2023 Metabolomics Interest Group Meeting Report

Meeting Co-coordinators:

A) Maryam Goudarzi, PhD, Charles River Laboratories

B) Thomas Horvath, PhD, Baylor College of Medicine & Texas Children's Hospital Microbiome Center

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

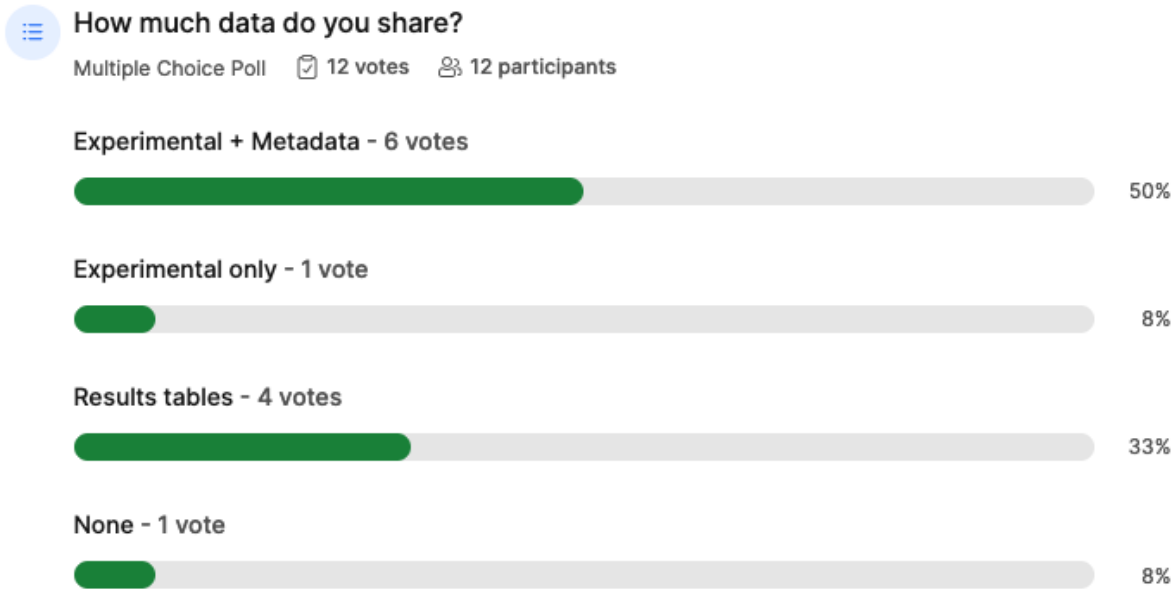
Meeting Overview

Meeting Title: FAIR Data Sharing Principles and Barriers: the New Data Management and Sharing (DMS) Policy

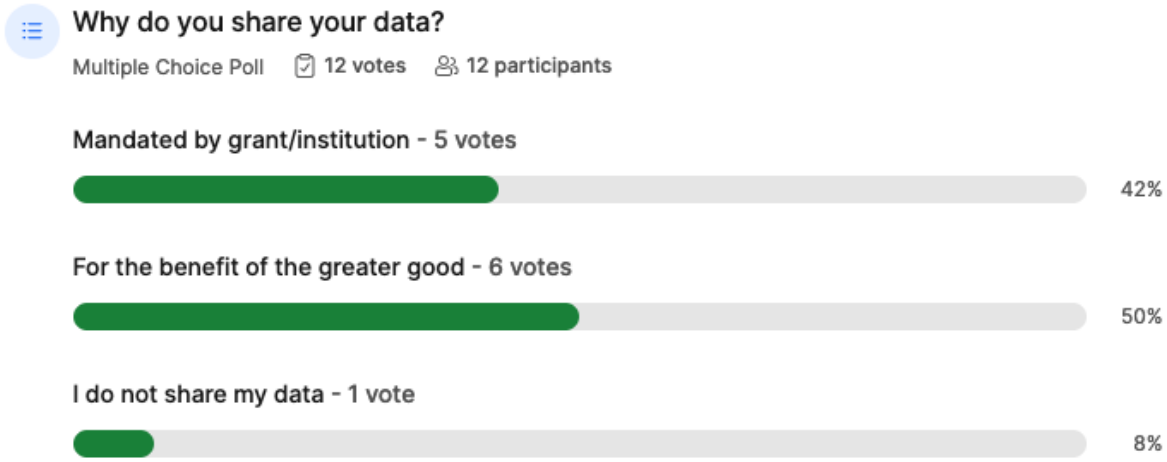
Meeting Theme

The overall goal of this workshop was to collect feedback from metabolomics practitioners on the new NIH Data Management and Sharing (DMS). We encouraged the attendees to share their experiences and barriers they face in sharing their data with an NIH representative. The attendees were polled at the start of the workshop on their current practices with respect to DMS. The poll questions were (insert screenshots):

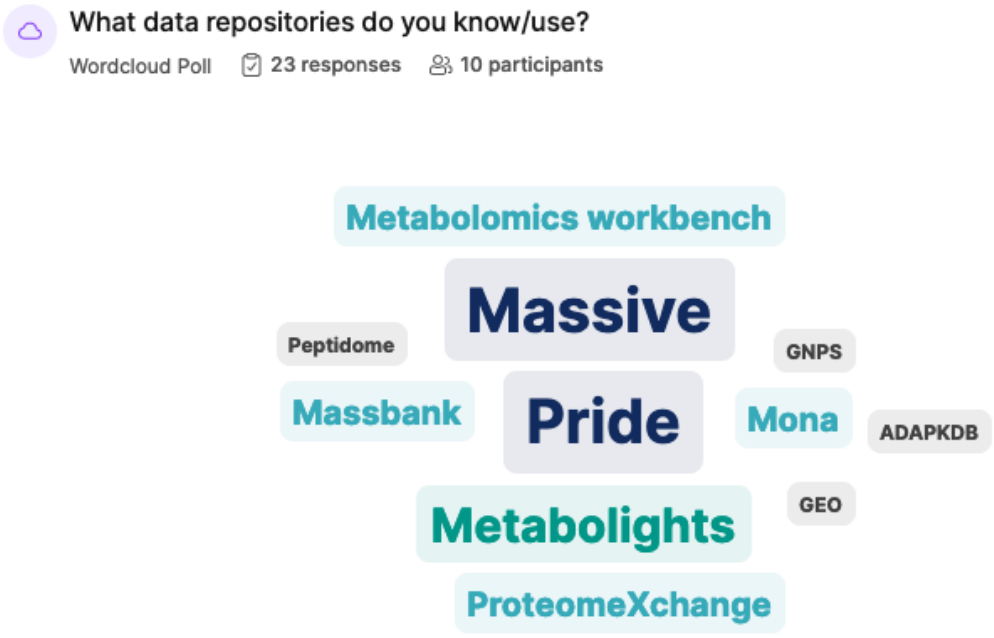
1. **Question 1:**



2. **Question 2:**



3. **Question 3:**



Dr. Keehwan Kwon, shared a few slides on DMS policy objectives and scope. The brief introduction included the plan for making experimental data generated using NIH funds to be Findable, Accessible, Interoperable, and Reproducible (FAIR). The attendees then were given the opportunity to drive the open discussion and share their concerns and experiences with DMS and data FAIRness with Dr. Kwon. The workshop organizers steered the discussions to gain more insight into the incentives and barriers that result in successful or failed attempts at data sharing by various labs – there was a particularly "spirited and healthy" debate regarding complying with DMS & FAIR within a research environment that is heavily dependent on vendor-specific data formats, i.e., LC/MS-based acquisition formats. This was done by proposing the following seed questions: the advantages and shortcomings of current data repositories, the necessary computing infrastructure to accommodate data sharing, deciding the proper amount of metadata to be shared with the raw data, the types of requirements that the industry (both

MS vendor and fee-for-service labs) should implement in their current workflows and software to accommodate DMS. These topics were discussed at length among the attendees and the discussion was free flowing.

Some key points brought up during the discussion include:

- Issues with how raw is raw data?
- Different versions of proprietary programs can result in different outcomes
- Why is the DMS plan not part of the grant review process?
- Does the NIH have long term plans for funding the Metabolomics Workbench?
- Contract Research Organization (CRO) issues with data sharing
- Need for working with the vendors more, better coordination with the open source community
- How should metadata be handled? People often do the bare minimum to get the submission to work