DAViDD: Initial data management solution for UNC's READDI AViDD Center

Terrell Russell, Ph.D
Executive Director
iRODS Consortium

May 28-31, 2024
iRODS User Group Meeting 2024
Amsterdam, Netherlands

The Rapidly Emerging Antiviral Drug Development Initiative AViDD Center (READDI-AC) is an NIH-funded public-private partnership focused on developing effective antiviral drugs to combat emerging viruses.

The READDI-AC at UNC-Chapel Hill is one of nine Antiviral Drug Discovery (AViDD) Centers funded by the US National Institute of Allergy and Infectious Disease (NIAID) at the National Institutes of Health.

$65M in 2022 - 40 Investigators, 23 Research Sites, 5 Countries

NIH Award 1U19AI171292-01

AViDD Center READDI AC

Rapidly Emerging Antiviral Drug Development Initiative

READDI-AC Mission

The response to viral outbreaks has historically been **reactive** – vaccines and medications are developed only after a new virus emerges. Our mission is to **proactively prepare** for emerging viruses by developing antiviral drugs that are active against more than one virus in a family. These **broad-spectrum antivirals** will help safeguard the well-being of communities worldwide against existing viruses and will be more likely to be effective against future novel viruses in the same family.

Four families:

- Coronaviruses - causes SARS, MERS, COVID-19
- Filoviruses - includes Ebola, Marburg
- Flaviviruses - includes West Nile, Dengue, Zika
- Alphaviruses - includes Chikungunya, Equine Encephalitis

AViDD Center
READDI AC
Rapidly Emerging Antiviral Drug Development Initiative

Timeline

RENCI, as a subawardee, was tasked to assess, design, and develop the data management solution for the READDI-AC project.

- Interviews - July-August 2022
- Survey - August 2022
  - Determination of existing lab workflows
  - Document types, variety, size, volume
  - Number and identity of humans in the loop
  - Opportunities for automation
  - Opportunities for cross-lab interactions
- Security considerations - Fall 2022
- Initial design of system - Fall 2022
- Paper evaluation - Fall 2022
- Initial implementation - Nov-Dec 2022
- Testing - Dec 2022
- Deployment - Jan 2023
- Evaluation - Q1 2023
- Iteration - through 2023

Discovery Questions

- If you use instruments in your work, what is the format of files they produce?
- Where do you currently record and store chemical or biological data? In what data format?
- What keywords or other terms do you use to search for previously recorded data?
- Do you use existing or public vocabularies, ontologies or other references?
- Are you familiar with FAIR data sharing principles?
- What are typical dataset sizes for each unit of work?
- What is a typical data generation rate for your lab / unit?
- What is a typical number of data files you generate per week?
- Do you protect the stored data (do you require secure login/authentication to access your data?
- How do you currently share your data with (i) your labmates, (ii) within UNC, (iii) with the rest of the world?
- What software do you use to process or visualize your data?
- Do you have a need to format your data for publication or presentation format?
- What steps are manually processed today? What steps are automated today?
- Where is manual processing required? Where can data processing be automated?
- What limitations are your lab / group / team running into?
- What is your highest priority or need for data capture or storage?

Discovery Findings

- **Not Big Data (yet)**
  - 1000s of files over the course of a year
  - Maybe 10s of GBs, but most much smaller
  - Human scale rate of ingest
- **A few formats, mostly open / convertible**
  - doc, pdf, xls, ppt, csv, txt, prism, jpg
- **Some electronic lab notebooks**
  - Mostly xls
  - Manually calculated / generated
- **Very little currently automated**
  - Manual transcription from paper notebooks
  - Graphing done in Excel or (rarely) Jupyter notebooks
- **No shared naming conventions**
  - For either data filenames or metadata
  - Sometimes consistent within a lab
    - Due to necessity
    - But not over time
- **Highest priority is access / sharing**
  - This project's data needs a 'home'
- **No centralized data repository**
- **No standardized data processing (raw to publication quality) and data upload protocols**
- **No versioning protocols**
- **Metadata currently non-existent**
- **Negative results / Failed attempts not recorded**
- **HEIGHTENED NEED for RDM due to new NIH reqs**

Design and Preparation

There was very little process to automate - we were starting from scratch and these labs did not have much in common. Different instruments, different chemistry, different software, different processes, different formats.

Not their fault - they'd never been required to coordinate and collaborate in the past except via publications. This was a new mandate.

There would be two projects:

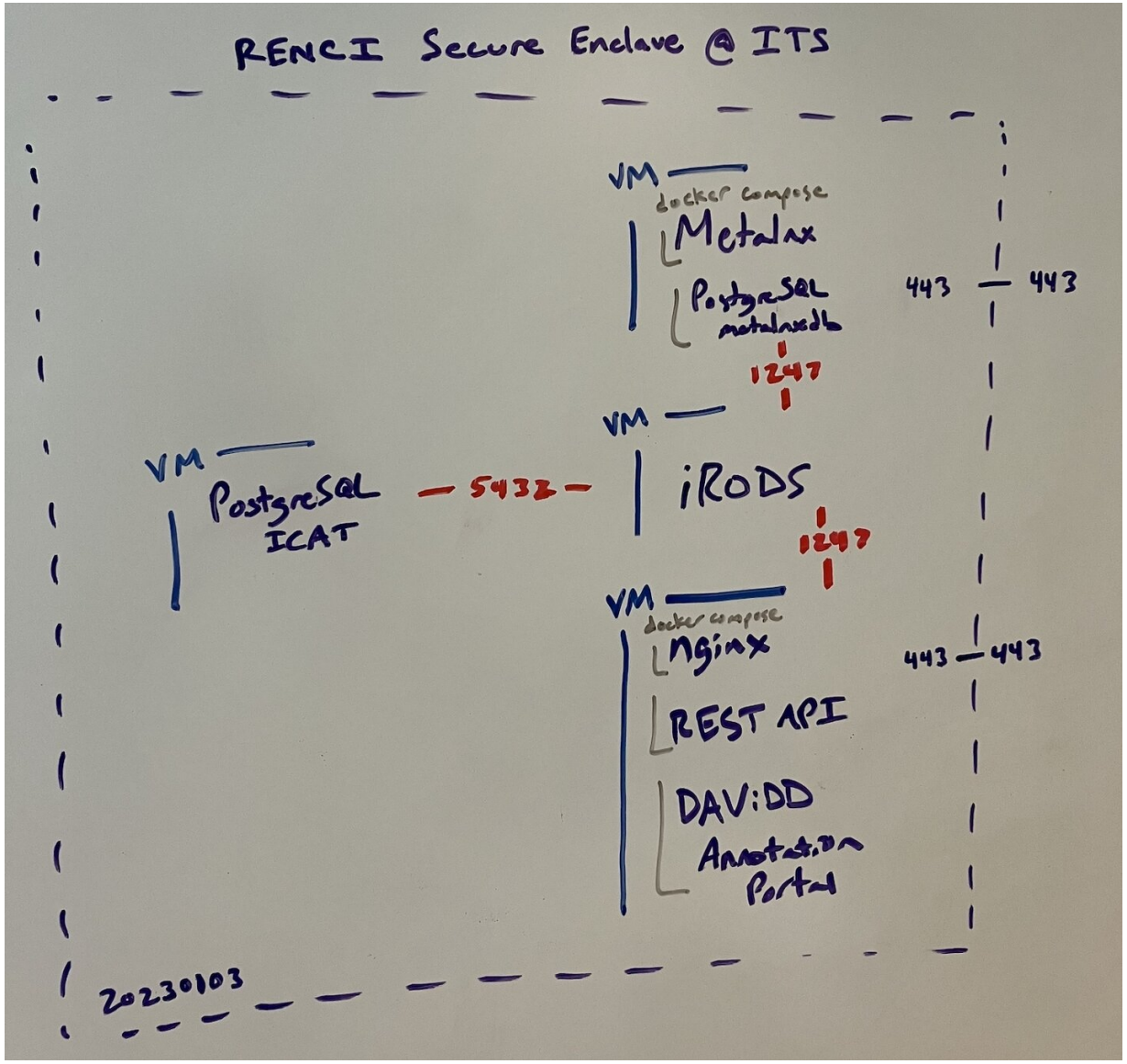
- People engineering
  - hardest part, scientists do not want to change their processes
  - requires many people to coordinate (expensive in time and effort)
- Software engineering
  - a few puzzles to solve, but nothing too daunting
  - security requirements demand working with other parties

Software Engineering Requirements

- federated login for otherwise unaffiliated researchers
- secure enclave
- just files, mostly spreadsheets
- some annotation
- automation where possible
- search
- available for analysis with existing tooling
    - probably via download

January 2023 - Initial Deployment

- 4 VMs
  - RENCI Secure Enclave
- docker compose
  - originally REST API
  - later HTTP API
- CILogon providing identity



DAViDD - Application and Policy

Angular Application

- upload
- assays
- search
- compound profile
- FAQ
- profile information

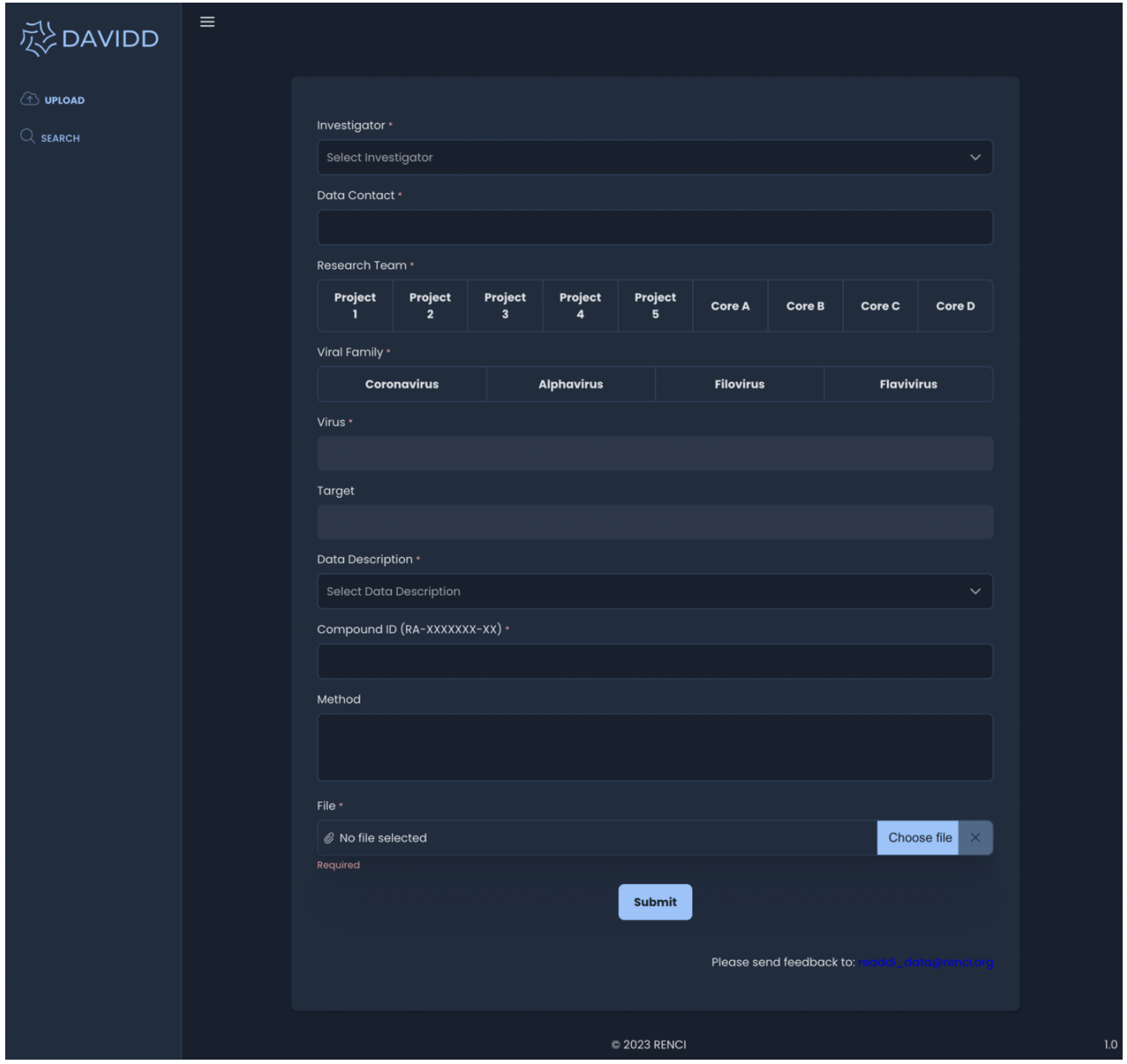
iRODS Policy - Four recurring rules

- irule davidd_add_sweeper_to_queue
- irule davidd_add_compound_profile_sweeper_to_queue
- irule davidd_add_compound_profile_remover_to_queue
- irule davidd_add_assays_sweeper_to_queue

February 2023 - Upload

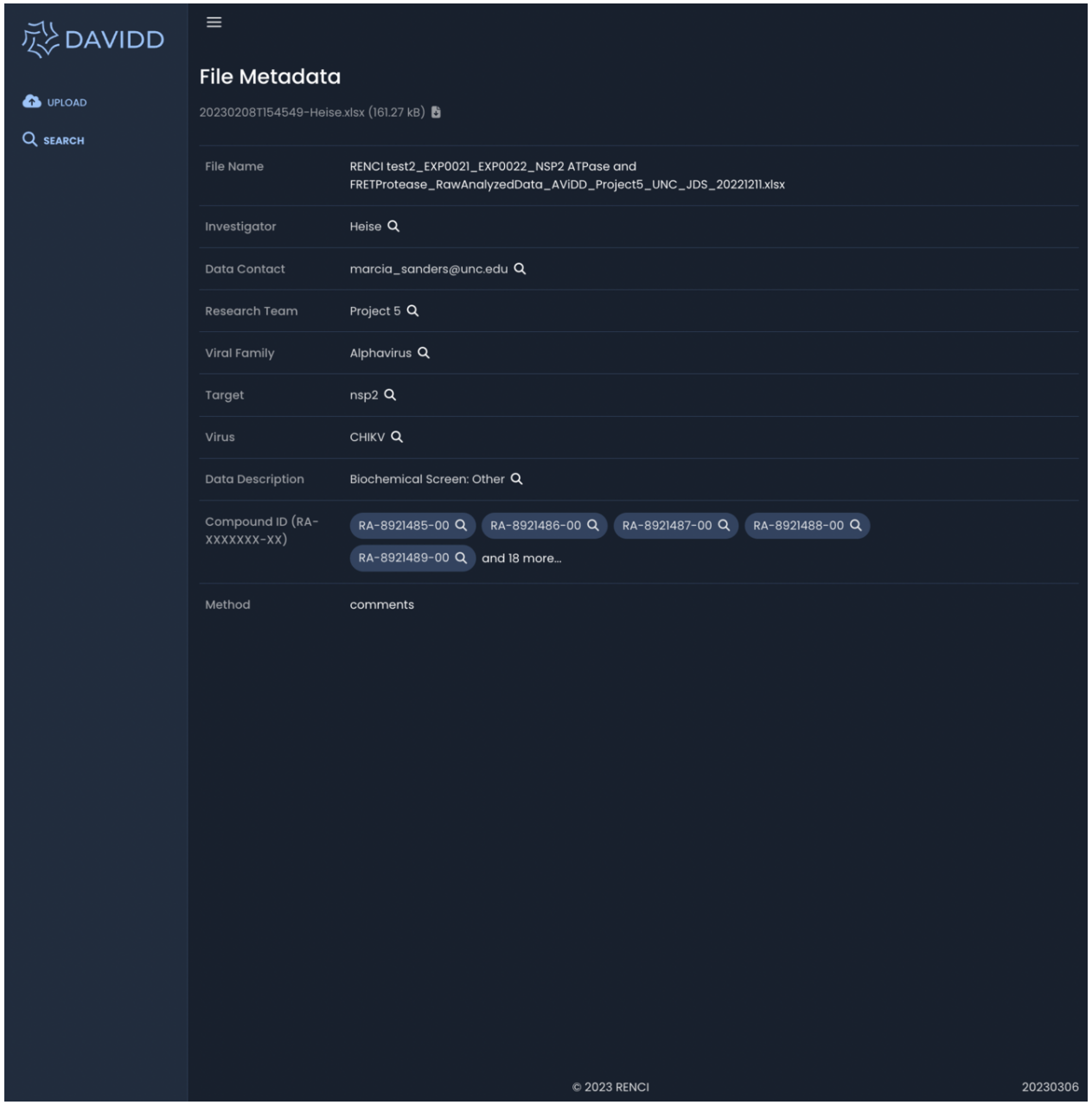
irule davidd_add_sweeper_to_queue

- davidd_find_and_parse_uploaded_files
- davidd_parse_and_place_jsonfile
  - parse python dict
  - prepare avus_to_add
  - decode file data, write it
  - associate avus



March 2023 - File Metadata

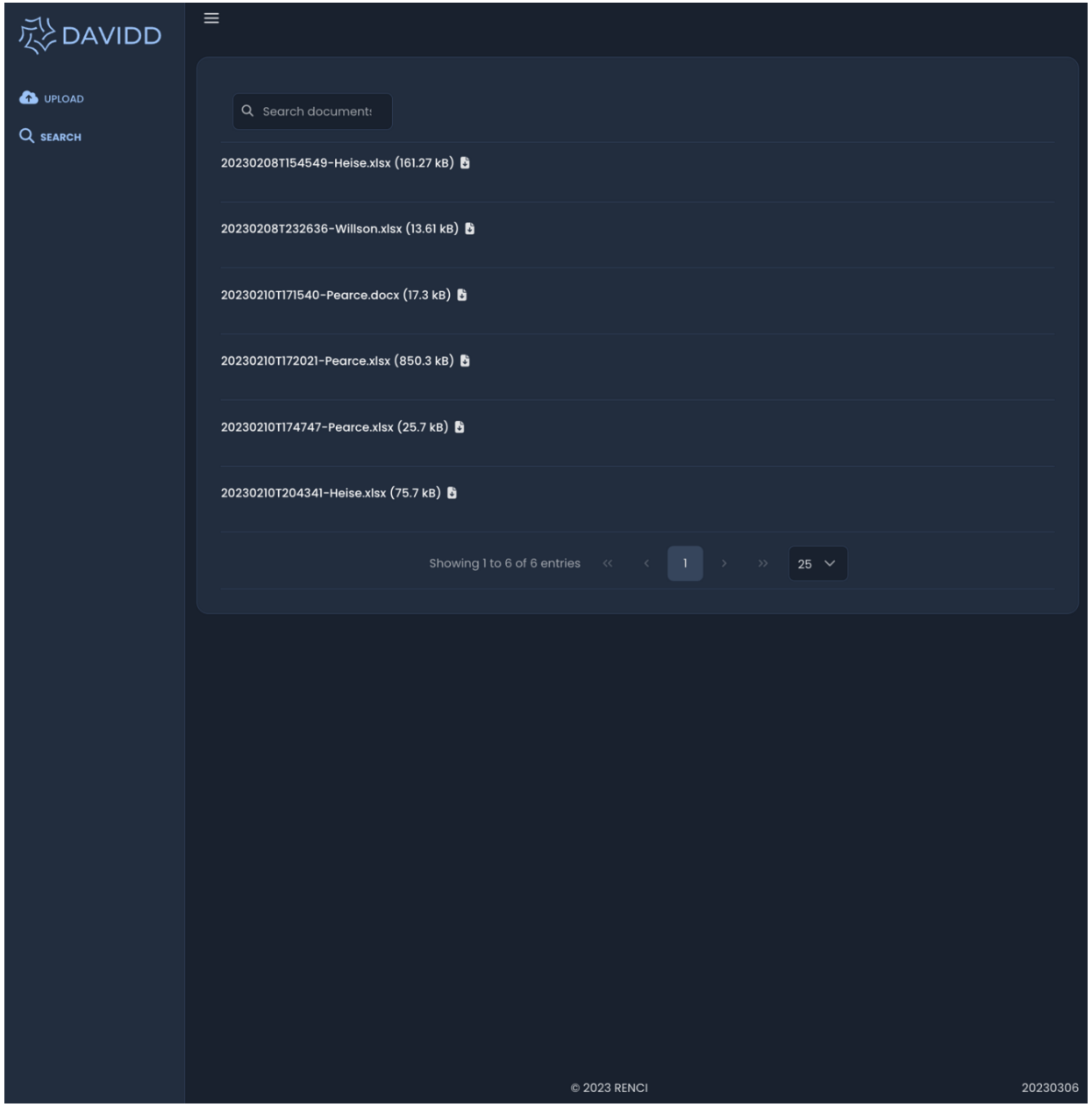
Associated metadata from upload form available to search and browse



March 2023 - Search

GenQuery

- matching on file name and metadata



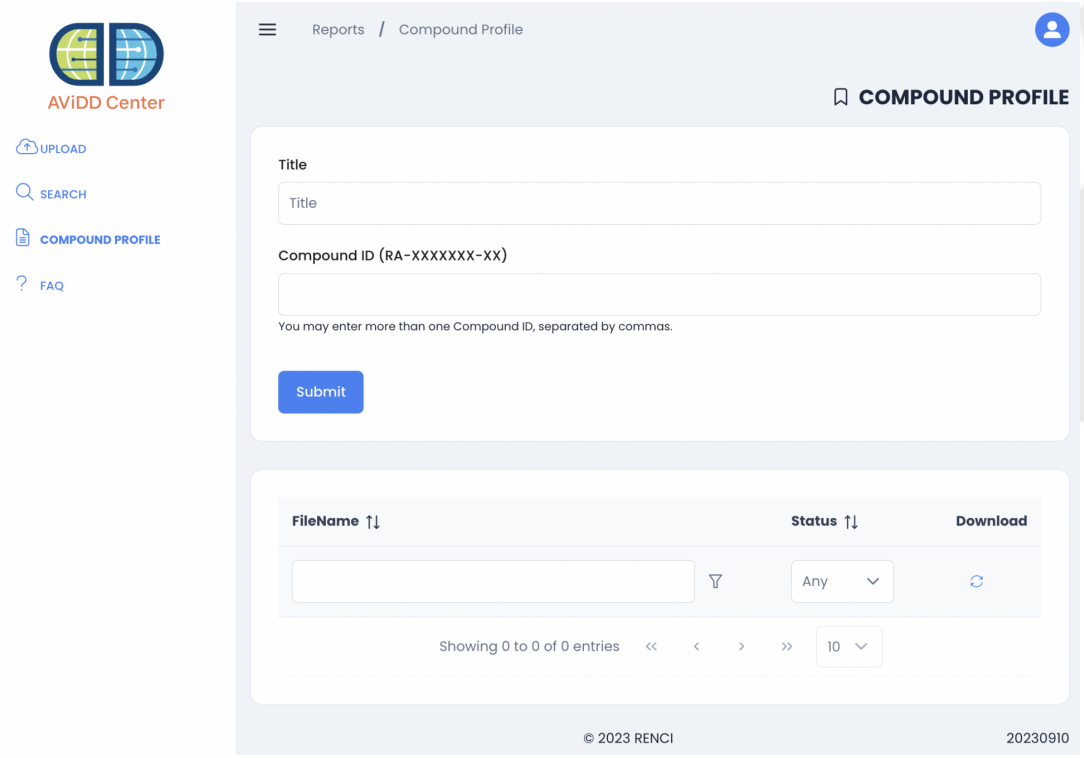
September 2023 - Compound Profile

irule davidd_add_compound_profile_sweeper_to_queue

- davidd_process_requested_profile
- davidd_process_queued_file
- davidd_walk_collection_for_compound_info
  - use openpyxl, read spreadsheets, populate new one

irule davidd_add_compound_profile_remover_to_queue

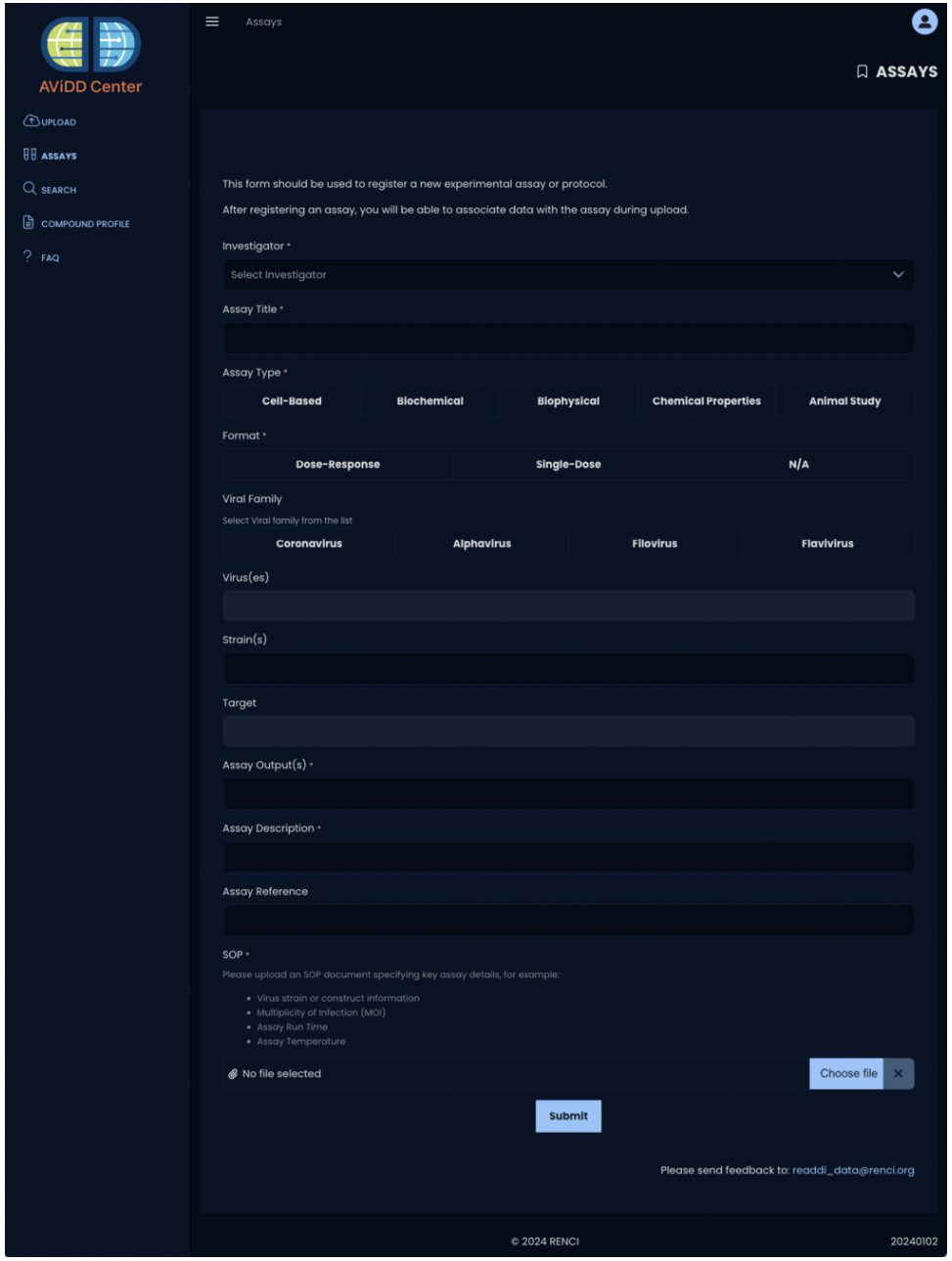
- davidd_remove_old_compound_profiles
  - defined by compound_profile_removal_age_in_minutes



January 2024 - Assays

irule davidd_add_assays_sweeper_to_queue

- davidd_find_and_parse_assay_files
  - davidd_parse_and_place_jsonfile



Summary

Discovery and prototyping were a success

- 4 labs interviewed
  - Many challenges identified and lessons learned
- 3 federated login architectures attempted
  - Selected CILogon.org

353 datafiles uploaded in the first year

- 105 Coronavirus
- 173 Alphavirus
- 27 Filovirus
- 48 Flavivirus

The Future

Having identified the main requirements and bench-to-data process, the project selected an existing commercial vendor for its extensive GUI and compound-specific analysis tooling.

RENCI continues to develop database-level tooling focused on chemical compound information and linkages with other tools in the ecosystem.

Acknowledgements

- NIH
- Ava Vargason, Nat Moorman, Ralph Baric, Tim Willson, Toni Baric
- Oleg Kapeljushnik, Kory Draughn, Alex Tropsha, Robert Hubal, Kelyne Kenmogne, Carrie Pasfield, Patrick Patton

Thank you!

Questions?