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Use of *Schinus molle* (Anacardiaceae) as a means of biological control against *Trialeurodes vaporariorum* (Aleyrodidae)

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Greenhouse whiteflies, *Trialeurodes vaporariorum*, are very small sucker-whipper-type pests of the family Aleyrodidae. They cause considerable damage to greenhouse crops in the first order and show resistance to chemical insecticides. In this context, we dedicated this study to the control of this pest through the active ingredients extracted from the leaf and fruit part of the pepper tree, *Schinus molle* by inhibiting the chemosensory protein responsible mainly for capturing external stimuli in these polyphagous insects. By applying molecular modeling methods, including molecular docking, using software Molegro Virtual Docker version 2012.5.5.0, we tested the bioinsecticide potency of seven inhibitors. The results obtained show that the molecule beta-elemol is the best chemosensory protein inhibitor with a score of –82.6648 Kcal/mol and that it forms strong bonds with the active site amino acids of the protein.

Keywords: *Trialeurodes vaporariorum*, *Schinus molle*, chemosensory protein, molecular modeling, inhibitor, bioinsecticide

INTRODUCTION

It is the law of nature that any living being will be the target of one or more enemies at one point in its life cycle (Suty, 2010; Yarou et al., 2017). Vegetable products are an essential component of our daily diet (James et al., 2010). They are, unfortunately, attacked by many types of insects, so the losses are considerable. This work contributes to the knowledge of the greenhouse whitefly, *T. vaporariorum*, commonly known as whitefly. *T. vaporariorum* is a polyphagous insect (Malausa et al., 1988) of the sucker-whipper type (https://www.agrimaroc.ma) of the order Hemiptera in the family Aleyrodidae. The greenhouse whitefly today seems to be cosmopolitan. It is found mainly in greenhouses and glass buildings. *T. vaporariorum* attacks vegetables, fruits, ornamental plants (Bellmann, 2006), and even weeds (https://www.agrimaroc.ma); it weakens them and stops their growth (Alford, 2012). Chemical insecticides are one of the most widely used pests control methods (Regnault-Roger et al., 1997). However, greenhouse whiteflies are resistant to these insecticides, and chemical control is therefore inefficient (hydroponie.fr) The intensive use of insecticides has consequences for the health of consumers: numerous studies report association between insecticides and carcinogenic diseases (prostate cancer, hematopoietic cancers), endocrine disruption,

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allergies, neurological and neurobehavioral effects, and effects on fertility and development (Inserm, 2013; Yarou et al., 2017). Insecticides also have negative impacts on the environment (surface and groundwater contamination, soil contamination, air contamination). The level of this impact depends on the degree of exposure resulting from their dispersions and concentrations in the environment and their ecotoxicological characteristics (Periquet et al., 2004; Yarou et al., 2017). Because of these risks to consumer health, the negative effect on the environment, and the high cost of insecticides (Champ et al., 1977; White, Leesch, 1995; Subramanyam, Hagstrum, 1995), current research is moving towards biological control methods. Biological control is the use of living organisms or their products to control other organisms considered to be harmful. There are two categories of methods or means of biological control: means without recourse to auxiliaries and those who resort to them. The biopesticide-based means of plant origin (James et al., 2010) had existed for a long time, but they were neglected with the advent of synthetic chemistry, mainly in the second half of the twentieth century. The use of biopesticides has many advantages: they restrict or eliminate the use of chemical insecticides, are less toxic, reduce the risks of developing resistance, offer consumers healthy products, maintain the biodiversity of biotopes, and degrade rapidly, reduce the risk of pollution (Rochefort et al., 2006). The self-defence of plants lies in the subtle chemistry of their toxins: if a plant is not attacked by an insect, this is due to its chemical defence. Many herbs that we use in our recipes and herbal teas produce volatile insect-repellent products. Today, we have more than 2000 plant species that can keep pests away (Pintureau, 2009). The pepper tree, *S. molle*, of the family Anacardiaceae is an example of an insect-repellent aromatic tree due to its chemical compounds in leaves and fruits. The purpose of our work was to test theoretically the bioefficacy of the active principles of *S. molle* on greenhouse whiteflies, *T. vaporariorum*, by molecular modeling methods.

MATERIALS AND METHODS

Preparation of inhibitors

Our work consisted in studying the interaction of the chemosensory protein (CSP) with a series of molecules extracted from the essential oils of the leaf part and fruit of the pepper tree, *S. molle*. The following inhibitors were studied: alpha-phellandrene, beta-elemol, limonene, beta-phellandrene, beta-eudesmol, alpha-eudesmol, and alpha-pinene. These inhibitors were chosen according to the most important yield in each part of the plant, leaf or fruit. The chemical structure of the seven inhibitors was obtained from the PubChem database (Tables 1 and 2). In this study, we drew the seven inhibitors with the software ChemDraw, v. 12.0.2.1076 and then saved them in the mol format. Then, we optimised these inhibitors with the software HyperChem, v. 8.0.10 and saved them in the mol format. Regarding molecular docking, we did it using software Molegro Virtual Docker, v. 2012.5.5.0 with the aim of finding the best conformation between the chemosensory protein 1N8U and the seven inhibitors, that is, we conducted a search for the most stable protein-inhibitor complex with the lowest energy level.

Table 1. **Chemical structures of the essential oil compounds of *S. molle* fruits** (https://pubchem.ncbi.nlm.nih.gov/source/DrugBank)

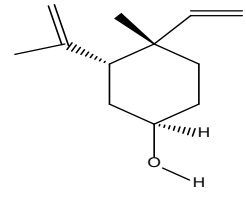
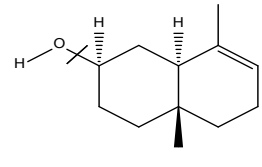
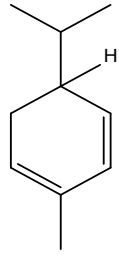
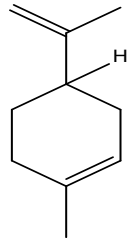
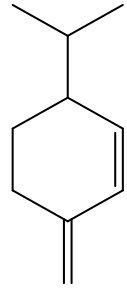
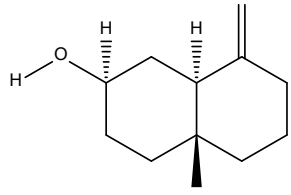
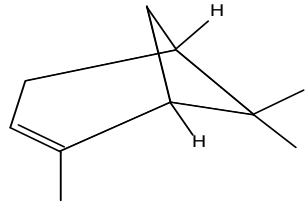
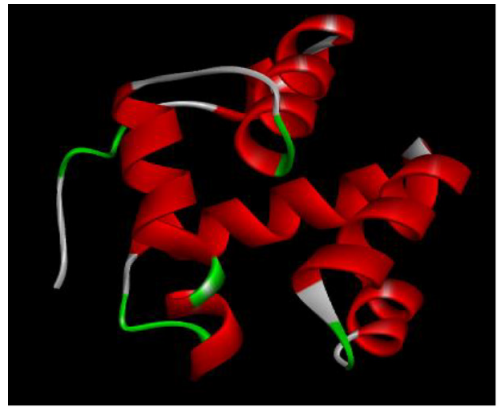
Chemical compounds	Chemical structures
Beta-elemol	
Alpha-eudesmol	

Table 2. **Chemical structures of the essential oil compounds of *S. molle* leaves** (https://pubchem.ncbi.nlm.nih.gov/source/DrugBank)

Chemical compounds	Chemical structures
Alpha-phellandrene	
Limonene	
Beta-phellandrene	
Beta-eudesmol	
Alpha-pinene	



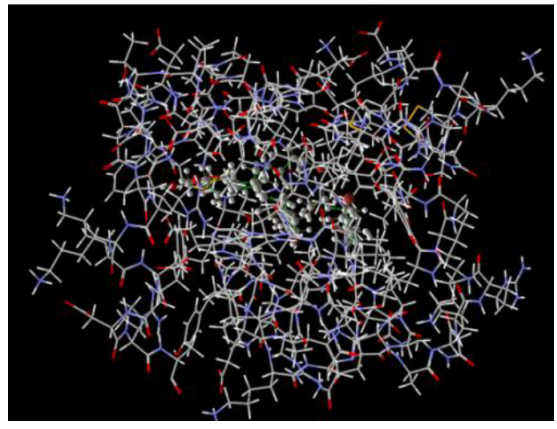


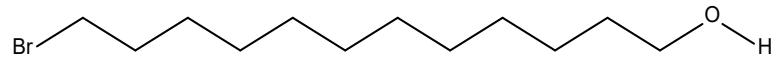
Fig. 1. Three-dimensional structure of the CSP with the PDB code 1N8U (https://www.rcsb.org)

Protein preparation

In our study, we downloaded the chemosensory protein under access code 1N8U from the database Protein Data Bank with a resolution of 1.8 Å (Fig. 1), which is within the interval of 1.5–2.5 Å. It is composed of a single polypeptide chain with 112 amino acids (Table 3) (www.rcsb.org).

We chose molecular modeling as a method for this study. This method is a bioinformatic tool that allows the study of biological phenomena at the atomic scale. Today, molecular modeling is increasingly used to study chemical reactions and protein dynamics (Hercend, 2012). It aims to predict the structure and reactivity of molecules. (https://www.unilim.fr/). The principle of molecular modeling consists in specifying, from calculations, the position of atoms in space and calculating the energy of the generated structure. The closest possible representation of reality will correspond to a structure of lower energy. Molecular modeling involves theoretical calculation methods including molecular mechanics and molecular docking.

Table 3. **Crystallographic data of the chemosensory protein 1N8U** (https://www.rcsb.org)

Protein	1N8U
Co-crystallization inhibitor	
	BROMO-DODECANOL
Molecular weight (KDa)	11.69
Polymer	1
Chain	A
Chain type	Polypeptide (L)
Length of the sequence	112 amino acids
Resolution (Å)	1.8

RESULTS AND DISCUSSION

Molecular docking. Using software Molegro Virtual Docker, v.2012.5.5.0, we have performed molecular docking between the chemosensory protein under access code 1N8U and the seven inhibitors in cavity 1 (we chose this cavity because it represents the largest active site) to compare the stability of complexes trained (Fig. 2).

The score values of the first poses that designate the conformations that best represent the seven inhibitors are given in Table 4.

The results of molecular docking led us to the following rankings:

$$S_{\text{beta-elemol}} < S_{\text{limonene}} < S_{\text{alpha-eudesmol}} < S_{\text{beta-eudesmol}} < S_{\text{beta-phellandrene}} < S_{\text{alpha-phellandrene}} < S_{\text{alpha-pinene}}$$

From the score ranking we can conclude that the 1N8U-beta-elemol complex is the most stable as it represents a better affinity with the lowest energy level compared to the others. The molecule bromo-dodecanol inhibitor of co-crystallization deactivates the function of the 1N8U protein. We note that there is not a big difference between the score values of the bromo-dodecanol (–103.714 Kcal/mol) and beta-elemol (–82.6648 Kcal/mol). So beta- elemol also deactivates the protein and inhibits it. We consider it a good bioinsecticide against the polyphagous *T. vaporariorum* and that the fruits of S. moll have a good bioinsecticide power.

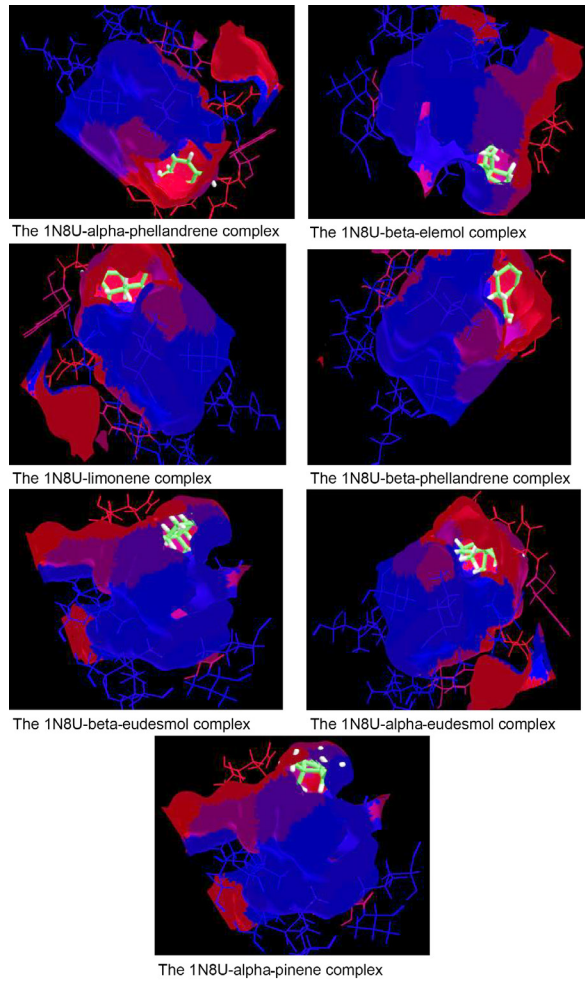


Fig. 2. Complexes formed after molecular docking

Table 4. **Molecular docking scores**

Inhibitors	Score (Kcal/mol)
Alpha-phellandrene	–63.6504
Beta-elemol	**–82.6648**
Limonene	–72.0394
Beta-phellandrene	–68.7278
Beta-eudesmol	–71.4398
Alpha-eudesmol	–71.8688
Alpha-pinene	–60.4802
Co-crystallisation inhibitor	–103.714

Determination of interactions. We determined the different amino acid interactions of cavity 1 of the 1N8U protein and the seven inhibitors using two software packages, Molegro Virtual Docker, v.2012.5.5.0 and BIOVIA Discovery Studio Visualizer, v.19.1.0.18287. Figure 3 shows the interactions established by the Molegro Virtual Docker software:

The interactions established with the BIOVIA Discovery Studio Visualizer software are represented in Fig. 4.

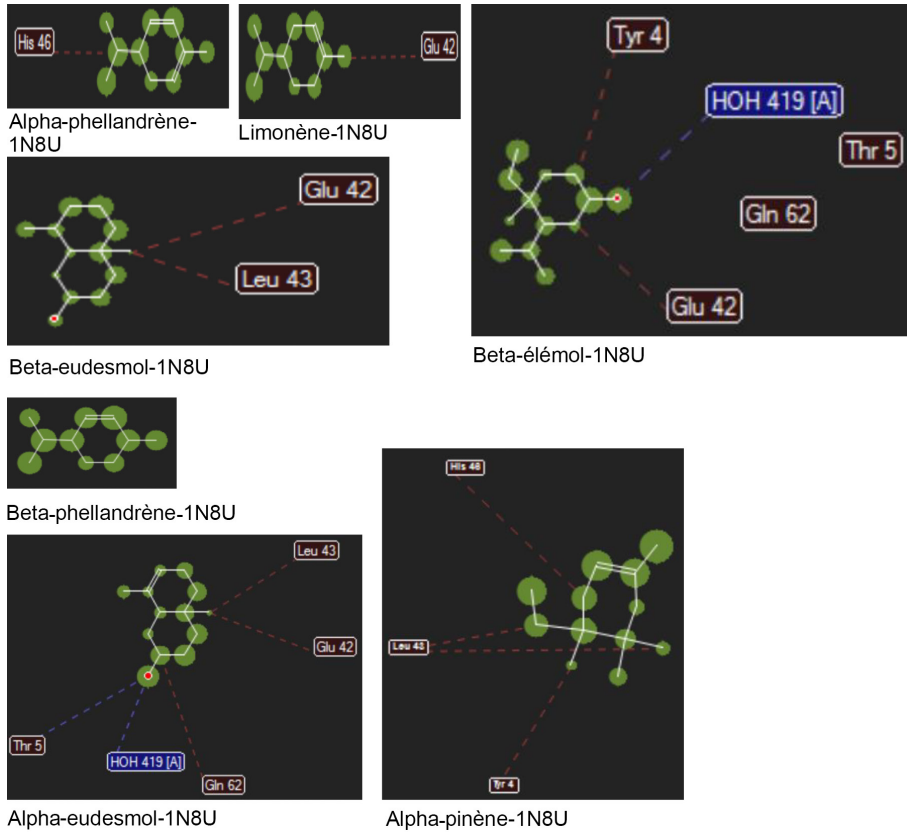


Fig. 3. Interactions between the amino acids in cavity 1 and the seven inhibitors.
--- steric bonds; --- hydrogen bonds

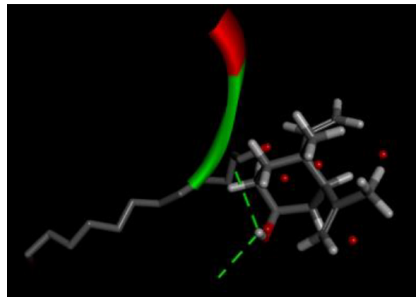


Fig. 4. Hydrogen interactions between the amino acids of cavity 1 and beta-elemol.
--- hydrogen bonds

The results of the interactions are represented in Table 5:

Based on the results in the table above, we observed that:

– the inhibitors formed steric interactions with the amino acids of cavity 1 of CSP 1N8U, apart from alpha-phellandrene, which did not form any interaction.

– beta-elemol formed two hydrogen bonds with glycine (GLY54) and glutamic acid (GLU63) of cavity 1.

– alpha-eudesmol formed a hydrogen bond with threonine (THR5).

As for the distances of the hydrogen bonds, we have as a rule:

• 2.5 Å < D < 3.1 Å => strong interaction;

• 3.1 Å < D < 3.55 Å => medium interaction;

• D > 3.55 Å => weak interaction (Imberty et al., 1991).

We then noticed that:

– the two hydrogen bonds between beta-elemol and the two amino acids GLY54, GLU63 belong to the range of strong interactions;

– the hydrogen bond formed between alpha-eudesmol and the THR5 amino acid belongs to the range of mean interactions.

We conclude that beta-elemol formed two steric bonds and two strong hydrogen bonds, which confirms its good complementarity with the 1N8U protein and the formation of a stable complex.

Cultivated plants would suffer considerable pre-harvest losses due to pests, diseases, and competitors. People must therefore protect their agricultural production, with respect to the environment and without harming public health. Whiteflies cause very serious damage to the crops they attack. Adults and larvae sting and suck sap from the leaves, which eventually fade. Over time, the growth stunts and leaves fall. As is the case with aphids, the larvae of the white fly also secrete a sweet and sticky substance (honeydew) that causes the appearance and development of a fungus called sooty mold. The leaves of the plants are then covered with a black or brown powder thus blocking

Table 5. **Distances and interactions between the amino acids of cavity 1 and the inhibitors**

1N8U				
Inhibitors	**Steric bonds**		**Hydrogen bonds**	
	Amino acids	**Distance (Å)**	**Amino acids**	**Distance (Å)**
Alpha-phellandrene	HIS46	3.16	/	/
Beta-elemol	TYR4	3.02	GLY54	2.93
	GLU42	2.74	GLU63	2.65
Limonene	GLU 42	2.85	/	/
Alpha-phellandrene	/	/	/	/
Beta-eudesmol	GLU42	2.76	/	
	LEU43	3.00		
Alpha-eudesmol	LEU43	3.02	THR5	3.28
	GLU42	2.90		
	GLN62	3.19	/	
Alpha-pinene	HIS46	2.99		
	LEU43	3.19	/	
	LEU43	3.14		
	TYR4	3.04		

photosynthesis; they turn yellow and die. In this context, the use of the pepper tree, *S. molle* (Anacardiaceae), as a means of biological control against *T. vaporariorum* (Aleyrodidae), pest of crops in greenhouses, was investigated. To this end, we applied molecular modeling methods, to theoretically, study the bioefficacy of the active principles extracted from the leaves and fruits of *S. molle* on the polyphagous *T. vaporariorum*; by inhibiting the chemosensory protein: mainly responsible for capturing external stimuli in these harmful insects and facilitating communication between adults for reproduction. Benabdelkader (2012) showed that the insecticidal effectiveness of an essential oil is due to the nature and chemical structure of its constituents. Thus, Aiboud (2011) demonstrated a very interesting insecticidal activity with regard to the fertility of female *Callosobruchus maculates* (Aiboud, 2011). Delimi et al. (2013) reported that the essential oil extracted from the white wormwood, Artemisia herba alba, is considered a disruptive insecticide for reproduction. The disruptive effect of some vegetable oils has been found by many studies. Thus our study on the effect of the essential oil of *S. molle* just confirms its disruptive effect on the adults of *T. vaporariorum* (Aleyrodidae). Senouci (2016) contributed to the use of essential oils of medicinal plants: *Marrubium vulgaris* and *Pistacia lentiscus* (Anacardiaceae) as a means of fight against the pests of the olive tree. Our study confirms the insecticidal power of the Anacardiaceae family, of which *S. molle* is a part (Senouci, 2016). Bouayad Alam (2015) proved the bio-insecticidal power of essential oils of some aromatic plants (Bouayad Alam, 2015) on another pest of greenhouse plants, *Tuta absoluta*. Agarwal et al. (2001) demonstrated the toxicity and repellency of the 1,8-cineol compound in eucalyptus against *Callosobruchus maculatus*, *Rhyzopertha dominica* (Coleoptera: Bostrychidea), and *Sarocladium oryzae*. The recurrence rate of repellency of this chemotype towards these three insect pests ranged from 65% to 74% (Agarwal et al., 2001). Yarou et al. (2017) added that the use of pesticide plants was proving to be an ancestral practice in Africa. Indeed, many plants are known and used for their biocidal activities (toxic, repellent, anti-appetizing) towards a wide range of pests (Yarou et al., 2017). Our results are in agreement with those reported by many authors who highlighted the effectiveness of many essential oils applied as bio-insecticide. The remarkable insecticidal potential of *S. molle* is due to the presence of beta-elemol, which is present in its fruits and proves that it has the bio-insecticidal power on the greenhouse whitefly. Biocidal plants can be used as foliar extracts (Mochiah et al., 2011; Dela et al., 2014) or in combination with other crops (Asare-Bediako et al., 2014; Baidoo et al., 2012). We can thus propose our farmers replace the hitherto-used insecticides to fight the greenhouse whitefly *T. vaporariorum* with the essential oil of the pepper tree, *S. mole*, in biological fight or integrated fight, thus protecting our health and our environment.

CONCLUSIONS

The purpose of our study was to test theoretically, by using molecular modeling methods, the inhibitory activity of seven molecules extracted from the leaf and fruit parts of the pepper tree, *S. molle* (Anacardiaceae), according to their highest yield with the chemosensory protein in greenhouse whiteflies, *T. vaporariorum* (Aleyrodidae). Chemosensory protein is responsible for the detection, transport of stimuli from the external environment, and their solubilisation in the aqueous environment that surrounds the sensory neurons. The molecular docking with Molegro Virtual Docker v.2012.5.5.0 allowed us to evaluate the affinity between the seven inhibitors and the chemosensory protein with the PDB 1N8U code, and to retain the beta-elemol molecule as the best inhibitor of the chemosensory protein with the best score of –82.6648 Kcal/mol. The results of the visualisation of the interactions between the seven inhibitors and the amino acids of the active site of the protein show that beta-elemol formed two strong hydrogen bonds and two steric bonds, which confirms the good

complementarity between beta-elemol and the chemosensory protein and the formation of the most stable complex. Finally, after conducting an overview of the disadvantages of chemical insecticides on human health and the environment, the results obtained in the present led us to judge the molecule beta-elemol extracted from fruit of *S. molle* as nontoxic and it has no effects on human health. As a result, these results led us to propose this molecule as a possible new inhibitor of the chemosensory protein and to confirm the bioinsecticidal power of *S. molle* fruit for the control of this harmful insect.

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SCHINUS MOLLE (ANACARDIACEAE) KAIP BIOLOGINĖS KONTROLĖS PRIEMONĖ NUO *TRIALEURODES VAPORARIORUM* (ALEYRODIDAE)

Santrauka

Šiltadaržinis baltasparnis (*Trialeurodes vaporariorum*) yra labai mažas Aleyrodidae šeimos vabzdys. Jis daro didelę žalą šiltnamio augalams ir yra atsparus cheminiams insekticidams. Tyrimas skirtas šio kenkėjo kontrolei naudojant iš pipirmedžio *Schinus molle* lapų ir vaisių dalių išgautas veikliąsias medžiagas, kurios slopina polifaginių vabzdžių chemosensorinį baltymą, fiksuojantį išorinius dirgiklius. Taikydami molekulinio modeliavimo metodus, įskaitant molekulinę jungtį, naudojome programinę įrangą „Molegro Virtual Docker“ (versija 2012.5.5.0) ir išbandėme septynių inhibitorių bioinsekticidinį stiprumą. Tyrimas rodo, kad esant –82,6648 Kcal/mol rezultatui, molekulė beta-elemolis sudaro stiprius ryšius su baltymo veikliosios vietos aminorūgštimis ir yra geriausias chemosensorinio baltymo inhibitorius.

Raktažodžiai: *Trialeurodes vaporariorum*, *Schinus molle*, chemosensorinis baltymas, molekulinis modeliavimas, inhibitorius, bioinsekticidas