

GNPS MASST Workshop

We want to show you how to make use of the (now) enormous amount of public metabolomics/small molecule/natural products data available. This totals nearly 1500 datasets which includes 196,727 LC/MS runs. MASST is one tool to help you query where else in all this data your spectrum might be found. You can read the publication here:

<https://www.nature.com/articles/s41587-019-0375-9>

Audience

The target audience is mass spectrometrists or natural products chemists that have MS/MS data of their samples and either have trouble identifying specific fragmentation spectra or just simply are curious where else their compounds are found.

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 and annotate (if possible)

Goals

1. Query with MASST from web import form
2. Query with MASST directly from Molecular Networking
3. Interpreting results
4. Follow up analyses after MASST

Zoom Etiquette

All participants will be muted by default and will not be able to chat everyone. If you would like to ask a question, please chat Alan Jarmusch or Mingxun Wang. 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.

Team

Mingxun Wang
Alan Jarmusch
Morgan Panitchpakdi
Emily Gentry

Workshop/Hackathon Link

Zoom - <https://ucsd.zoom.us/j/98351548626>

Meeting PW: 013501

Agenda

Wednesday, April 22, 2020, @ 9-12 AM (PST)

9:00 AM - 9:30 AM

1. Overview of MASST (<https://ccms-ucsd.github.io/GNPSDocumentation/masst/>)
 - a. Web Query Form - <https://masst.ucsd.edu/>
 - b. Exploring Demo Results - <https://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=235f9656654f4486b1cf4c5cc61b1f1b>
 - c. Downstream Analysis - Molecular Networking ([Example](#))

9:30 AM - 10:30 AM

2. Hands-on Session/QA

Example Data

[Example MASST for Stenothricin](#)

[Example Molecular Networking from MASST Search](#)

[Example Molecular Networking to MASST Query](#)

Presentation Slides

Will be placed [here](#) closer to the event.

Fun Things

MASST Usage:

