Computational evaluation of the insecticidal potential of heptane extract compounds from *Pyrostegia venusta* against *Helicoverpa armigera* and *Anticarsia gemmatalis*

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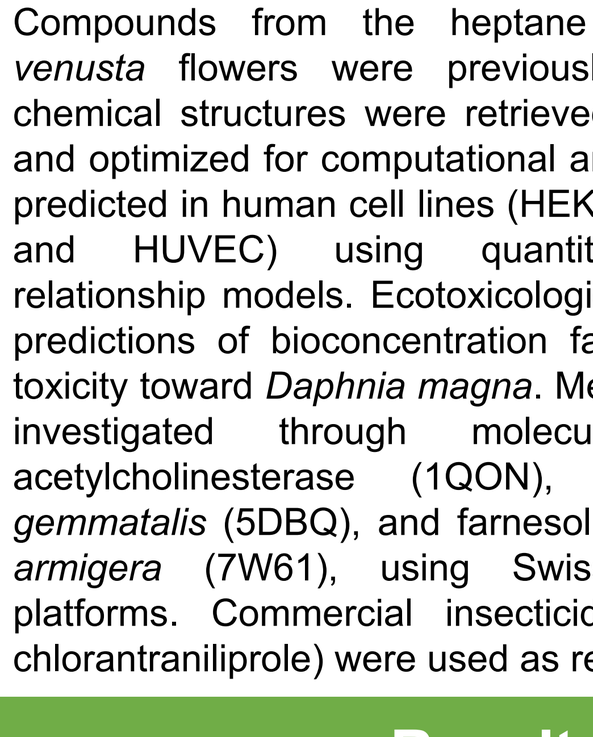
Introduction

Soybean is one of the world's major agricultural commodities and a cornerstone of the Brazilian economy. However, lepidopteran pests such as *Helicoverpa armigera* and *Anticarsia gemmatalis* can cause yield losses exceeding 30% and billion-dollar economic damage per growing season. In this context, the prospection of plant-derived insecticidal molecules combined with *in silico* approaches emerges as a promising and sustainable strategy.

Methodology

Compounds from the heptane extract of *Pyrostegia venusta* flowers were previously identified, and their chemical structures were retrieved from public databases and optimized for computational analyses. Cytotoxicity was predicted in human cell lines (HEK-293, HEK-293T, HaCaT, and HUVEC) using quantitative structure–activity relationship models. Ecotoxicological assessment included predictions of bioconcentration factor (BCF) and aquatic toxicity toward *Daphnia magna*. Mechanisms of action were investigated through molecular docking against acetylcholinesterase (1QON), thioredoxin from *A. gemmatalis* (5DBQ), and farnesol dehydrogenase from *H. armigera* (7W61), using SwissDock and CB-Dock2 platforms. Commercial insecticides (flubendiamide and chlorantraniliprole) were used as reference compounds

Results



In silico ecotoxicity predictions indicated that the compounds from the heptane extract exhibited low to moderate bioaccumulation potential (Figure A) when compared to the commercial compound CT1. In the toxicity prediction for *Daphnia magna* (Figure B), the compounds showed lower values than the CT1 control (7.4 $-\text{Log}_{10}$ mol/L), suggesting lower relative toxicity.

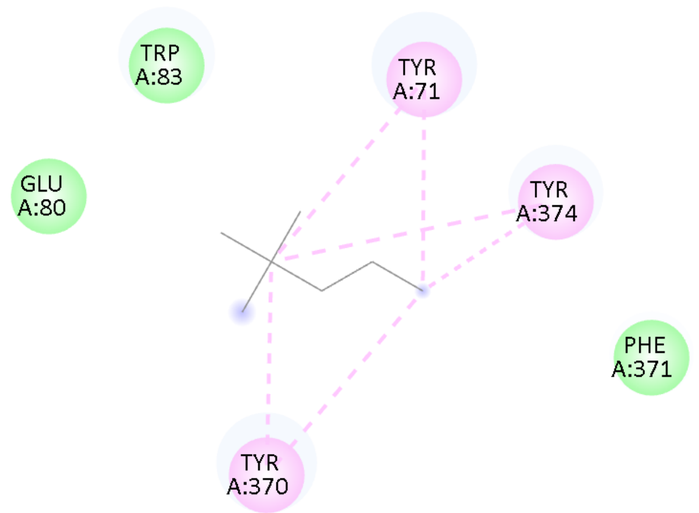
Table 1. Computational prediction of the cytotoxicity (pIC_{50}) of compounds from the heptane floral extract of *Pyrostegia venusta* in different human cell lines.

	C1	C2	C3	C4	C5	C6	CT1
HEK-293	4.9057	3.7189	2.8262	5.1290	4.3937	4.1683	4.4887
HEK-293T	3.8577	4.1882	4.3314	3.8975	4.2095	3.9073	5.0371
HUVEC	5.1073	4.6451	4.9494	4.4120	4.2551	4.6113	5.6197
HaCaT	4.8584	4.9447	5.2519	5.1432	5.1598	4.7395	4.9410

Table 2. Prediction of the cytotoxicity of compounds from the heptane floral extract of *Pyrostegia vebusta* in different human cell lines by computational methodology.

Title 1	Ligante	SwissDock AC Score	SwissDock ΔG (kcal/mol)	SwissDock FullFitness
5DBQ Thioredoxin	C5	-22.019922	-5.52	-1590.41
	C6	-14.942758	-6.18	-1583.62
	CT1	-24.683469	-6.72	-1583.13
7W61 Farnesol dehydrogenase	C5	-26.082070	-6.02	-1274.63
	C6	-19.422992	-6.27	-1266.27
	CT1	-27.695948	-7.79	-1272.07
1QON AChE	C5	-23.840242	-5.96	-2244.54
	C6	-16.381083	-6.22	-2236.61
	CT1	-27.141668	-7.42	-2236.81

Molecular docking showed stable ligand binding to AChE, predominantly mediated by π–π and π–alkyl interactions with TYR A:71, TYR A:370, and TYR A:374, along with hydrophobic contacts involving TRP A:83 and PHE A:371. GLU A:80 was positioned adjacent to the ligand, suggesting a secondary role in molecular orientation. This interaction pattern is consistent with the classical mechanism of acetylcholinesterase inhibition.



Conclusion

In silico analyses indicate that compounds from the heptane extract of *Pyrostegia venusta* exhibit relevant molecular affinity toward entomological targets and a favorable preliminary safety profile, supporting their potential as insecticidal candidates and warranting further in vitro experimental validation.