

**Abstract:**

Wheat is one of the main crops that play a significant role in feeding the hungry world and improving the food security. *Wheat streak mosaic virus* is one of the most important viral infections in the wheat which its prevalence is increasing in Iran. NIa protein as a vital protein in this virus has some important functions including viral replication and proteolytic digestion of virus polyprotein. The aim of the present study was to purify NIa protein and its interaction considering with antiviral compounds at the molecular level. This study was performed in two parts: bioinformatics and laboratory studies. In the bioinformatics study, third structure of the NIa protein was investigated and modeled using ITASSER server. Interaction of this protein with plant derived organic compounds including catechin, caffeic acid, glabridin, limonene and scopoletin was considered by molecular docking method. In the laboratory studies, NIa protein-coding gene was isolated from *Wheat streak mosaic virus*, Meymeh isolate and its sequence was determined. NIa gene expression and post-induction time optimization were performed to produce the significant amount of protein. Purification of recombinant protein was done by affinity chromatography. Auto-cleavage activity of NIa protein was confirmed using protease inhibitors as control. Interaction of the purified protein with catechin and caffeic acid and *Calendula officinalis*, *Dracocephalum* and liquorice extracts was considered using UV-vis spectroscopy. The results of bioinformatics part showed that the modeled NIa protein had a high structural disorder. Molecular docking results indicated that the compounds with lower bond energy and more hydrogen bonds had the more stable complex with NIa. Laboratory results showed that maximum protein expression was occurred within 2 h after induction. UV-vis spectroscopy results showed the liquorice extract had more effect on the protein absorption amount in comparison with two other extracts. Catechin also had more effect on the protein absorption compared to caffeic acid. In general, each of the compounds that had lower binding energy in interaction with NIa protein in silico condition had more effect on the protein absorption in vitro condition. Finding of this study can provide an effective way to biologically control of agricultural epidemic diseases.

**Key words:** NIa protein, Gene expression, Interaction, Biological compounds.



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**Cloning and studying of NIa gene expression related to  
wheat streak mosaic virus and its interaction with some  
herbal compounds**

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