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

- Finalized on PDB structures 1MS0 and 1MS8 for TcTS and 1LML for gp63.
- 1MS0 and 1MS8 differ in resolution, so checked for similarity using VMD alignment
- Learned how to do virtual screening and practiced screening with the NCI Set II database compounds
- Successfully screened prepared 1MS8 and 1MRS proteins and waiting for results on ranking
- Continued reading on the background of Autodock and structural mechanisms of TcTS

TENTATIVE PLANS

- Continue virtual screening with the NCI database and move onto the NADI database
- Skype with Dr. Bourne and Chirag on progress made and to be made
- Analyze results of screening and begin visualization process of selected results
- Continue reading on protein background, Autodock and SMAP

CULTURAL ASPECT

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