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

Jenny Jia Xin Liang
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University of California, San Diego
Universiti Sains Malaysia

#### **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**

- Did virtual screening on 1MS8 and 1LML with the NCI and NADI databases
- Prepared Autodock files and uploaded to the server
- Continued reading on the background of Autodock and structural mechanisms of TcTS and 1LML.
- ·Visualized the grid box for each active site to confirm
- Talked to Dr. Bourne about the progress and kept in touch with Li and Chirag

## TENTATIVE PLANS

- Prepare SMAP files through Putty for 1MS8 and 1LML receptor screening and have Chirag and Li look over it.
- Analyze results of virtual screening and prepare visualizations for report
- ·Continue reading on protein background, Autodock and SMAP
- Start using SMAP
- Keep in touch with UCSD mentors

#### SUCCESSES AND SETBACKS

Virtual screening with Autodock 3.0 was successful, however the road to getting there was full of obstacles

Figured out which proteins would be best to use for screening

No major setbacks! Just need to read and learn more from the people in lab.

# **CULTURAL ASPECT**









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