Molecular docking studies of antimalarial compounds from extract of *Cecropia obtusifolia.*

Yolotl Moreno-Hernández [1], Zendy Evelyn Olivo-Vidal [2*] and Carlos Alberto Lobato-Tapia [3]

[1] Departamento de Salud, El Colegio de la Frontera Sur Unidad Villahermosa, Carretera Villahermosa – Reforma, Km. 15.5 Ra. Guineo Segunda sección. Villahermosa, Tabasco. México C.P. 8628

[2*]Departamento de Salud, El Colegio de la Frontera Sur Unidad Villahermosa, Carretera Villahermosa – Reforma, Km. 15.5 Ra. Guineo Segunda sección. Villahermosa, Tabasco. México C.P. 8628; ozendy@ecosur.mx; Tel. (993) 3136110 Ext. 3402

[3]Departamento de Ciencias Químico-Biológicas, Universidad de las Américas Puebla. Ex Hacienda Sta. Catarina Mártir S/N. San Andrés Cholula, Puebla. México C.P. 72810

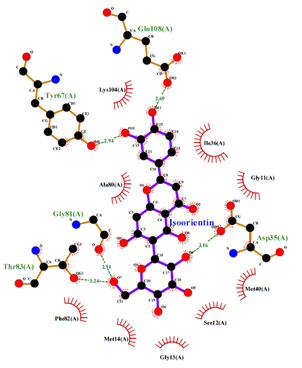
Introduction

Malaria is a disease that affect many people in the world. In México, malaria still a disease with active zones especially in the states of Chiapas and southern Chihuahua where several communities are affected year after year. According to previous studies, a moderate antimalarial effect has been attributed of some Cecropia species in countries like Brazil, Panama and Colombia. To date in México, it doesn't exist studies have been evaluations of the possible antimalarial activity of *Cecropia Obtisifolia* Bertol.

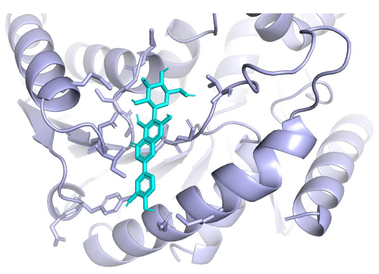
Objective identify the main metabolites present in acetonic extract of *C. Obtusifolia* and evaluate their possible antimalarial activity *in silico* analysis.

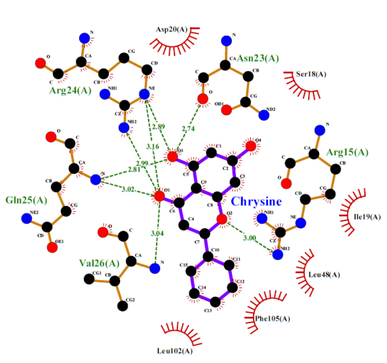
Methods

An acetonic extraction of *C. Obtusifolia* leaves was carried out and by means of Thin Layer Chromatography (TLC) and HPLC the main compounds were identified. This compounds were evaluated with specific molecular docking studies using four different malaria targets with PDB codes 1CET, 1PZ4, 2BL9 and 4ZL4 using AutodockVina and visualized using LigPlot+ and PyMOL.

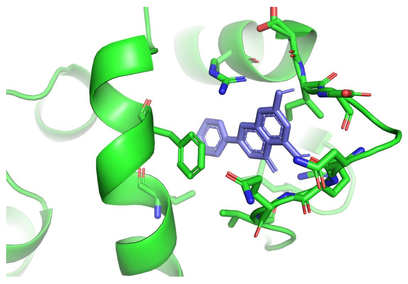


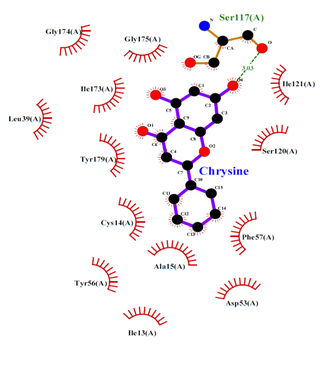
1cet_isoo_complex



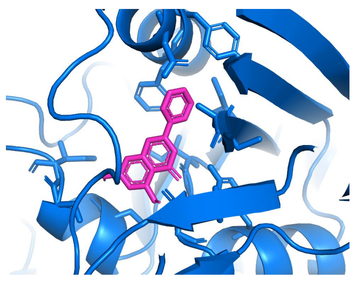


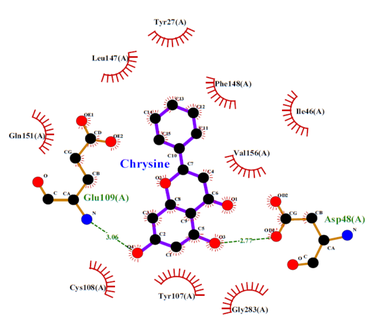
1pz4_chry_complex



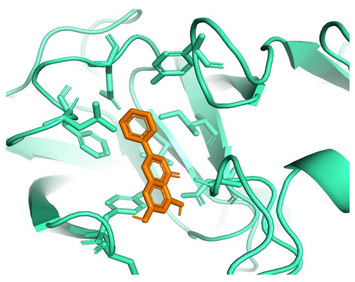


2bl9_chry_complex





4zl4_chry_complex



Molecular docking results (kcal/mol)

	1CET	1PZ4	2BL9	4ZL4
α- amyrin	-7.9	-6.0	-7.9	-8.2
Chrysine	-7.8	-9.6	-8.7	-9.6
Isoorientin	-9.1	-7.0	-8.6	-8.3
Ursolic acid	-7.7	-6.5	-7.8	-7.8
Chloroquine	-6.3			
Fatty acid (16C)		-6.9		
Pyrimethamine			-7.6	
WEHI-842				-8.2

Results

The docking studies showed that the ligands docked well with the targets, resulting in the next strongest binding energies between ligands and targets (kcal/mol): isoorientin-1CET (-9.1), chrysine-1PZ4 (-9.6 kcal/mol), chrysine-2BL9 (-8.7) and chrysine-4ZL4 (-9.6).

Conclusions

These binding affinities were stronger than the control ligands. Analysis of the results suggests that isoorientin and chrysine could act as an anti-malaria agent.

References

Boletín Epidemiológico. (2021). SINAVE México. [Consultado en 2022].
Rivera-Mondragón A. et al. (2019) Phytochem. Lett, 31, pp. 118-120.
Pettersen EF, et al. (2004) Comput Chem. Oct;25(13):1605-12.
Eberhardt, J. et al. (2021) J Chem Inf Model. 61(8):3891-3898.
Schrödinger, L., & DeLano, W. (2020). PyMOL.
Wallace AC, et al. (1996) Protein Eng. 8: 127-134.