

EGC-442 SARS-CoV-2 Spike and ACE2 protein-protein interactions database

Abstract

SARS-CoV-2 protein interactions are essential for viral replication and pathogenesis. To better understand these interactions, we have created a database using AWS (Amazon Web Services) to store data extracted from protein simulations. This database can be used to study the structure and function of SARS-CoV-2 proteins and their interactions with each other and with host cell proteins.

Introduction

Under the advisement of Dr. Chloe Yixin Xie, the team worked on improving an existing database used to store protein-protein interaction data. The current database was self-hosted on individual computers, which made collaboration and sharing of research data difficult.

The team was tasked to research and design a new database. The existing database was to be researched to determine whether it can be re-used, and if not, make changes and improvements to it for better future scalability.

Project Goals

- Investigate the existing database to determine whether it's usable for research on protein-virus interactions
- Determine the improvements needed in the new database design
- Validate the functionality of the database by importing test data into it

Materials and Methods

An AWS RDS instance was created with a salt bridges table, a donor table, and an acceptor table. Using VMD simulations, data is extracted from protein interaction simulations and inserted using a python script into the database.

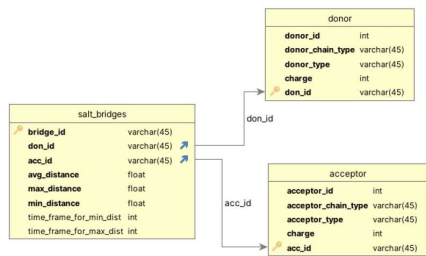


Figure 1. New database structure design

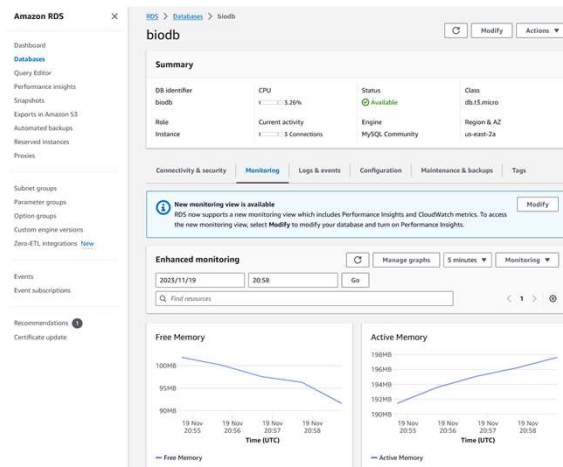


Figure 2. Screenshot of newly created RDS instance

Figure 3. Example of data in acceptor table

Figure 4. Example of data in Donor table

Figure 5. Example of data in salt_bridges table

Results

The RDS instance successfully accepted data from data extracted from VMD simulations, allowing more accessible research of protein-protein interaction data.

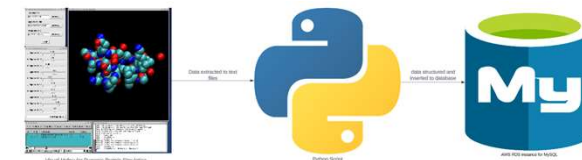


Figure 6. Data flow from VMD Simulations, to python, to MySQL (AWS)

Acknowledgments

Dr. Chloe Yixin Xie – Project Owner
Dr. Jack zheng – Capstone Instructor

Contact Information/ Website

