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Research Article

Sequence Characteristics of Dammarenediol Synthase in Medicinal Plant *Panax notoginseng*

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ABSTRACT

Panax notoginseng is a commonly used herb in Traditional Chinese Medicine. It is a traditional herb plant of for manufacturing compound Danshen dripping pills, Yunnanbaiyao, et al. Dammarenediol synthase is one of its important ingredients. Some sequence characteristics, such as theoretical isoelectric point, hydrophobicity, molecular properties, transmembrane region, secondary structure and tertiary structure, of dammarenediol synthase in *Panax notoginseng* are studied in this paper. All results of the study would be benefit for further study on the medicinal properties of *Panax notoginseng*.

Introduction

In traditional Chinese medicine, *Panax notoginseng* is widely used in treating bruises, coronary heart disease, angina, cerebrovascular sequelae, hypertension and other diseases. So far, dozens of different monomer xanthan ingredients form *Panax notoginseng* are studied for their important usage in medicine [1-5]. There are hundreds of varieties of proprietary Chinese medicines about *Panax notoginseng* for sale in Chinese. The *Panax notarization* industry has shown a rapid development in recent years. Many scientists studied on Panax notoginseng and its ingredients, Dan Jiang, et al. explored the molecular cloning and squalene synthase function in Panax notoginseng [6]. Pengguo Xia, et al. studied the saponins accumulation characteristics in Panax notoginseng during its different growing stages [7]. Form the perspective of qualitatively, the regulation of intestinal microbiota on the metabolism of Panax notoginseng saponins is studied by Jingcheng Xiao, et al [8]. Co-overexpressions of 3-hydroxy-3-methylglutaryl CoA reductase and squalene synthase genes could enhance the triterpenoid saponins biosynthesis in Panax notoginseng cells according to the study by Bing Deng, et al. [9]. Ting Wang, et al. systematically analyzed the traditional usages including phytochemistry, pharmacology and toxicology of Panax notoginseng [10]. Cuiping Miao, et al. studied the properties of rhizospheric fungi in Panax notoginseng and the authors tent to think that the rhizospheric fungi may provide for antagonism to host phytopathogens [11]. Thu Dang Kim, et al [12]. Qinbo Yang, et al [13]. Peiwei Wang, et al [14]. Mao Qian, et al [15]. Shi Sun, et al [16], all explored the anticancer effects of saponin in Panax notoginseng. When the bioinformatics is concerned, Wan-jing Liu, et al. studied the HMGS and HMGR genes from Panax notoginseng form the cloning and bioinformatics Analysis methods [17]. Pengguo Xia, et al. tent to think that the wild Panax vietnamensis, et al. may increase the genetic diversity in Panax notoginseng [18]. Many other functions and properties of *Panax notoginseng* are all explored by lots of scholars [19-25]. In this paper, main physical characteristics dammarenediol synthase in *Panax notoginseng* is studied from

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the bioinformatics view, and the status and function of *Panax notoginseng* in the development of traditional Chinese medicine is also summarized.

Materials and Methods

Literatures published by PubMed, SinoMed, Embase and so on are summarized and analyzed to reveal the value of *Panax notoginseng*. The protein sequences data of dammarenediol synthase is from NCBI, and the accession number is AED99865.1.

Some prediction systems are used in this study, such as: (1) http://web.expasy.org/protparam/ [26] is used to predict the molecular weights, theoretical isoelectric point, et al, of the dammarenediol synthase. (2) http://web.expasy.org/protscale/ is used to analyze the hydrophilic property of dammarenediol synthase [26]. (3) http://www.cbs.dtu.dk/services/TMHMM/ is used to predict the transmembrane region of dammarenediol synthase [27]: (4) Signal peptide properties of dammarenediol synthase is analyzed via

http://www.cbs.dtu.dk/services/SignalP/ [28].

(5)SOPMA protein secondary structure prediction online system is used to study on dammarenediol synthase secondary structure information [29]. (6) The tertiary structure of dammarenediol synthase is predicted via the web [30]: https://swissmodel.expasy.org. Phosphorylation of dammarenediol synthase is studied via the NetPhos system [31].

Results and Discussion

Protparam system is a famous tool for studying the fundamental properties of a protein molecular. The predict result is shown in the Table 1 and Figure 1. The number of amino acids is 767, the molecular weight is 88170.83, the theoretical pI is 6.47, the negatively and positively residues are respectively 91 and 85. the molecular instability index of dammarenediol synthase is 39.71. In addition, the result shows that the molecular formula of dammarenediol synthase is $C_{3992}H_{6074}N_{1066}O_{1124}S_{37}$. From the composition (Figure 1), the result shows that the most abundant amino acids are: Ile (75), Asp (58) and Glu (56), et al.

Table 1: Physical and chemical property analysis of dammarenediol synthase

Parameter	Results
Number of amino acids	767
Molecular weight	88170.83
Theoretical pI	6.47
Total number of atoms	12293
Aliphatic index	79.22
Negatively residues (Asp + Glu)	91
Positively residues (Arg + Lys)	85
Instability index	39.71

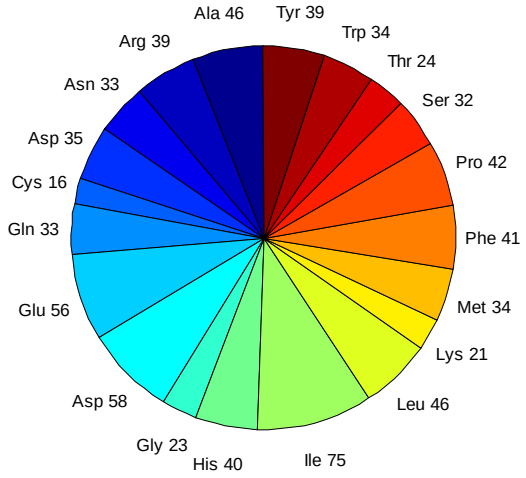

Fig 1:Amino acid composition of dammarenediol synthase

The hydrophobicity map of dammarenediol synthase is predicted via using the Hphoh. / Kyte & Doolittle scale in ExPASy's ProtScale system (see Figure 2). As it can be seen from Figure 2, the number of hydrophobic and hydrophilic amino acid residues of the dammarenediol synthase is more than the hydrophobic amino acid residues, and the peptide is biased towards hydrophobic.

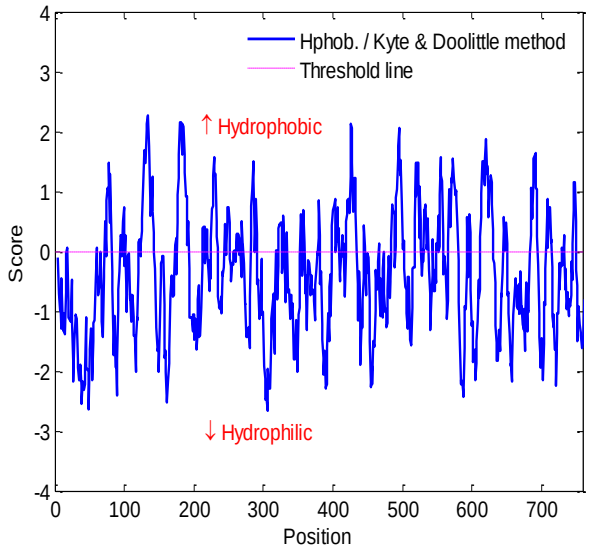

Fig 2:Hydrophobic characteristics of dammarenediol synthase

The transmembrane region of the dammarenediol synthase molecular is predicted via the TMHMM system, and its result is as shown in Figure 3. The results show that transmembrane region is at the position of about the 630 residue, and it is the only one the transmembrane region form the prediction result. At both sides of the transmembrane region, the peptide chains are respectively in the membrane and out of the membrane.

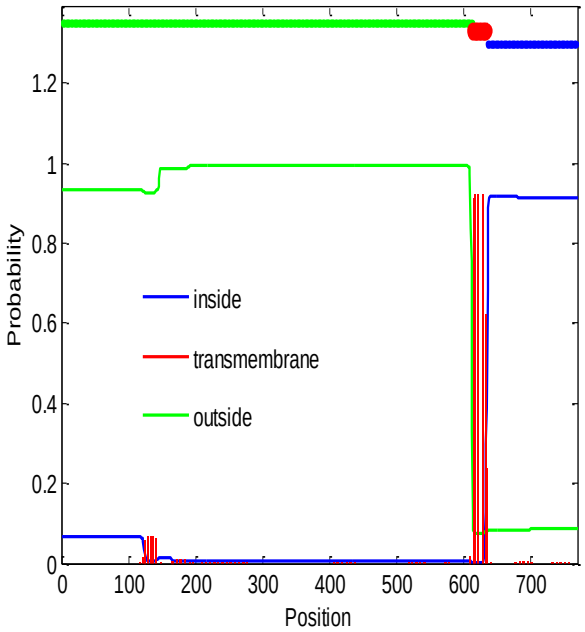

Fig 3: Transmembrane region prediction of dammarenediol synthase

The signal peptide is a short peptide with a typically length 5-30 amino acids. SignalP is used to predict the dammarenediol synthase, and the result is shown in Figure 4. The result shows that the max. C is at the 10th residue with its value of 0.113. The max. Y is at the 46th residue and its max value is 0.113, last, the max. S is at the 40th residue with the max value 0.129. C-score is the signal peptide cleavage site value, S-score is the signal peptide value, Y-score is the integrated score of shear point. Predictive results show that S-score of dammarenediol synthase is much smaller than the standard value 0.5, which denotes that in this sequence, there is no signal peptide.

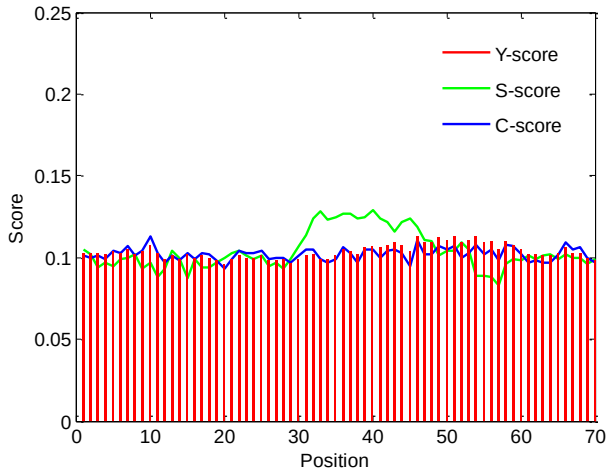

Figure 4: Signal peptide analysis of dammarenediol synthase

The SOPMA prediction system is used for predicting the secondary structure of the dammarenediol synthase. The parameters setting are number of conformational states: 4 (Helix, Sheet, Turn, and Coil), Similarity threshold is 8, output width is 80, and the Window width is 17. The secondary structure predicted result of the dammarenediol synthase is shown in Figure 5. From the result, there is 35.98% Alpha helix (Hh), 17.21% Extended strand (Ee), 11.21% Beta turn (Tt) and 35.59% Random coil (Cc) in the dammarenediol synthase.

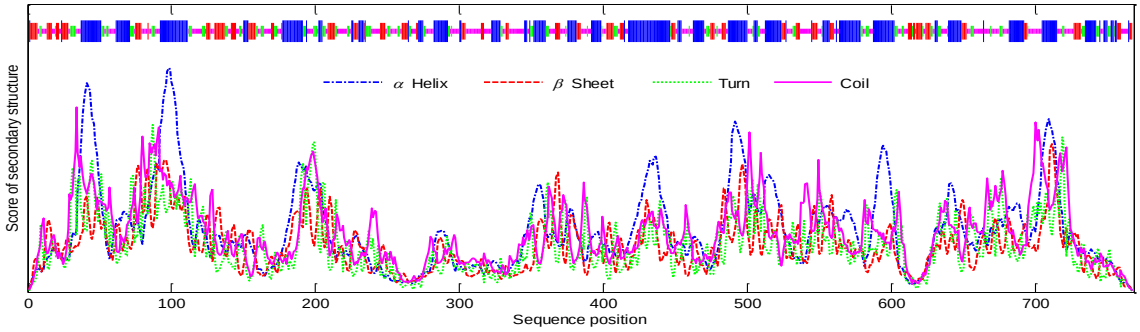

Figure 5:Secondary structure prediction result of the dammarenediol synthase

Three-dimensional structure of the dammarenediol synthase is predicted and the result is shown in Figure 6. As can be seen from Figure 6, it can be seen that there is no signal peptide in the structure. The prediction result shows that the dammarenediol synthase structure is 39.72% similar to lanosterol synthase, 0.84 Coverage to the sequence of lanosterol synthase (92-758). Total Seq Similarity is 0.4.

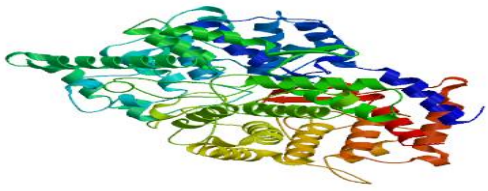

Figure 6. Tertiary structure of dammarenediol synthase

The NetPhos online system for protein phosphorylation site prediction is used to study the phosphorylation sites of the dammarenediol synthase. The prediction result is shown in Figure 7. There are 12 phosphorylation sites for tyrosine, 18 phosphorylation sites for threonine and 23 phosphorylation sites for serine. All of these phosphorylation sites value are more than 0.5, in the Figure 7, the phosphorylation potential value less than 0.5 are neglected.

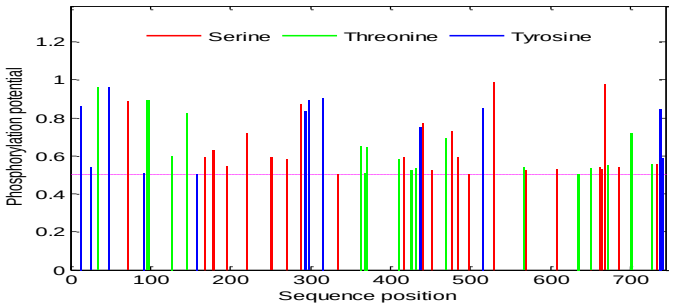

Figure 7. Phosphorylation site prediction results of the dammarenediol synthase

For dammarenediol synthase in Panax notoginseng, there are many other properties need to be explored, and in fact lots of scientists are devoting at this area [31, 32], such as many scientists study its function from different aspect [33], in fact, for the specific mechanism of medicinal ingredients of Panax notoginseng, it still need further study [34].

Conclusion

In this study, the sequence characteristics and biological information contained in dammarenediol synthase are systematically studied via the common prediction system such as its basic physical and chemical properties, three-dimensional structure, phosphorylation site and so on. All these properties of the dammarenediol synthase are studied in order to understand the structural characteristics of dammarenediol synthase and reveal its further usages in medicine. With the advancement of science and technology, some new characteristics of dammarenediol synthase are still need to be studied to make the *Panax notoginseng* research into a new stage.

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