2022 Metabolomics Interest Group Meeting Report

Meeting Co-coordinators:

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C) Tytus Mak, PhD, NIST Mass Spectrometry Data Center

Meeting Overview

Meeting Title: Democratizing Metabolomics: Lessons learned and future directions from US regional core facilities
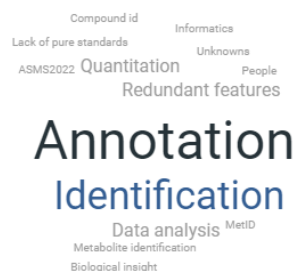
Meeting Theme

The workshop was opened by a welcome message from the co-coordinators and a brief overview on its format and focus. We also took a live Slido poll from the audience in attendance (we opted to not live-stream the meeting) on the main challenges they face in their metabolomics data analysis, and what were the software tools that they commonly use to help us decide the best theme for next year's workshop. From the results of the poll it's evident that compound ID is the key challenge the attendees face followed by data analysis tools. The most popular software among the responders was Compound Discoverer and Progenesis followed by several community-driven and open source tools (see figures 1-2). Over half the 29 responders self-identified as student (17%)/postdoc (7%)/early-career up to 10 years post-PhD (41%) while 38% self-identified as senior level scientist.

This workshop aimed at highlighting the resources that exist in NIH Regional Comprehensive Metabolomics Resource Cores (RCMRCs). RCMRCs are at the forefront of bioanalytical innovation, and have played a pivotal role in the inexorable rise of metabolomics as a critical platform for life science, environmental, and clinical

What is the main challenge you face with your metabolomics data?   25

Compound id   Informatics
Lack of pure standards   Unknowns
ASMS2022 Quantitation   People
Redundant features

Annotation
Identification
Data analysis MetID
Metabolite identification
Biological insight

What data processing software do you use?   28

Agilent and custom   In house code
MassHunter   In-house software
Progenesis   Proprietary
Elements
Compound discoverer
MSDIAL MSDIAL MZmine depends Xcms Inhouse
Stuff we code   Tbd
Python   Custom
LC Binbase
Compound discover MZmine
Compound Discovers

research. This workshop aimed at learning from their decade-long expertise as NIH-funded US regional cores through the eyes of each invited core director/ representative. The invited representatives that presented at the workshop included:

- Prof. Timothy Garrett, Co-Director of the Southeast Center for Integrated Metabolomics (SECIM)
- Dr. Uri Keshet, Manager of West Coast Metabolomics Center at UC Davis (WC3MRC)
- Dr. Maureen Kachman, Managing Director of Michigan Regional Comprehensive Metabolomics Research Core (MRC2)
- Dr. Douglas Sheeley, Program Leader of the NIH Metabolomics Common Fund

Each core representative was given 5 minutes and option to present up to 2 slides to highlight their distinct services and core competencies. These presentations were followed by a 15 minute overview given by a representative from the NIH Metabolomics Common Fund, Dr. Sheeley, on current consortium efforts. The rest of the workshop   was dedicated to an open panel discussion with the audience. The discussion was very engaging and very much driven by audience participation. Some of the questioned that were discussed at length   with the audience included:

1. What is the most important lesson that you've learned since the funding of your RCMRC?
2. What's gone well and what can be improved?
3. What data management strategies have you used?
4. Do you provide "raw" data to customers? Are they the vendor "raw" files or open source mzML/mzXML files?
5. It has been a decade since the RCMRCs have been established, what do you see happening in the next 10 years?