GNPS ReDU Workshop/Hackathon

We want to introduce **ReDU** (Reanalysis of Data User Interface), redu.ucsd.edu, and familiarize the community with how to contribute data to ReDU, the unique analysis tools available in ReDU, and how ReDU integrates with the tools you already love in GNPS.

Audience

The target audience is mass spectrometrists, natural products chemists, and all other researchers. We encourage the participation of people that have mzXML/mzML converted MS data deposited in MassIVE.

Participation Requirements

1. Enthusiasm!
2. Zoom Video Conferencing Software
3. GNPS Account (https://gnps.ucsd.edu/ProteoSAFe/static/gnps-splash.jsp)
4. Data to upload to MassIVE (or already uploaded), GNPS molecular networking, GNPS feature based molecular networking, or GNPS library search task ID, and/or interesting questions to ask about repository MS data analysis

Goals

1. Become familiar with ReDU and documentation (https://ccms-ucsd.github.io/GNPSDocumentation/ReDU/)
2. Create and upload ReDU-compliant metadata
3. Project your data onto the ReDU database
4. Find out information about your favorite chemical with Chemical Explorer in ReDU
5. Compare annotations between cohorts via Group Comparator in ReDU
6. Re-analyze ReDU data via GNPS molecular networking

Workshop/Hackathon Link

https://ucsd.zoom.us/j/94195852297
Password: 024250

Zoom Etiquette

All participants will be muted upon entry. If you would like to ask a question, please chat Mingxun Wang, Alan Jarmusch. We can then unmute you to start a discussion. If you think we're going too fast, you can also select go slower/faster in the feedback options in the top right of the zoom meeting. There will be periods of time for questions.

Agenda

Wednesday, May 6th, 2020, @ 9-11:00 AM (Pacific Time)
9:00 AM - 9:30 AM

1. Overview of ReDU and review of steps to contribute data
    a. Brief overview of ReDU (explore PCA of ReDU data)
    b. Complete ReDU metadata
    c. ReDU update process/lifecycle

9:30 AM - 10:30 AM

2. Data Analysis Tools
    a. Explore your favorite chemical in Chemical Explorer and explore the sample information associations
    b. Project data onto the ReDU database (if you have a task ID you can use it!)
    c. Learn how to use the file selector and launch
        i. Group comparator
        ii. Re-analysis of data using molecular networking in GNPS
            1. See our previous workshop for more information about molecular networking (https://www.youtube.com/watch?v=PqTuex0nsGk&t=5485s) and the documentation at GNPS (gnps.ucsd.edu)

10:30 AM - 11:00 AM

3. Questions and discussion

Team

Alan Jarmusch
Mingxun Wang
Chrissy Aceves
Julia Gauglitz

Documentation Links

General Info:

ReDU homepage - LINK
ReDU documentation - LINK

Contributing Data:

Step-by-Step Direction - LINK
File Upload - LINK
ReDU sample information template - LINK

Analysis Tool Info:

GNPS Molecular Networking - LINK

Presentation Slides

Will be placed here closer to the event.