# Computationally Accelerating Protein-Ligand Matching: A Case Study on Leishmaniasis

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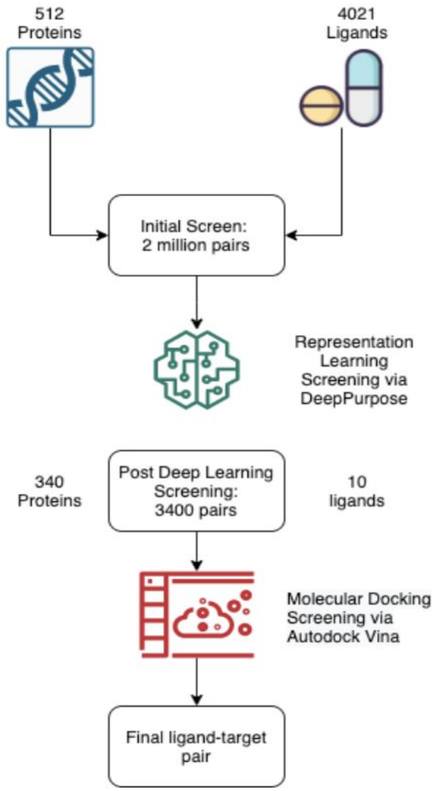
## BACKGROUND & PROBLEM

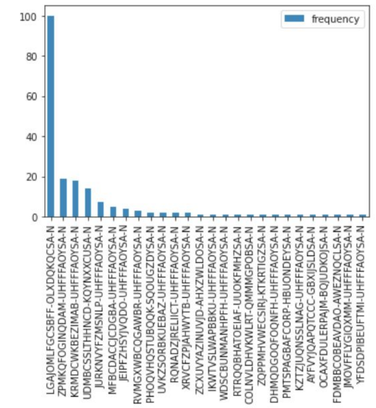
- Out of 12,000 diseases, only 5,000 have treatments. The 7,000 others belongs to the rare diseases category and aren't target of major drug discovery programs
- Drug repurposing is a promising approach to find cure for these diseases
- Protein-Ligand Docking is one important step of the drug repurposing pipeline
- There have been new, lighter approaches powered by Deep Learning: How do they compare to conventional molecular docking methods?

## METHODS and APPROACH

- We used a list of Leishmaniasis associated targets from the 2020 Deep Learning Indaba Challenge
- We used the Deep Purpose Library to rank drugs for each target
- We ran molecular docking for each target against ligands using Autodock Vina 4
- We compare the predictions of the two methods
  - Rank correlation
  - Overlap of top 10/50 target
  - Median rank assigned by deep learning methods to top drug found by molecular docking

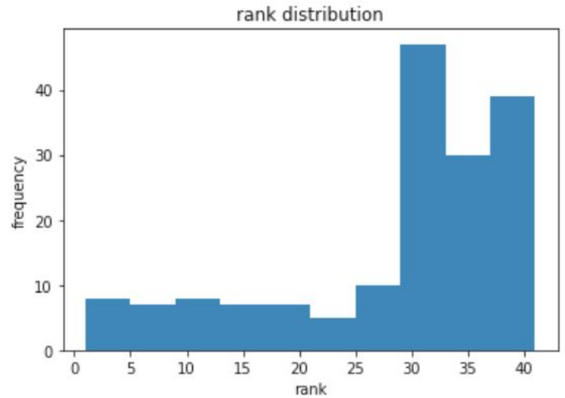



## Results




(b) Top 1

Frequency of drug's appearance at the top of the list for each target




Rank assigned by deep learning methods to top drug according to molecular docking

## CONCLUSION AND FUTURE WORK

- Deep Learning methods are helpful at coming up with a shortlist and reduce the search space from 4,000 drugs to ±250
- However, the top drug predicted by Deep Learning rarely matches the top drug predicted by molecular docking methods. The median rank assigned by Deep Purpose to Autodock Vina 4 target is 29.
- Next step: Extend Analysis to other diseases

**References:**

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