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Abstract Book

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VIRTUAL SCREENING OF PLANTS EXTRACTS WITH ANTI-CHAGASIC ACTIVITY GUIDED BY OMICS DATA

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Background:

Chagas disease is caused by the protozoan parasite *Trypanosoma cruzi* and their treatment consists in the use of two nitro heterocyclic compounds that both present high toxicity and low effectiveness during the chronic phase.

Cymbopogon citratus extracts have been shown to alleviate the chronic phase symptoms of the disease, reducing amastigote nests and inflammatory infiltrates in the heart tissue of infected mice.

In this work we used bioinformatics tools to mine public functional genomics databases along with chemoinformatics tools and molecular docking to understand the action mechanism at the molecular level of *C. citratus* extract in chagasic cardiomyopathy.

Results:

The GSE41089 dataset from NCBI GEO contains 14154 genes that were processed for analysis. Genes with log Fold Change > 1 and adjusted p-value < 0.05 were considered over-expressed, resulting in 1465 that met the conditions for further analysis.

Functional gene enrichment analysis prioritized Gene Ontology terms associated with innate immune response and the most significatives biological pathways affected were those relationed to release of cytokines.

Genes in the top-enriched pathways that are known to be affected by the *C. citratus* ingredients, were selected as potential protein targets, resulting in 6 candidates.

Molecular docking of active plant ingredients were performed on the candidate targets to identify potential inhibitors. Promising results were found particularly for one of the candidate targets, Ptgs2 (prostaglandin-endoperoxide synthase 2). Compounds such as Nerolidol, Farnesol and Oleic Acid show quite similar binding modes and comparable anchoring strength than that of the enzyme substrate.

Conclusions

The results show that the combination of omics analysis with molecular docking is a promising strategy to understand the action mechanisms of plants extracts against chagas disease. The information obtained will allow us to search for healthier and less harmful treatments against *T. cruzi*.

Poster Session: http://bit.ly/cab2c-2021-posters

Poster Gomez Chavez et al: https://youtu.be/fAG-H_rwy2g