2024 ASMS Metabolomics Interest Group Workshop Report

Co-coordinators

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- Tytus Mak, PhD, NIST Mass Spectrometry Data Center

Timeslot

5:45 – 7:00 pm, Monday, June 3, 2024

Topic

LC-MS data processing software for untargeted metabolomics and exposomics: commercial and open-source solutions

Goals

The workshop aims to bring together both software developers for and users of software tools for mass spectrometry-based untargeted metabolomics and exposomics. It provides an interactive platform for both the developers and users to exchange ideas and address needs for software tools in the metabolomics and exposomics research and application community.

Attendance

Based on the survey responses, more than 170 people attended the workshop.

Agenda

- Introduction (3 min)
- Short introduction of software tools (30 min with 3.5 min each including 0.5 min changeover, no more than 5 slides)
    - Open source
        - MZmine — Ansgar Korf
        - MS-DIAL — Hiroshi Tsugawa
    - Commercial
        - Progenesis/MARS (Waters): — Roy Martin
        - Compound Discoverer (Thermo Fisher): — Ralf Tautenhahn
        - MassHunter (Agilent) — James Pyke
        - MetaboScape (Bruker) — Heiko Neuweger
        - SciexOS (Sciex) — Rebekah Sayers
- Survey at https://www.slido.com (15 min)
- Guided panel discussion and Q/A (25 min) — All presenters and participants

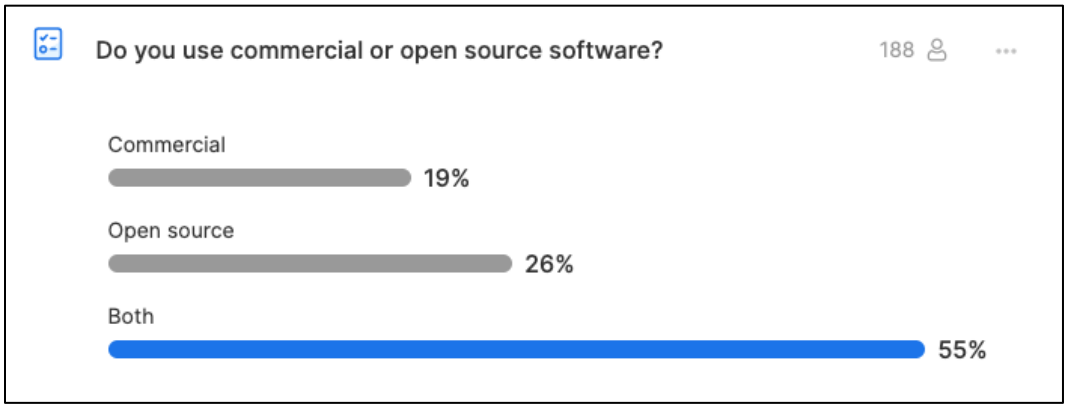
Survey

This survey is to obtain feedback from the workshop participants regarding their specific needs, including needs for new features and their user experiences of existing features of the software tools. A total of 7 questions were asked.

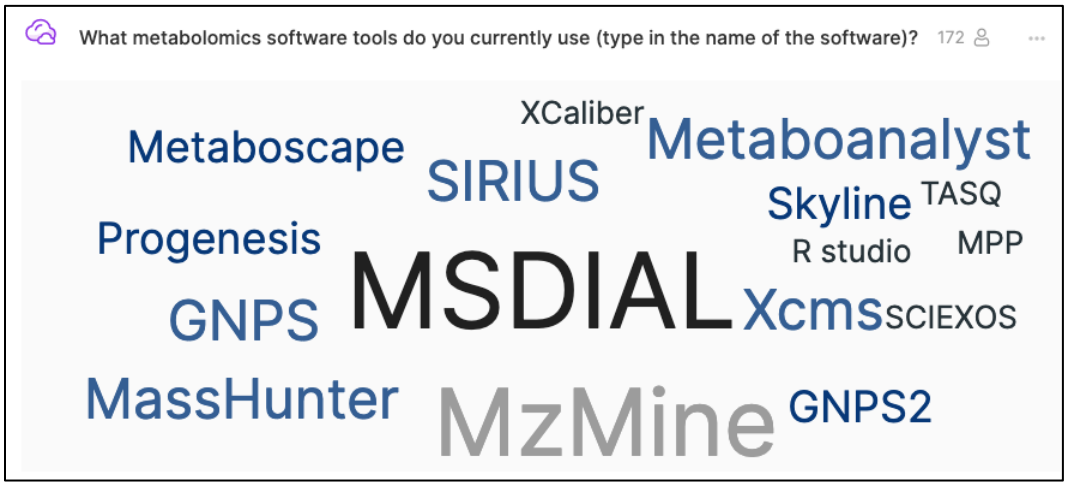
1. Do you use commercial or open-source software tools?
2. What metabolomics software tools do you currently use (type in the name of the software)?
3. How long have you been using your primary LC-MS data processing workflow?
4. What are the most important features you look for in data processing software? (Pick 3)
5. What are the significant challenges or limitations with your current software? (Pick 3)
6. What factors influence your choice between commercial and open-source LC-MS data processing software? (Select all that apply)
7. What new features would you like to see in metabolomics software tools in the future?

Survey Results

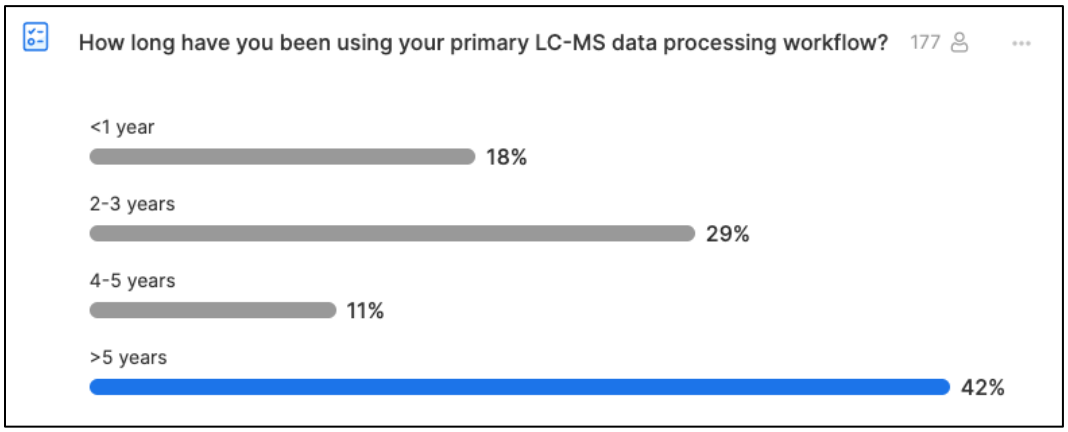
1. Question 1



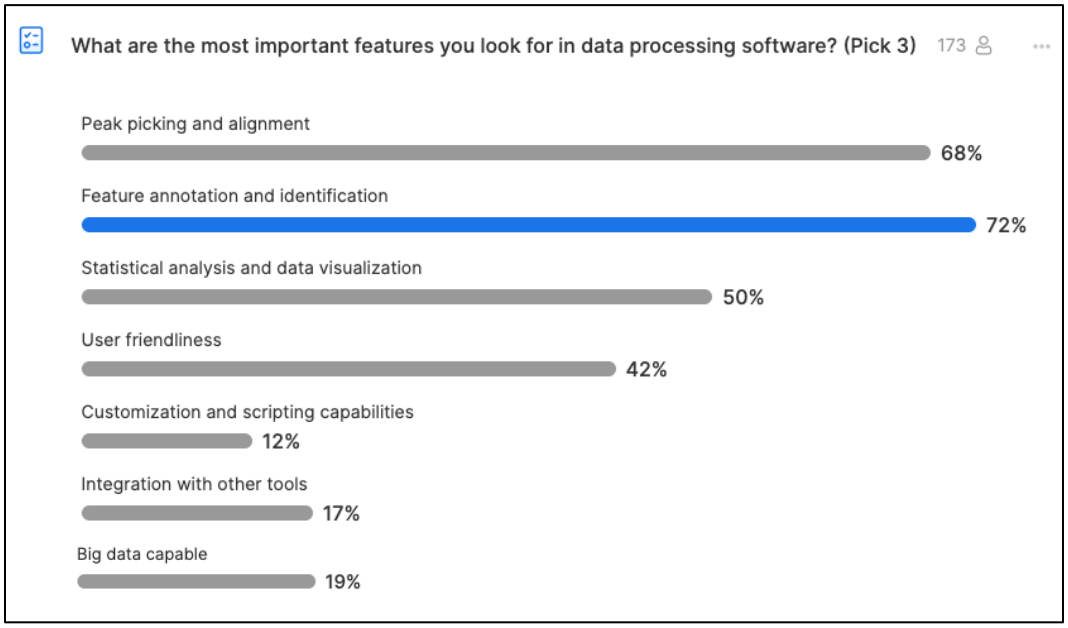
2. Question 2



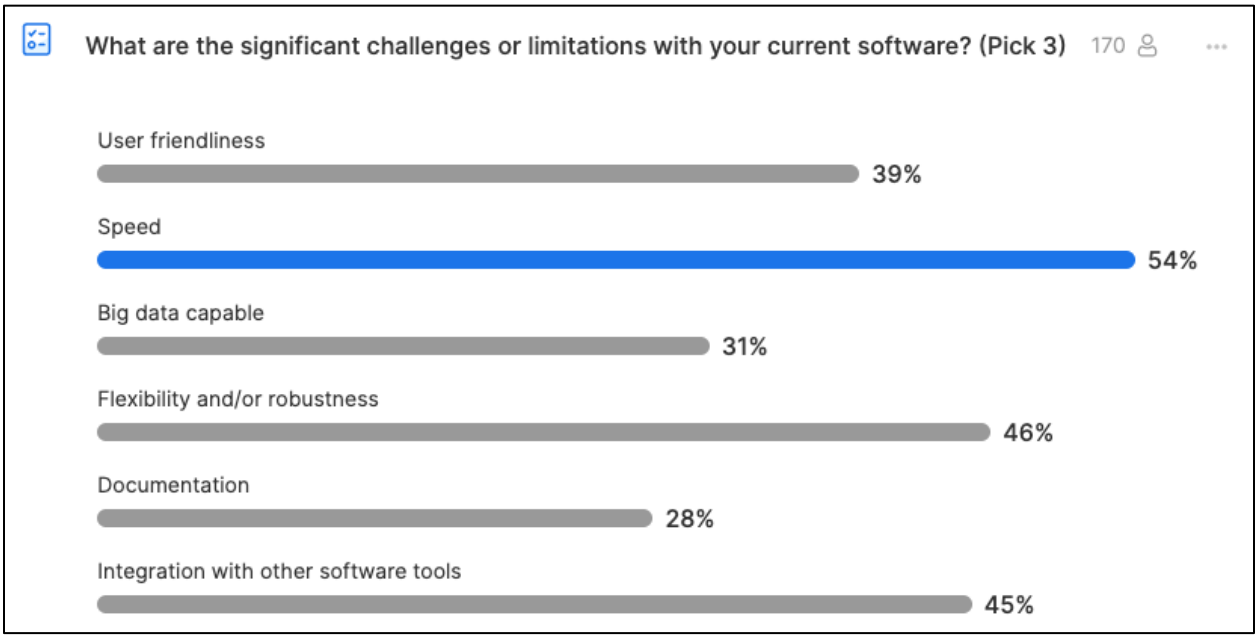
3. Question 3



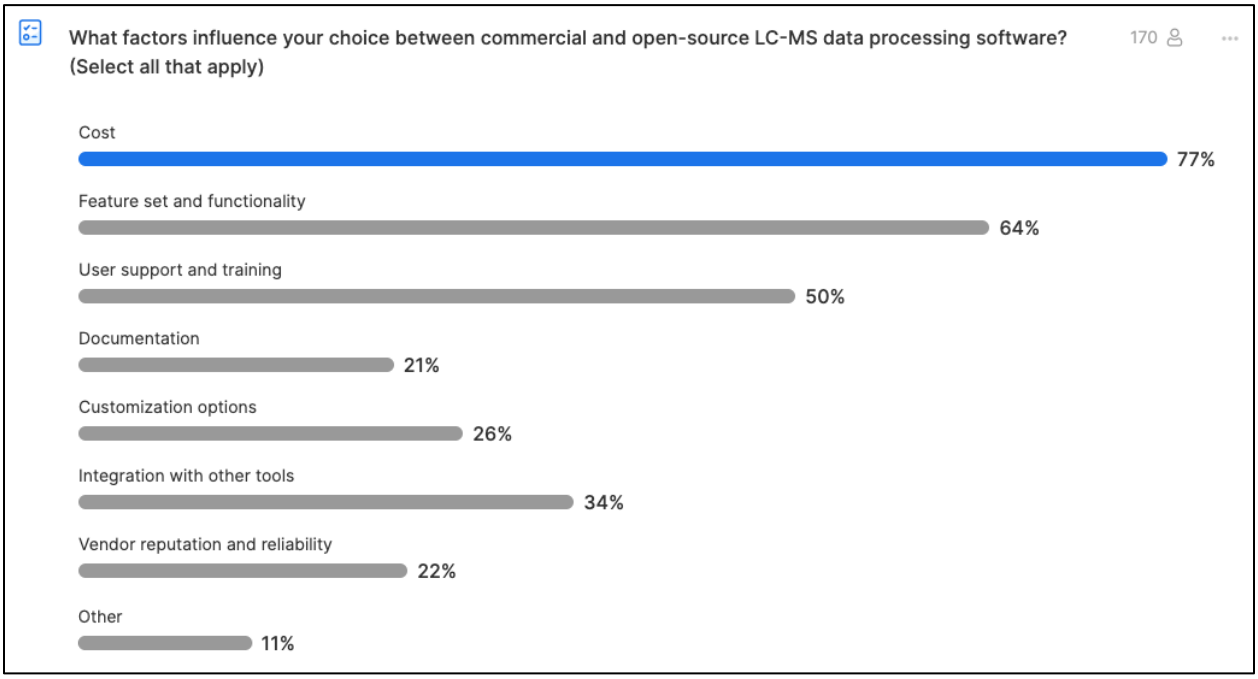
4. Question 4



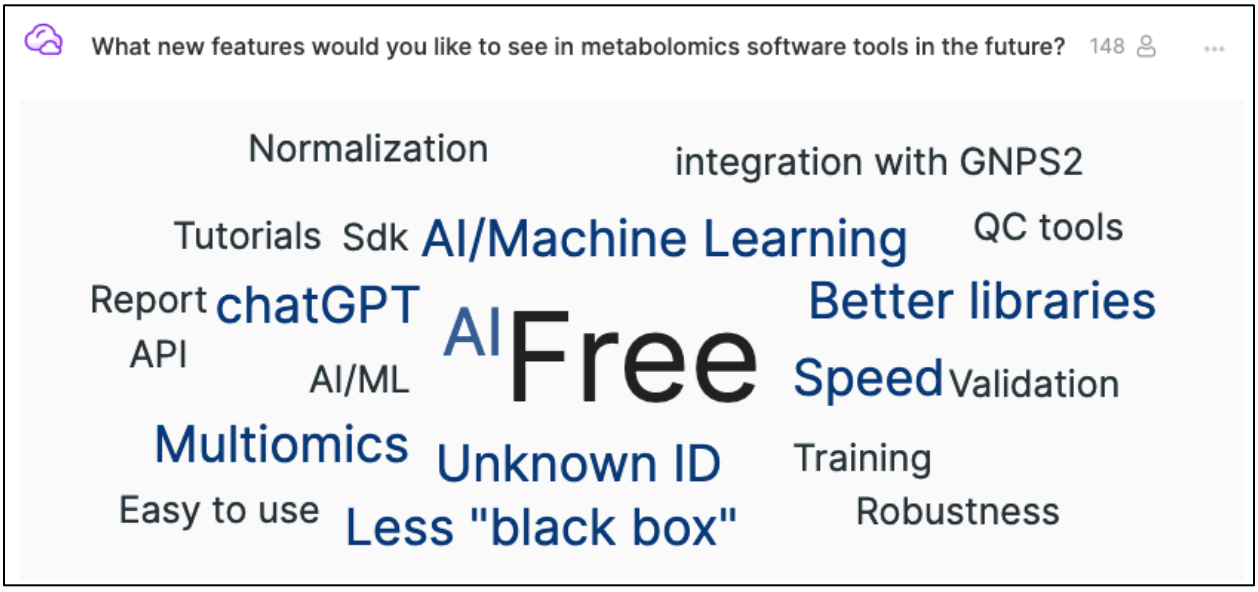
5. Question 5



6. Question 6



7. Question 7



Open Panel Discussion Questions and Topics

- **For the panel:** What are the biggest challenges you face in understanding the specific needs of researchers using your software for untargeted metabolomics and exposomics studies?
- **For the audience:** What are the most significant difficulties you encounter when trying to communicate your data processing needs and desired functionalities to software developers?
- **For the panel:** How can software developers contribute to improving data reproducibility and standardization in untargeted metabolomics and exposomics research?
- **For the audience:** What are your views on the importance of data format standardization and interoperability between different LC-MS data processing software platforms?

Photos From the Workshop


Active poll
Do you use commercial or open source software?
Join at
slido.com
#2352 294
21%
52%
27%
Both 52%
Open source 27%
Commercial 21%


4 participants typing
What metabolomics software tools do you currently use (type in the name of the software)?
Join at
slido.com
#2352 294
Wikipedia
Profinder
Omeka Flow
Shimadzu
SCIEXOS
Python
Proteowizard
Proprietary
SIRIUS
Genedata
Mass Hunter
SCILS Lab
Explorer
Trace finder
XCaliber
SCIEX
GNPS
MzMine
Metaboanalyst
compound discovery
TASQ
MS DIAL
Xcms(R)
ElMaven
Xcms
MSDIAL
Metaboscape
MPP
SCIEX OS
Xcalibur
Compound Discoverer
Spectrus processor
XCML
MSFINDER
Progenesis
MassHunter
Pubchem
GNPS2
LipidSearch
Fiuoromatch
Skyline
Pivotal wizard
Xmsannotator
compounddiscovery and
MarkerView
Xmsanalyzer
Rstudio


TECAN
healthcare