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Ligand-Protein Interactions of Cymbopogon citratus Compounds and Their Implications for Chagas Disease Treatment

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Background: The chronic stage of Chagas disease is characterized by severe cardiomyopathy caused by infection with the parasite Trypanosoma cruzi. Through molecular dynamics simulations, compounds derived from *Cymbopogon citratus* have demonstrated promising potential as ligands for proteins involved in this stage of the disease, displaying favorable binding energies. These interactions between the ligand-protein complexes may explain the observed effects of relieving this pathology by reducing amastigote nets and inflammatory infiltrates in the cardiac tissue of mice.

In this study, we analyzed the key interactions between compounds derived from *Cymbopogon citratus* and the most significant proteins associated with Chagas disease in mice.

Results: Ptgs2, Hck, and Csf1r complexes have demonstrated excellent binding free energies (ΔGbind) compared to specific inhibitors targeting these proteins. An analysis based on Quantum Theory of Atoms in Molecules (QTAIM) revealed that, in the case of Ptgs2, it exhibits a high affinity for binding to molecules with both a polar and non-polar (unsaturated) moiety, such as certain terpenes. This is attributed to the characteristic triad in its active site, consisting of arginine, tyrosine, and aspartic acid, which can attract the polar part of ligands. Furthermore, due to the presence of numerous non-polar residues in the active site, a significant number of non-polar interactions are formed, stabilizing the interaction with the formed complexes.

Similarly, Hck and Csf1r also show a strong tendency to bind to terpenes with structural unsaturations, leading to the formation of numerous non-polar interactions within the complexes. Although these non-polar interactions are weaker compared to polar interactions, they still contribute to stabilizing and forming a high affinity with these complexes.

Conclusions: This study highlights the importance of interactions between compounds derived from *Cymbopogon citratus* and key proteins involved in Chagas disease in mice. Furthermore, the fact that multiple compounds bind to different target proteins suggests that the observed alleviation of symptoms in the chronic phase of Chagas disease may be due to a collective action of multiple molecules on different targets. These findings encourage further investigation of *Cymbopogon citratus* as a potential alternative for Chagas disease treatment.