

Introduction

- Drug discovery is cost-effective and time-consuming taking about 10-15 years and over 2.5 billion funding.
- The global **COVID-19** outbreak emphasizes the importance of a more quicker, cheaper and effective drug discovery.
- Collaborative drug discovery using AI provides a cheaper, effective and quicker drug discovery.

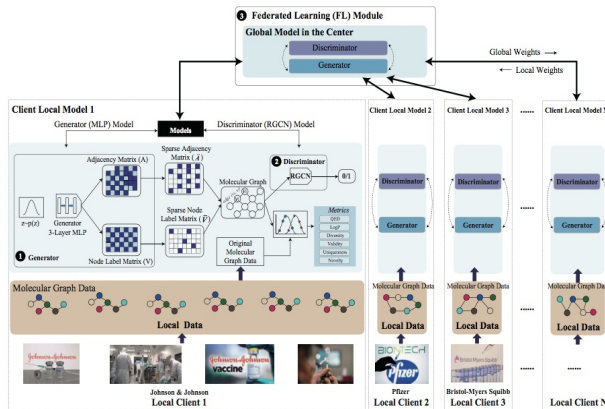


Objectives

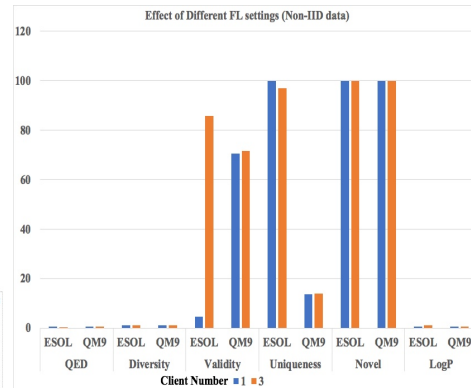
- Design a framework that can generate molecular drugs.
- Demonstrate that drug generation over many clients (federation) can be more effective.
- Framework should be able to generate high drug-likeness, novel and valid molecules.

Methods

- Generator as a multilayer-perceptron.
- Discriminator as Relational graph convolution network.
- Random noise from normal distribution as input to generator.
- Federated learning provides an option to select number of clients to participate in drug generation.
- Evaluation metrics are drug-likeness, validity, novel, diversity, uniqueness and logP scores.



Results



Conclusions

- Results show that drug generation over several clients yields higher performance compared to single client.
- Emphasizes the need for several pharmaceutical companies to collaboratively perform drug discovery during disease outbreak for effective and quick drug discovery.