**Antioxidant Properties of Lycium barbarum Extracts**

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| **Abstract**  Lycium barbarum (Goji berry) belongs to the Lycium genus. Lycium barbarum is a plant of Asian origin and its fruit has some pharmaceutical features exerting antioxidant and anticancer effects. To this end, the functional components constitute polysaccharides, polyphenols, flavonoids, carotenoids, and their derivatives. These compounds can neutralize free radicals by affecting the maintenance of cellular homeostasis and intracellular signalling pathways. Lycium barbarum is rich in antioxidants that fight free radicals in the body. Therefore, it may help slow the aging process, reduce cellular damage, and sustain overall health. The plant also produces vitamin C which helps strengthen the immune system. GC-MS analysis was performed to determine the content of Lycium barbarum extracts. Activities of the identified molecules against antioxidant proteins, PDB ID: 1HD2, and 4Z8D, were assessed. |
| Keywords: Antioxidant, GC-MS, Lycium barbarum, Molecular docking. |

1. **Introduction**

Lycium barbarum L., is a medicinal plant, growing all over the world. It is famous with its fruit, called wolfberry or goji berry. Almost a hundred thousand tons of it is produced by China alone. This country knows this plant for almost 2,500 years. The fruit of this plant has been a traditional medicine as anti-aging, antioxidant, antidiabetic, anticancer, cytoprotective, neuroprotective, and immunomodulatory agent [1-3]. It contains carotenoids, phenylpropanoids, flavonoids, polyphenols, and polysaccharides. Its polysaccharides, vitamins, betaine and mixed extracts of goji berry elicit anti-aging effects and improve eyesight [4].

L. barbarum polysaccharides (LBPs) are a group of water-soluble glycoconjugates with a molecular weight between 10-2300 kDa and they form around 6% of dry fruit weight [5]. LBPs are the bioactive components of L. barbarum. The biological functions of LBPs appear to be complex and multifaceted.

1. **Materials and Methods**

**2.1. Polysaccharides**

Aqueous extractions at medium and high temperatures have revealed that L. barbarum L. possesses douzens of polysaccharides within a molecular range between 10 and 2300 kDa [3]. Additional means such as physical or enzymatic breakdown of the extracts have been added in some of the experimental procedures. Such treatments have seemed to increase the overall LBP yield. Some other extraction startegies have involved a combiantion of the several extraction methods [6]. Similar results have been reported from extractions with ultrasound-enhanced subcritical water [7].

In recent years sophisticated instrumental extraction approaches, involving gel permeation and ion exchange chromatography, high-performance liquid chromatography (HPLC), size exclusion chromatography (SEC), and hybrid membrane technology, have been introduced [8]. These novelties have also enabled the researchers to gather some information on the extracted LPS conformations [9,10].

**2.2. Phenolic compounds**

**2.2.1. Flavonoids and Anthocyanidins**

Flavonoids apigenin and luteolin possess 2-phenyl-1 benzopyran-4-one skeletons. L. barbarum L. flavones quercetin, myricetin, and routine, possess a 3-hydroxyflavone skeleton [11]. Routine and quercetin appear to dominate the fruit LPBs [12,13].

Extraction yield and diversity of flavonoids have seemed to differ with the solvent, water, alcohols or their combinations, commonly used in earlier efforts. Recents studeis have preferred instrumental extractions, like gas chromatography-mass spectrometry (GC-MS), and capillary zone electrophoresis (CZE), HPLC-MS (Yang et al. 2021b), and solvents such as DESs (deep eutectic solvents), and "green solvents" including cheaper and biodegradable ingradients. Extraction in DESs has resulted in very high amounts of myricetin and routine, morin [14], and a very impportant flavanone naringenin [15].

Chromene pigments anthocyanidins is the coloring agent of L. ruthenicum. In some of the studies, a good number of anthocyanins have been extracted using UPLC-Triple-TOF/MS and UPLC-Q-Orbitrap methods [16]. These results have indicated that the type and yield of anthocyanin depended on the approach chosen [10].

**2.2.2. Phenolic acids**

Lycium species appear to be very good producers of phenolic acids: gallic acid, vanillic acid, 2,4-dihydroxybenzoic, veratronic acid, benzoic acid, salicylic acid, syringic acid, protocatechuic acid, chlorogenic acid, caffeic acid, p-coumaric acid, and ferulic acid [13]. Extraction methods have generally involved sophisticated instrumentation, mainly HPLC-MS, and GC-MS as weel as electrophoresis chemiluminescence (CE-CL) with solid phase extraction (SPE) [10,17].

**2.2.3. Other phenolic compounds**

As well as Lycium fruit, its roots have aslo been used as the phenolic compound source. And so far, fruit phenolics have included cannabicin D, cannabicin E, cannabicin F, threo-cannabicin H, erythro-cannabicin H, melongenamide D, grosamide, O-hydroxybenzene acetic acid, phloretic acid, dihydroferulic acid, and ethyl dihydroferulate. In other parts of the plant phenolic acid amides N-trans-feruloyl tyramine, N-trans-feruloyl 3-methoxytyramine, lysiumite A, N-trans-p-coumaroyl tyramine, N-cis-p-coumaroyl tyramine, N-feruloyl agmatine have been found [10,13].

**2.3. Molecular docking**

Molecular docking calculations are performed to compare the biological activities of molecules against biological materials. The program developed by Maestro Molecular modeling platform (version 12.8) by Schrödinger [18] was used for molecular docking calculations. Calculations are made up of several steps. Each step is done differently. In the first step, the protein preparation module [19] 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 [20] is prepared for calculations using optimized structures. The Glide ligand docking module [21] was used to examine the interactions between the molecules and the cancer protein after preparation. Calculations were made using the OPLS4 method in all calculations. Finally, ADME/T analysis (absorption, distribution, metabolism, excretion and toxicity) will be performed to examine the drug potential of the studied molecules. The Qik-prop module [22] of the Schrödinger software was used to predict the effects and reactions of molecules in human metabolism.

1. **Results and Discussion**
   1. **Antioxidant activity of goji leaves**

Goji leaves also appear to be a very rich source of both polyphenols and polysaccharides. Detection methods have mainly involved DPPH (free radical scavenging activity assay), TEAC (Trolox equivalent antioxidant capacity), HAPX (hemoglobin ascorbate peroxidase activity inhibition assay), and superoxide anion scavenging capacity assay. The compounds identified with the antioxidant activity mainly comprised polyphenols [23]. Here some other observations made have suggested that room temperature influenced the molecular diversity of the phenolic content [24]. Environmental samples have also been found to yield superior phenolic yields. Polysaccharides have been proven to be a significant DPPH, superoxide, and hydroxyl radicals scavengers in in vitro assays. Their in vivo antioxidant performance however remains a mystery for some of the researchers [25]. Evidence in this direction supports this concern [26]. One in vivo result however has pointed to the other direction that in diabetic rats ethyl acetate fraction of LCL could meaningfully lessen the amount of malondialdehyde at certain concentrations and increase the activities of radical scavenging enzymes, including catalase, superoxide dismutase, and glutathione peroxidase [27,28].

* 1. **The potential of goji in the food industry**

Industrial products of Goji fruit have found place in the shelves of food markets. In comparison, the leaves lag far behind and most of it is currently thrown away as waste, probably because Goji is a seasonal product and its leaves constitute a mass that is difficult to harvest and to preserve. On the other hand, the chemical composition and biological activities of Goji leave extracts, including above–mentioned compounds, flavonoids, alkaloids, polysaccharides, promise a brighter future as to its industrial use especially in bakery [29], because it can justly replace synthetic flour supplements. It can also lengthen the shelf life of meat products [30]. Calcium bind to LBLP through ionic interactions, and LBLP binds abundant calcium with uronic acid. Besides, crystallized cellulose contain high amounts of silicon and [31]. These findings might imply that Goji leaves are rich in mineral-based macromolecules [28].

Goji leaves, when used directly, can be toxic and decompose in gastrointestinal tract [32]. Encapsulation of leave extracts can avoid this problem [33]. Liposomes can also be used as efficient carriers of polyphenolic extracts [33-35].

* 1. **Molecular docking result**

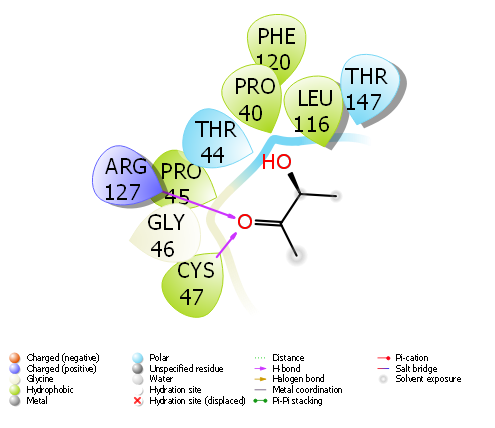
The outcomes from the GC-MS analysis have unveiled a diverse array of chemical compounds within the Coriandrum sativum. Each of these compounds has been identified, and their names are meticulously presented in Table 1, offering comprehensive details for each.

Molecular docking is a computer simulation method that models the interaction of a target molecule (usually a protein) and a small molecule (ligand) [36,37]. This method is used in many areas such as drug design, understanding biological interactions and discovery of biochemical processes [38].

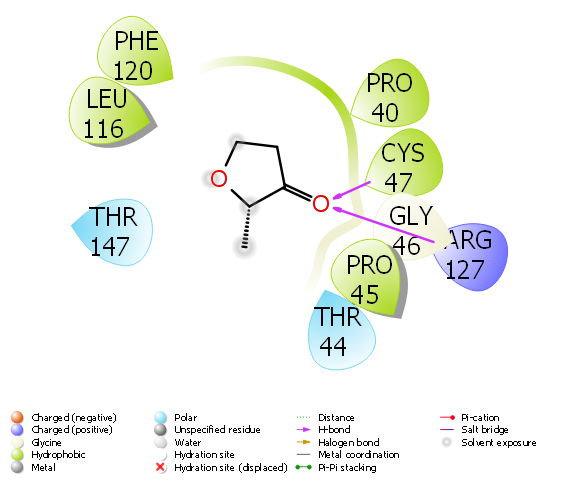
Essentially, molecular docking attempts to predict how a ligand binds to a target protein and how stable that binding is [39]. This is used to identify potential drug candidates or understand biological interaction mechanisms [40].

In this investigation, the effectiveness of the compounds enumerated in Table 1 was individually appraised against prostate cancer proteins via molecular docking computations [41,42]. These computations generated a multitude of parameters alongside their associated numerical values, playing a pivotal role in appraising the interactions and potential effectiveness of these compounds against prostate cancer proteins [43-45].

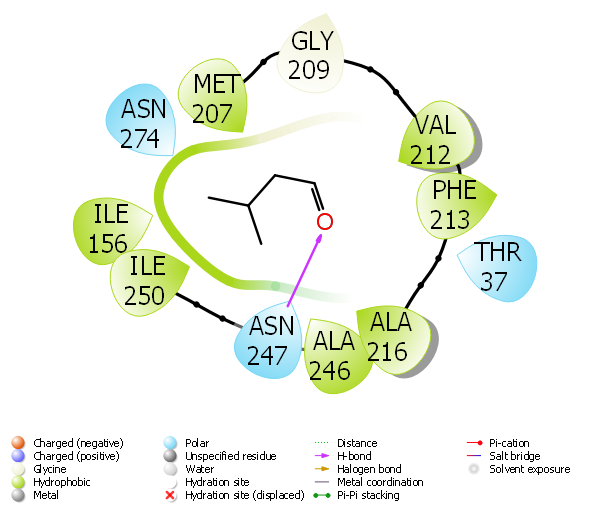
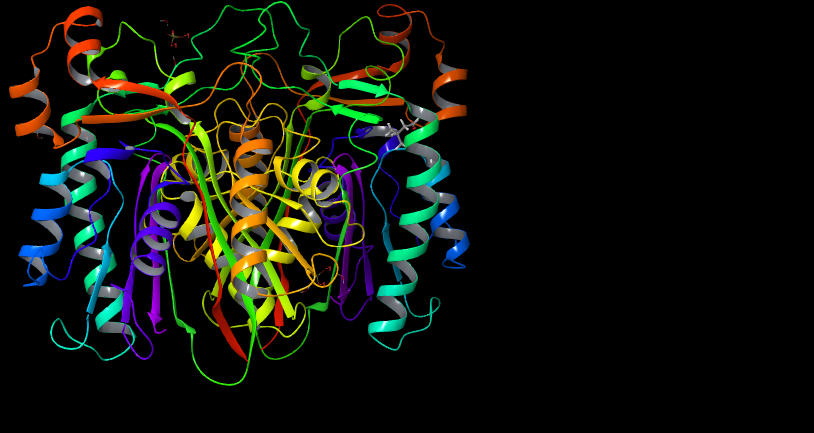
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| **Table 1**. Numerical values of the docking parameters of molecule against enzymes | | | | | | | | | | | | | |
| 1HD2 | Docking Score | Glide ligand efficiency | Glide hbond | Glide evdw | Glide ecoul | Glide emodel | | Glide energy | | Glide einternal | | Glide posenum | |
| Butanal, 3-methyl | -4.14 | -0.69 | -0.32 | -10.61 | -2.73 | | -16.91 | | -13.34 | | 0.52 | | 229 | |
| 3-Hydroxy-2-butanone | -4.67 | -0.78 | -0.15 | -7.90 | -8.11 | | -21.12 | | -16.01 | | 0.15 | | 383 | |
| 2-Methyltetrahydrofuran-3-one | -4.72 | -0.67 | -0.12 | -13.12 | -1.78 | | -19.48 | | -14.90 | | 0.00 | | 221 | |
| 1-Methoxy-2-propanone | -4.29 | -0.71 | -0.39 | -10.18 | -4.20 | | -18.55 | | -14.38 | | 0.46 | | 124 | |
| 2,3-Butanediol | -3.65 | -0.61 | 0.00 | -1.77 | -13.87 | | -18.56 | | -15.65 | | 1.92 | | 267 | |
| 1-Butanol, 3-methyl- | -3.14 | -0.52 | -0.40 | -9.83 | -5.11 | | -16.84 | | -14.94 | | 1.44 | | 60 | |
| 1-Pentanol | -1.55 | -0.26 | -0.37 | -9.63 | -4.17 | | -14.48 | | -13.80 | | 1.21 | | 210 | |
| Ethyl lactate | -3.30 | -0.41 | -0.28 | -5.59 | -10.98 | | -20.40 | | -16.57 | | 0.50 | | 376 | |
| 2-Pentanone | -4.00 | -0.67 | -0.07 | -11.22 | -1.50 | | -15.57 | | -12.71 | | 1.94 | | 286 | |
| Pentanal | -2.61 | -0.43 | -0.07 | -11.65 | -1.71 | | -14.70 | | -13.35 | | 2.20 | | 287 | |
| 4Z8D | Docking Score | Glide ligand efficiency | Glide hbond | Glide evdw | Glide ecoul | Glide emodel | | Glide energy | | Glide einternal | | Glide posenum | |
| Butanal, 3-methyl | -5.41 | -0.90 | -0.32 | -12.80 | -3.08 | -21.12 | | -15.89 | | 0.01 | | 191 | |
| Acetic Acid | -3.84 | -0.96 | -0.40 | -0.72 | -7.10 | -14.48 | | -7.82 | | 0.00 | | 4 | |
| 3-Hydroxy-2-butanone | -5.28 | -0.88 | -0.30 | -10.92 | -6.44 | -22.85 | | -17.36 | | 0.20 | | 259 | |
| 2-Methyltetrahydrofuran-3-one | -5.91 | -0.84 | -0.42 | -15.62 | -1.48 | -23.29 | | -17.10 | | 0.00 | | 123 | |
| 1-Methoxy-2-propanone | -4.97 | -0.83 | -0.61 | -12.43 | -3.10 | -20.38 | | -15.54 | | 0.10 | | 371 | |
| 2,3-Butanediol | -4.57 | -0.76 | -0.84 | -13.42 | -7.75 | -26.61 | | -21.17 | | 0.62 | | 219 | |
| 1-Butanol, 3-methyl- | -4.54 | -0.76 | -0.86 | -8.74 | -6.97 | -19.10 | | -15.71 | | 1.60 | | 291 | |
| 1-Pentanol | -3.29 | -0.55 | -0.85 | -9.78 | -6.82 | -19.42 | | -16.60 | | 0.73 | | 222 | |
| Ethyl lactate | -3.76 | -0.47 | 0.00 | -14.40 | -6.55 | -25.54 | | -20.95 | | 1.03 | | 165 | |
| 2-Pentanone | -5.32 | -0.89 | -0.32 | -11.51 | -3.11 | -19.75 | | -14.61 | | 0.06 | | 285 | |
| Pentanal | -4.69 | -0.78 | -0.61 | -12.81 | -2.72 | -19.51 | | -15.53 | | 1.00 | | 27 | |



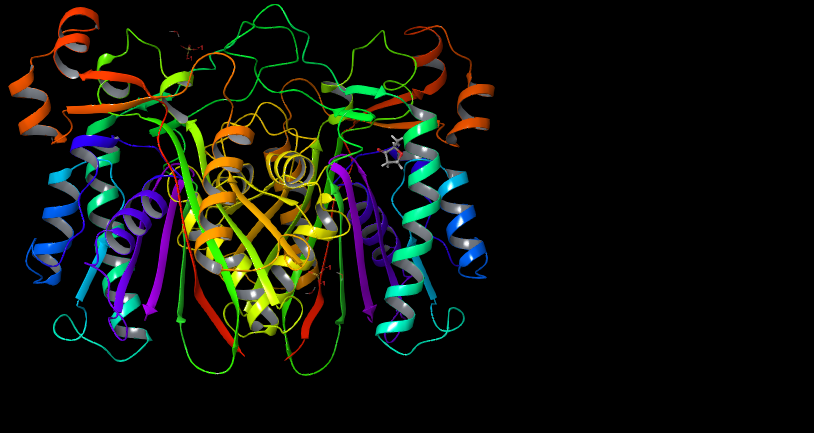
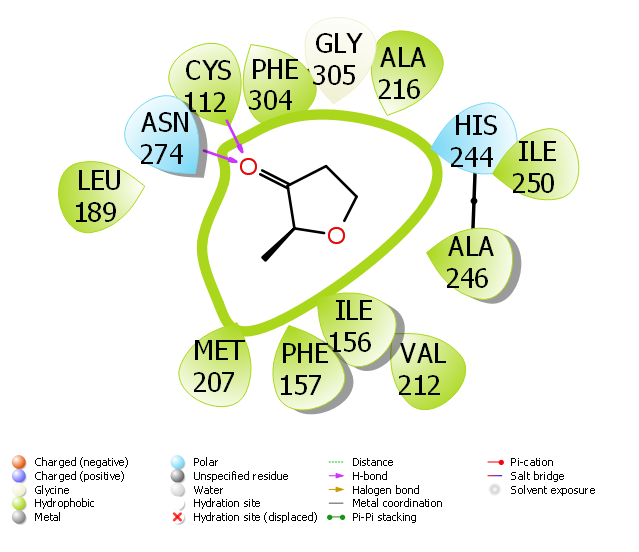
**Figure 1**. 2-Methyltetrahydrofuran-3-one's Interactions with Proteins Related to anti-oxidant protein (PDB ID: 1HD2)



**Figure 2**. 3-Hydroxy-2-butanone 's Interactions with Proteins Related to anti-oxidant protein (PDB ID: 1HD2)

**Figure 3**. 2-Methyltetrahydrofuran-3-one's Interactions with Proteins Related to anti-oxidant protein (PDB ID: 4Z8D)



**Figure 4**. Ethyl linolenate's Interactions with Proteins Related to anti-oxidant protein (PDB ID: 4Z8D)

The docking score, a vital metric derived from the calculations, holds a pivotal role in the comparative analysis of the activities of the molecules examined in your research [46,47]. It is noteworthy that the molecule exhibiting the most negative numerical value for the docking score is regarded as having the highest activity among the tested compounds [48,49]. This parameter serves as a key tool in evaluating the potential effectiveness of these molecules in their designated roles, such as inhibiting prostate cancer proteins [50,51].

1. **Conclusion**

Goji fruit and leaves are rich in mineral-rich polysaccharides, phenolic compounds, alkaloids and minerals and exhibit various biological activities such as antioxidant, anti-inflammatory, anti-diabetic and anti-microbial activities. Moreover, the proteins obtained from Goji leaves deserve to be researched and studied. Goji leaves may be a good alternative to Goji berries for people who prefer to consume less sugar and more dietary fibre. However, before any use recommendations can be made for products based on Goji leaves, clinical evidence and strict procedures for their safety and quality are indispensable.

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