ADVANCEMENT OF CHAGAS DISEASE TREATMENT THROUGH THE IDENTIFICATION OF POTENTIAL NATURAL PRODUCT TARGETS IN THE *TRYPANOSOMA CRUZI* PROTEOME

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RATIONALE

Chagas disease, (American Trypanosomiasis), is a tropical disease linked to *Trypanosoma cruzi,* a protozoan parasite infection which can be spread via triatomine insects and contact with bodily fluids. Approximately 8-10 million people in Latin American countries have Chagas which is most prevalent in rural areas. Current drugs, Nifurtimox and Benznidazole, are effective treatments for the disease in acute phases, but are limited in the chronic stages and display detrimental side effects. Further research and annotation of the *T. cruzi* proteome is critical in polypharmaceutical advancement or repositioning of existing drugs .

PROPOSED RESEARCH

- Identification of natural products that might be effective against Chagas through the screening of the natural based drug library against the surface proteins Transialidase and GP63 of the *T. Cruzi* proteome.

- Search for similar binding sites across the *T. Cruzi* proteome and determine if identified natural products display similar affinity

PROGRESS

- Finished screening on Autodock and ranked all results
- Visualized top 10 output results for IMS8 using VMD and prepared a table for potential interactions between atoms using the cap of 2-4 Angstroms
- Went over SMAP with Chirag and Li and successfully finished running 1MS8 against the T. Cruzi proteome

TENTATIVE PLANS

- Prepare SMAP files for 1LML GP63 protein.
- Find out command to rank results according to P-Value significance
- Decide on which compounds to run against results of SMAP and continue with docking
- Visualize and gather all images for report
- Continue reading on theory of programs and T-Cruzi mechanism
- Try to get all the data prior to the next report
- Go over any questions with Sy Bing, Li and Chirag

SUCCESSES AND SETBACKS

- Finally done with virtual screening with the two databases
- Ran SMAP successfully
- However, recording possible interactions is taking longer than expected and will require extra time

CULTURAL ASPECT

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