# Bioconductor Community Advisory Board (CAB) Agenda

Sept 11, 2025

1 pm GMT Apr – Oct '25 10 pm GMT Nov '25 – Mar '26

Members: Aedin, Enis, Hédia, Janani, Jasmine, Jiefei, Johannes, Kevin, Kozo, Leo, Lluís, Lori, Maria, Mengbo, Nicole, Oluwatobilola (Tobi), Stevie, Umar, Xueyi, Zahraa

Attending: Lori, Enis, Stevie, Tobi, Maria, Johannes, Aedin, Janani, Zahraa, Kevin, Hedia,

Leo

Regrets: Kozo

Guests:

Schedule

:00 - :5 Welcome + Review minutes from previous meeting for posting

<u>August Minutes</u>

### Sign up for discussion

Sign Up for CAB lead discussion

We need a volunteer for October, November and December

## :06-:35 CAB Led Discussion [Johannes]

#### Interoperability of software for mass spectrometry in Bioconductor and beyond

- A variety of software for metabolomics data analysis exists, some in R and Python, but also GUIs (e.g. MS-DIAL, mzmine, SIRIUS, ...).
- Goal: reduce re-implementations, simplify data/result exchange for a better "user experience".
- Events/efforts in 2025
  - <u>EuBIC-MS developer meeting</u>. Hackathon to facilitate R/Python integration -> SpectriPy package was revamped, and is not part of Bioconductor, published in <u>JOSS</u>. SpectriPy translates MS data structures between R and Python, allows combined R/Python MS data analyses (e.g. using Quarto). Integration of Bioconductor's packages around Spectra and Python's matchms and spectrum utils libraries.
  - o HUPO-PSI (Proteomics Standards Initiative) meeting: mzTab-M working group (led by Nils Hoffmann with Kozo, Steffen Neumann, Philippine Louail and myself also part of it). mzTab-M is a text-based file format to report metabolomics data analysis results. Agreed to rethink the file format to a) enable also storing/representing intermediate results and b) improve and standardize reporting of final annotation results. a: enable sharing of

- **intermediate results** between main metabolomics data preprocessing softwares MS-DIAL, mzmine, and Bioconductor's xcms.
- <u>ELIXIR Biohackathon</u>. mzTab-M / <u>proteomics and metabolomics file format interoperability</u>.
- Plans and outlook (from my perspective): get developers from the different software get together and collaborate to define and implement interoperability between their tools. Worked/works well between Python and R. Hope is that mzTab-M will also simplify integration with GUI-based tools.
- At the moment it's focused on developers any suggestions on how to involve the community (users) would be great.
- Maybe one option: develop workshops/tutorials explaining the integrative analyses?
   CAB feedback: workshops run at field-specific conference(s) to get the user community involved.
- Own experience with Python/R integration in R/Bioconductor: not too straight forward. Also, because reticulate now uses new system for package management.
   And BBS system was not working at the beginning.
- <a href="https://rformassspectrometry.github.io/Metabonaut/">https://rformassspectrometry.github.io/Metabonaut/</a> docker-based resource with tutorials. Would there be a cloud service available (from Bioconductor) to run/host that? ELIXIR?
- Maria: have a look at <a href="https://biocpy.github.io/tutorial/">https://biocpy.github.io/tutorial/</a> for Python users that want to use/get access to Bioconductor/R.
- Hedia: check <u>posit cloud</u> to run workflows (Free version: 1GB main memory limit; Instructor version: ~\$10/month).
- Enis: Galaxy has training resources, but not possible to host an instance (RStudio environments) year round.

#### :35-:45 CAB/TAB exchange:

## TAB -> CAB:

- Lost Azure support so currently have no windows builds. Looking into NIH funding to restore
- Invited Speaker on R coding assistant (ChatR)
- Governance: See Charter below. Would like it reviewed and encourage comments in the document

## CAB -> TAB:

Aedin and Maria suggested forwarding Windows requirements as they might be able to link with European cloud support

#### **Discussion of Drafted Charter**

### :46-:50 Bioconductor Licensing

- Vince has requested we discuss what license is applied to the logo.

- Does the section regarding licenses in <a href="https://contributions.bioconductor.org/license.html">https://contributions.bioconductor.org/license.html</a> need any update or clarification?
   Aedin: <a href="https://creativecommons.org/share-your-work/cclicenses/">https://creativecommons.org/share-your-work/cclicenses/</a>
- <a href="https://www.r-project.org/logo/">https://www.r-project.org/logo/</a> [Action @jo]: make PR to the Bioconductor page adding the text/license from the R-page.

## :50-:50 Kevin's package

Lluís found a maintainer for EnhancedVolcano

## :50-:60 CAB Elections [Stevie]

Voting closed. Open discussion on candidates and review of voting procedure