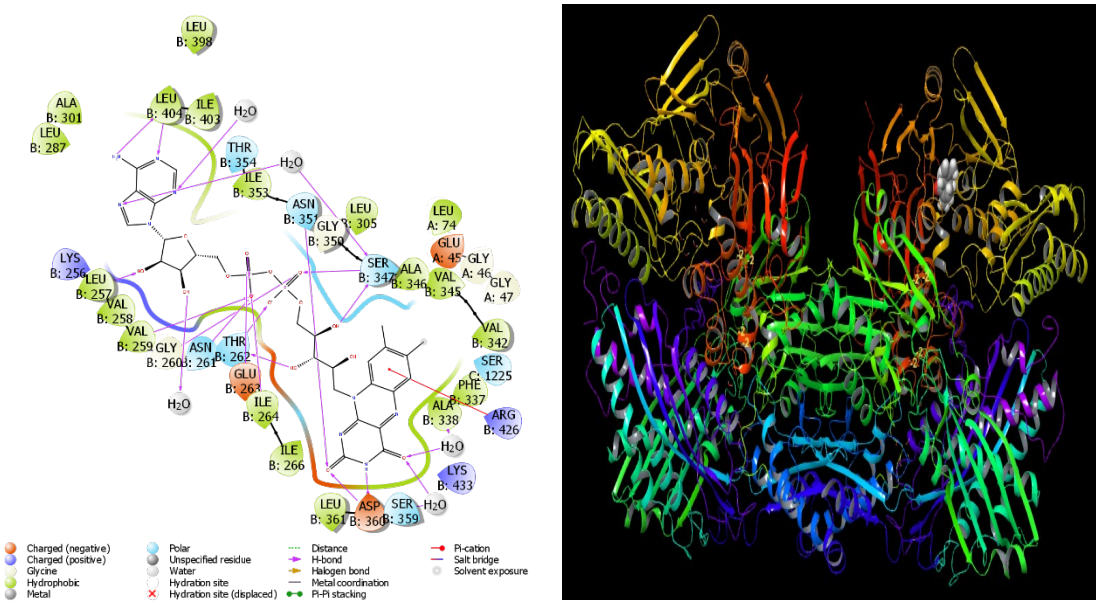

Fig. 4 Presentation interactions of Ar-turmerone with BXO protein

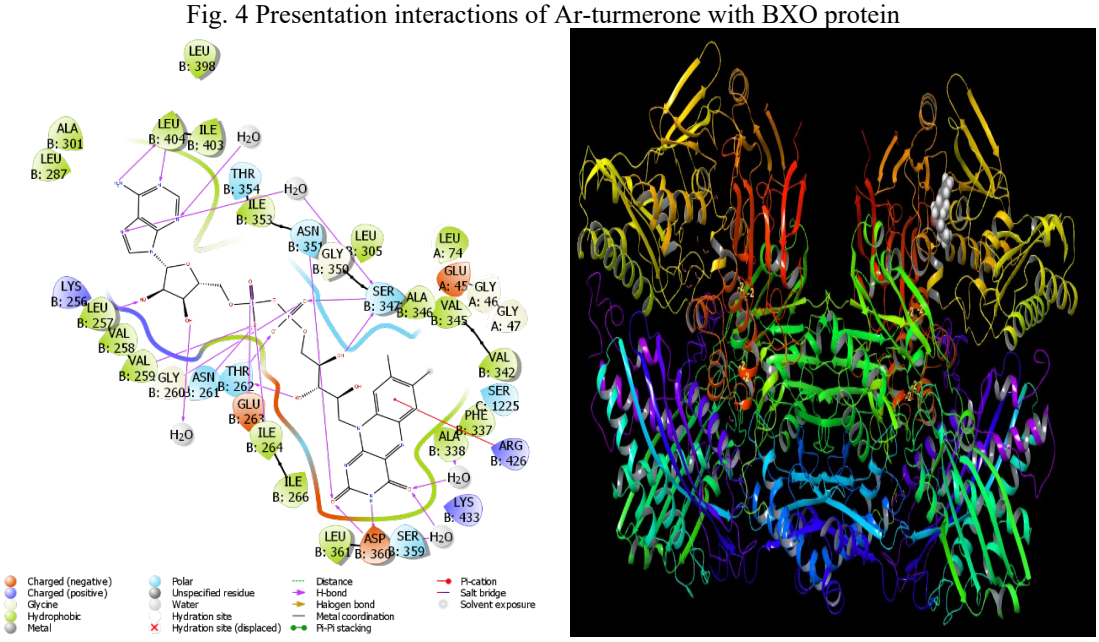

Fig. 5 Presentation interactions of Carvone with BXO protein

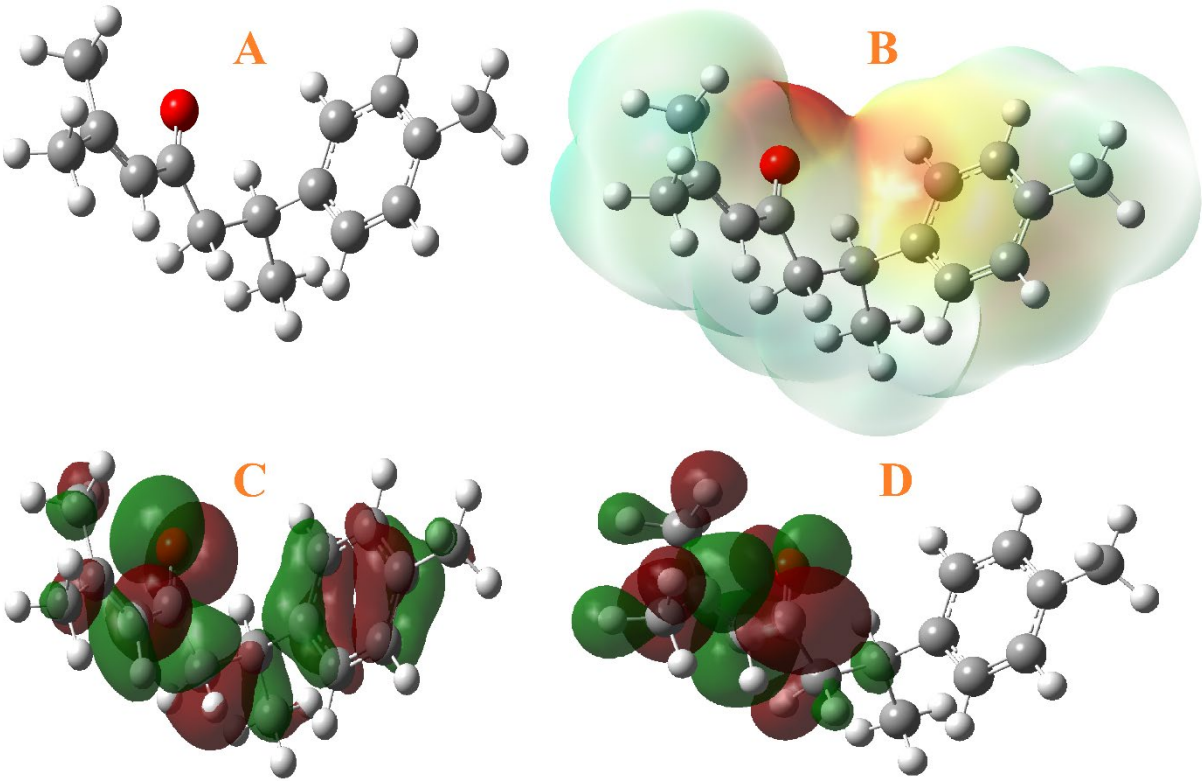

Fig. 6. Representations of optimize structure, HOMO, LUMO, and ESP of X

Many parameters are derived from molecular docking calculations, which are used to describe the chemical interactions between molecules and proteins, are given Table 2. Glide ligand efficiency parameter shows the efficiency of ligand molecules. Glide hbond, Glide evdw, and Glide ecoul parameters are numerical values of chemical interactions of molecules with antioxidant proteins [25]. The remaining parameters are take numerical data about the exposure between molecules and antioxidant proteins [26,28].

With the Gaussian calculations made, the calculation of the molecule with the highest activity was made in the HF/6-31++G(d,p) basis set. With these calculations, the active sites of the molecule were predicted [29-32]. The red colored regions are the regions with the highest electron density. It is expected to interact with the protein by making nucleophilic attacks from these regions [34-36].

4. Conclusions

As a result of the theoretical calculations, the activities of the chemicals in the extract of the turmeric (*C. longa* L.) plant against antioxidant proteins were examined. Docetaxel molecule was used as reference molecule. It was observed that Borneol molecule was higher than the reference Docetaxel molecule against both proteins.

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