International Journal of Advance and Applied Research
www.ijaar.co.in
ISSN – 2347-7075 Impact Factor – 7.328
Peer Reviewed Bi-Monthly
Vol.4 No.29 July-Aug 2023

In silico Characterization of dragline silk proteins from the spider, Trichonephila clavipes using Computational Tools and Servers

Deepali Sangale[1], Sandip Chordiya[2], Vitthal Nale[3]
[1,2,3]Department of Zoology, Tuljaram Chaturchand College of Arts, Science & Commerce, Baramati, (Autonomous) Pune (MS).Savitribai phule pune university, Pune (MS) India.
Corresponding Author- Dr.Deepali sangale
Email- wayasedr@gmail.com
DOI-10.5281/zenodo.8363284

Abstract

In this paper, dragline silk fibroin proteins of spider (SFs) retrieved from NCBI (National Center for Biotechnology Information) database is analyzed and characterized using in silico tools. Primary structure analysis shows that the dragline silk fibroin is hydrophobic in nature due to the high content of non-polar residues. The existence of very few amounts of cystein in SFs shows absence of disulphide links in the silk fibroin proteins. The presence of extensive hydrogen bonds may provide the stability to protein. The aliphatic index calculated by ExPasy's ProtParam concludes that SFs may be stable at wide range of temperature. Secondary structure analysis shows that most of the silk fibroin protein have predominant random coil, α-helix structure, and β-helical structure secondary structure. The very high random coil structural content of spider is due to the rich content of highly flexible glycine and hydrophobic alanine amino acids. The homology model created by SWISS-MODEL. The reliability of the modeled structure was confirmed using PROCHECK and QMEAN programs. a 3D structure of spider silk fibroin has been predicted from its amino acid sequence. This homology modeling based structure will provide an insight to its functional aspects and further studies which are based on tertiary structure of protein. The current analysis contributes to our understanding of proteins expressed by the silk gland of silk-producing insects such as spider. Together, these findings contribute to our understanding regarding the structural and functional significance of the dragline silk proteins of spider.

Key words: Silk; Silk fibroin protein; Computational analysis; Homology modeling

Introduction

Silk is an extracorporeal, protein based, fibrous structural material secreted by labial glands in arthropods. Many of the insects, arachnids and myriapods produce the silk but silk worm and spider are the most well-known silk producers (Tahir et al., 2019). Spiders have capability to produce numerous diverse types of silk. Spider silk is biocompatible, biodegradable, and rivals some of the best synthetic materials in terms of strength and toughness (Perera D et al., 2022) Although interrelated, these silks have been revealed to differ in their physical properties and composition of amino acid. Significantly recent importance has been concentrated on the dragline silk of *Trichonephila clavipes*. The *Trichonephila clavipes* makes dragline silk fibers with unbeatable toughness, as *T. clavipes* produce seven diverse kinds of silk that are used for different ecological purposes. Each of the different silks is associated with its own specialized type of silk gland. Each silk gland consists of silk proteins, of which the dominant proteins are spidroins (Sandra M et al., 2020; Hinman and Lewis, 1992) remarkable properties of the fiber, whose mechanical performance and hierarchical organization are still unmatched by the most sophisticated artificial materials (Malay D et al., 2022).

The silk fibers have been used for decades as sutures in biomedical application (Moy et al., 1991) and have potential as scaffolds in tissue engineering (Min et al., 2004; Dal et al., 2003). Many report the other applications of silk fibroin in medical,