

# Australasian Computational Proteomics Community Meeting

Public document

## Zoom link

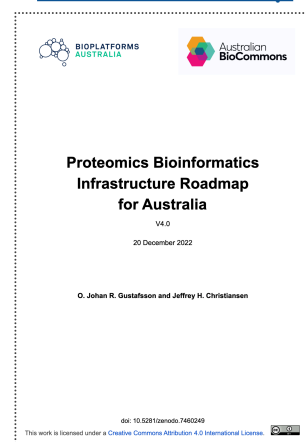
[Join the Google Group](#) to receive regular updates  
and automatic community meeting invitations.

### Why does this community meet?

This group meets so that members of the community can:

- [Hear from other researchers](#) about how they are approaching and leveraging computational proteomics
- [Learn more](#) about recent developments in bioinformatics that impact proteomics
- Share knowledge, make connections, and collaborate!
- [Contribute to discussions](#) that will inform how the BioCommons addresses bioinformatics challenges facing proteomics researchers
- [Ask](#) BioCommons anything!

### [Read the roadmap](#)



## Tuesday 30th of September 2025

11:00 am (AWST), 12:30 pm (ACST), 13:00 pm (AEST)

Chair: Johan Gustafsson (Australian BioCommons)

Minutes: Collectively recorded

## Zoom link

## In attendance

| Please add your name and affiliation here |                                |  |
|-------------------------------------------|--------------------------------|--|
| Johan Gustafsson, BioCommons              | Julia Broadbent, UoM           |  |
| Will Klare, APAF                          | Michela Mitchell, UoA and WCHN |  |
| Ignatius Pang, APAF                       | Yuheng Zhu, USYD               |  |
| Narjis Fatima, Kolling                    | Ben Crossett, USyd             |  |
| Angela Juhasz, ECU                        |                                |  |
| Yaan Kit Ng, UoM                          |                                |  |
| Dr Shivalaxmi Manchukonda                 |                                |  |

## Agenda + Minutes

| Item                                                       | Item / Description                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
|------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Welcome to meeting &amp; intros</b><br>Johan Gustafsson | An introduction to the <a href="#">Australian BioCommons</a><br>The <a href="#">Proteomics bioinformatics community</a>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| <b>Presentation</b>                                        | <p><b>“User friendly proteogenomics with GenomeProt”</b><br/>A/Prof Benjamin L Parker (University of Melbourne)</p> <ul style="list-style-type: none"><li>• Goal: to fully understand the regulatory processes converting genotypes to phenotypes</li><li>• Proteomics used to improve annotation of protein coding genes (Jaffe et al. 2004)</li><li>• Building patient specific databases of expressed ORFs</li><li>• You could use standard or extended databases (e.g. OpenProt), but these may contain isoforms that aren't actually expressed</li><li>• Several proteogenomics tools exist<ul style="list-style-type: none"><li>◦ Missing GUI</li><li>◦ Lack intuitive annotations required for downstream proteomics</li><li>◦ No built in visualisation</li></ul></li><li>• GenomeProt workflow</li><li>• Database generation -&gt; FASTA -&gt; proteomics analysis -&gt; integration</li><li>• Steps<ul style="list-style-type: none"><li>◦ Generate custom proteogenomic database based on RNAseq</li><li>◦ Download FASTA and metadata files<ul style="list-style-type: none"><li>■ GenomeProt will map all ORFs to UniProt, then OpenProt, and create detailed FASTA headers along with detailed metadata</li><li>■ Examples of potential ORFs detected with GenomeProt</li><li>■ Protein coding</li><li>■ lncRNA</li></ul></li><li>◦ Perform proteomics / database search and upload results to the viewer</li></ul></li></ul> |

- Testing
  - Mouse osteoblast cell line
  - Long read RNA-seq (nanopore)
  - GenomeProt database gen
  - Whole cell lysate -> multi-dimensional LC-MS/MS
  - Question: Impact of number of ORFs in the database?
    - #peptides and #proteins look similar, for all databases
    - As database gets larger, greater score cut off needed to achieve 1% FDR
    - Small database: more "sensitive", more proteins at lower scores but misses ORFs
    - Large database: less "sensitive", require higher scores, but gain in ORFs

### Questions

- If I have a whole genome sequencing data, can I create a library with only sequences (between two tryptic digestion points) that have been mutated? I would like to use this mutated library to detect genetic mutations using proteomic.
- 

### Community resources

- Join the [Slack group](#)
- GitHub organisation <https://github.com/Australian-Computational-Proteomics>
- Proteomics Learning Library Collection
  - Example [https://australianbiocommons.github.io/Community-Library/structural\\_biology](https://australianbiocommons.github.io/Community-Library/structural_biology)
  - You can add resources to [this spreadsheet](#)
- Inviting international experts in applications of AI to mass spectrometry
  -  AI in the life sciences - Dr Tine Claeys and Dr Veit Schwämmle
  - DONE, revisit for next year as well?

### Updates

- [Other BioCommons events](#), including webinars, workshops and community meetings
- ACF: <https://australasiancorefacilities.org/>
- WEBINAR SERIES: AI in the life sciences: Exploring possibilities, inspiring change  
<https://www.biocommons.org.au/events/ai-series-2025>
  -  AI in the life sciences - Dr Tine Claeys and Dr Veit Schwämmle
- WEBINAR SERIES: Leveraging deep learning to design custom protein-binding proteins  
<https://www.biocommons.org.au/events/protein-binder-series>
- APAF is currently hiring for a six-months fixed-term full-time bioinformatics role starting in January 2026. Please find the hyperlink to apply here:  
Closing date of Wednesday 22<sup>nd</sup> of October at 11:59pm (AEST).

|                              |                                                                            |
|------------------------------|----------------------------------------------------------------------------|
| Macquarie Careers (internal) | <a href="#">View Job Posting Details - Workday</a>                         |
| Macquarie Careers (external) | <a href="#">Careers at Macquarie</a>                                       |
| Seek                         | <a href="#">Analytical Technician Job in North Ryde, Sydney NSW - SEEK</a> |

|                                                                                                                                             |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
|---------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <div> <div>LinkedIn</div> <div> <a href="#">(24) Analytical Technician - Bioinformatics   Macquarie University   LinkedIn</a> </div> </div> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| <p><b>Add your item(s) for discussion here</b></p> <p>Anyone can add an item here!</p>                                                      | <ul style="list-style-type: none"> <li>Reminder: Bioinformatics Forum after this meeting             <ul style="list-style-type: none"> <li>Immediately after the meeting ( 2 pm AEST) , the community will be able to virtually join a Bioinformatics Forum where A/Prof Matt Padula will talk about the <i>"challenges of proteome and proteoform analysis, discuss the short-comings of current methodologies, and attempt to propose potential solutions"</i>. <a href="#">Zoom link</a></li> </ul> </li> </ul> |
| <p>The next meeting is in 2026!</p>                                                                                                         |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |

## Tuesday 22nd of July 2025 - cancelled

11:00 am (AWST), 12:30 pm (ACST), 13:00 pm (AEST)

Chair: Johan Gustafsson (Australian BioCommons)

Minutes: Collectively recorded

### In attendance

| Please add your name and affiliation here |  |  |
|-------------------------------------------|--|--|
| Johan Gustafsson, BioCommons              |  |  |

### Agenda + Minutes

| Item                                                                  | Item / Description                                                                                                                                                                                                                                                                                                                                        |
|-----------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <p><b>Welcome to meeting &amp; intros</b></p> <p>Johan Gustafsson</p> | <p>An introduction to the <a href="#">Australian BioCommons</a></p> <p>The <a href="#">Proteomics bioinformatics community</a></p> <p>Community leadership and invitation to join the effort 😊</p> <p>Contact Johan if you would like to be involved in these discussions</p> <p><a href="mailto:johan@biocommons.org.au">johan@biocommons.org.au</a></p> |
| <p><b>AusOMICS debrief</b></p>                                        | <p><b>"AusOMICS debrief"</b></p> <p>Group discussion and round table, facilitated by Johan</p>                                                                                                                                                                                                                                                            |

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|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | <ul style="list-style-type: none"> <li>• Key takeaways</li> <li>• New developments?</li> <li>• Challenges raised?</li> </ul> <p>Questions</p> <ul style="list-style-type: none"> <li>•</li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| <p><b>Community resources &amp; Open discussion</b></p> <ul style="list-style-type: none"> <li>• Join the <a href="#">new Slack group</a></li> <li>• GitHub organisation <a href="https://github.com/Australian-Computational-Proteomics">https://github.com/Australian-Computational-Proteomics</a></li> <li>• Proteomics Learning Library Collection <ul style="list-style-type: none"> <li>◦ Example <a href="https://australianbiocommons.github.io/Learning-Library/structural_biology">https://australianbiocommons.github.io/Learning-Library/structural_biology</a></li> <li>◦ You can add resources to <a href="#">this spreadsheet</a></li> </ul> </li> <li>• Inviting international experts in applications of AI to mass spectrometry - <b>in progress</b></li> </ul> <p><b>Community feedback</b></p> <ul style="list-style-type: none"> <li>• Resources required, and other challenges?</li> <li>•</li> </ul> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| <p><b>Updates</b></p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | <ul style="list-style-type: none"> <li>• <a href="#">Other BioCommons events</a>, including webinars, workshops and community meetings</li> <li>• ACF: <a href="https://australasiancorefacilities.org/">https://australasiancorefacilities.org/</a></li> <li>• WEBINAR SERIES: AI in the life sciences: Exploring possibilities, inspiring change <a href="https://www.biocommons.org.au/events/ai-series-2025">https://www.biocommons.org.au/events/ai-series-2025</a></li> <li>• WEBINAR SERIES: Leveraging deep learning to design custom protein-binding proteins <a href="https://www.biocommons.org.au/events/protein-binder-series">https://www.biocommons.org.au/events/protein-binder-series</a></li> <li>• New roadmap <ul style="list-style-type: none"> <li>◦ Michie, K. A., Litfin, T., Beecroft, S. J., Collins, B., Czabotar, P., Downton, M., Doyle, M. T., Ghosal, D., Grinter, R., Knott, G. J., Samaha, G., Christiansen, J. H., &amp; Gustafsson, O. J. R. (2025). Australian Structural Biology Deep-Learning Infrastructure Roadmap. Zenodo. <a href="https://doi.org/10.5281/zenodo.15786982">https://doi.org/10.5281/zenodo.15786982</a></li> </ul> </li> <li>•</li> </ul> |
| <p><b>Add your item(s) for discussion here</b><br/>Anyone can add an item here!</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | <ul style="list-style-type: none"> <li>• Sanders, J., Wen, B., Rudnick, P.A. et al. A transformer model for de novo sequencing of data-independent acquisition mass spectrometry data. Nat Methods (2025). <a href="https://doi.org/10.1038/s41592-025-02718-y">https://doi.org/10.1038/s41592-025-02718-y</a></li> <li>•</li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| <p><b>Next meeting is on 30th September 2025</b></p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |

## Tuesday 13th of May 2025

11:00 am (AWST), 12:30 pm (ACST), 13:00 pm (AEST)

### Zoom link

**Chair:** Johan Gustafsson (Australian BioCommons)

**Minutes:** Collectively recorded

### In attendance

| Please add your name and affiliation here |                            |  |
|-------------------------------------------|----------------------------|--|
| Johan Gustafsson, BioCommons              | Desmond Li, SydneyMS, USYD |  |
|                                           | Keiran Rowell, UNSW        |  |
| Nikeisha Caruana, Unimelb                 | Julia Broadbent, Unimelb   |  |
| Rob Goode, CSIRO                          | Joel Steele, MPMP - Monash |  |
| Caitlin Finney, Westmead Institute        | Ignatius Pang, APAF        |  |
| Artur Shvetcov, Westmead Institute        | Will Klare, APAF           |  |
| Kristina Gagalova, Curtin University      |                            |  |
| Mailie Gall, Standardbiotools             |                            |  |
|                                           |                            |  |

### Agenda + Minutes

| Item                                                       | Item / Description                                                                                                                                                                                                                                                                                                                     |
|------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Welcome to meeting &amp; intros</b><br>Johan Gustafsson | An introduction to the <a href="#">Australian BioCommons</a><br>The <a href="#">Proteomics bioinformatics community</a><br><br>Community leadership and invitation to join the effort 😊<br>Contact Johan if you would like to be involved in these discussions<br><a href="mailto:johan@biocommons.org.au">johan@biocommons.org.au</a> |
| <b>Presentation</b>                                        | “Proteomics with explainable machine learning: a pathway to experimental and clinical                                                                                                                                                                                                                                                  |

|                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
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|                            | <p><b>translation”</b><br/> Dr. Artur Shvetcov (Translational Dementia Research Group, Westmead Institute for Medical Research)</p> <ul style="list-style-type: none"> <li>• CSF proteome of APOE4 carriers with and without impairment</li> <li>• Alzheimer”s Disease Neuroimaging Initiative (ADNI) dataset</li> <li>• <a href="https://adni.loni.usc.edu/">https://adni.loni.usc.edu/</a></li> <li>• See publication: <i>Proteome profiling of cerebrospinal fluid using machine learning shows a unique protein signature associated with APOE4 genotype</i><br/> <a href="https://doi.org/10.1111/ace.14439">https://doi.org/10.1111/ace.14439</a></li> <li>• GNPC <a href="https://www.neuroproteome.org/">https://www.neuroproteome.org/</a></li> </ul> <p><b>Questions</b></p> <ul style="list-style-type: none"> <li>• Does the plasma proteome give an indication of what effects or pathways are upregulated in the brain? <ul style="list-style-type: none"> <li>◦ Just showing main points from the study</li> <li>◦ Didn’t show enrichments, which was significant work</li> <li>◦ Did find connections / similarities between plasma and CSF</li> </ul> </li> <li>• Advice for others that would like to apply ML methods? <ul style="list-style-type: none"> <li>◦ Keep it simple</li> <li>◦ Focus on the question, then pick the method</li> <li>◦ Also focus on the end user? Is it biomarker development? Is it for clinical diagnostics? Something else?</li> </ul> </li> </ul>                                                                                                                                                                         |
| <p><b>Presentation</b></p> | <p><b>“Proteomics and Machine Learning–Based Approach to Decipher Subcellular Proteome of Mouse Heart”</b><br/> Dr. David Greening (Baker Heart and Diabetes Institute)</p> <ul style="list-style-type: none"> <li>• Publication: <a href="https://www.mcponline.org/article/S1535-9476(25)00050-7/fulltext">https://www.mcponline.org/article/S1535-9476(25)00050-7/fulltext</a> <ul style="list-style-type: none"> <li>◦ DOI <a href="https://doi.org/10.1016/j.mcpro.2025.100952">https://doi.org/10.1016/j.mcpro.2025.100952</a></li> </ul> </li> <li>• Multiomics to illuminate EC vesicle biology</li> <li>• Look at abundance and ultrasmall amounts</li> <li>• Apply ML and other algorithms to understand complex biology in more detail</li> <li>• Heart <ul style="list-style-type: none"> <li>◦ Regional -&gt; Cellular -&gt; Subcellular</li> <li>◦ Covering limited profiling through to comprehensive mapping</li> <li>◦ Molecular spatial composition of heart is missing</li> </ul> </li> <li>• 450 markers associated with 16 subcellular niches</li> <li>• How can this map be improved?</li> <li>• Evaluated support vector machine (SVM), random forest (RF), extreme gradient boosting (XGB) <ul style="list-style-type: none"> <li>◦ SVM: high dimensional space, memory efficient</li> <li>◦ RF: high accuracy, less overfitting, handles missing data, effective with a wide range of features</li> <li>◦ XGB: high performance, flexible, handling missing values, limits overfitting</li> </ul> </li> <li>• Choice of method depends on data and task</li> <li>• Model evaluation metrics -&gt; accuracy, precision, recall, F1-score</li> </ul> |

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
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|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | <ul style="list-style-type: none"> <li>• Always ask: why are you using a model? What is it you are actually trying to do?</li> <li>• Selected SVM and RF for the study</li> </ul> <p><b>Questions</b></p> <ul style="list-style-type: none"> <li>• Features? Proteins and their localisation</li> <li>• Number of n's? <ul style="list-style-type: none"> <li>◦ 6 hearts for dev of fractionation</li> <li>◦ Replicates across 2 broad groups (6 and 6)</li> <li>◦ Validation in independent hearts using targeted experimental approaches</li> <li>◦ Total is 24</li> <li>◦ Age matched male mice</li> <li>◦ No injury, no perturbation</li> <li>◦ Applying to multiple other groups now</li> </ul> </li> </ul> |
| <p><b>Community resources &amp; Open discussion</b></p> <ul style="list-style-type: none"> <li>• Join the <a href="#">new Slack group</a></li> <li>• GitHub organisation <a href="https://github.com/Australian-Computational-Proteomics">https://github.com/Australian-Computational-Proteomics</a></li> <li>• Proteomics Learning Library Collection <ul style="list-style-type: none"> <li>◦ Example <a href="https://australianbiocommons.github.io/Learning-Library/structural_biology">https://australianbiocommons.github.io/Learning-Library/structural_biology</a></li> <li>◦ You can add resources to <a href="#">this spreadsheet</a></li> </ul> </li> <li>• Inviting international experts in applications of AI to mass spectrometry - in progress</li> </ul> <p><b>Community feedback</b></p> <ul style="list-style-type: none"> <li>• Resources required, and other challenges?</li> <li>• To be discussed in detail at AusOMICS as well</li> </ul> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| Updates                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | <ul style="list-style-type: none"> <li>• <a href="#">Galaxy Training Academy 2025</a> - happening this week!</li> <li>• <a href="#">Other BioCommons events</a>, including webinars, workshops and community meetings <ul style="list-style-type: none"> <li>◦ <a href="#">CO-WORKING: Sharing your bioinformatics workflows to make them findable and citable</a></li> </ul> </li> <li>• AusOMICS 2025: <a href="https://www.ausomics.com/">https://www.ausomics.com/</a></li> <li>• ACF: <a href="https://australasiancorefacilities.org/">https://australasiancorefacilities.org/</a></li> <li>• </li> </ul>                                                                                                  |
| Add your item(s) for discussion here<br>Anyone can add an item here!                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <ul style="list-style-type: none"> <li>• </li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| Next meeting is on 22nd July 2025                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |



## Tuesday 4th of March 2025

10:00 am (AWST), 12:00 pm (AEST), 12:30 pm (ACST), 13:00 pm (AEDT)

### Zoom link

**Chair:** Johan Gustafsson (Australian BioCommons)

**Minutes:** Collectively recorded

### In attendance

| Please add your name and affiliation here                                      |                                                          |                            |
|--------------------------------------------------------------------------------|----------------------------------------------------------|----------------------------|
| Johan Gustafsson, BioCommons                                                   | Clifford Young, UniSA                                    | Abarna Murugan, APAF       |
| William Klare, APAF                                                            | Muhammad (Maz) ALI, VCCRI, UNSW                          | Desmond Li, SydneyMS, USYD |
| Mahya Bahmani, CSIRO                                                           | Tiff Nelson, Australian BioCommons                       | Laura Dagley, WEHI         |
| Ignatius Pang, APAF                                                            | Muhammad Zenaidee, APAF                                  | Jumana Yousef, WEHI        |
| Yunqi Wu, APAF                                                                 | Jeff CHristiansen, BioCommons                            |                            |
| Rob Goode, CSIRO                                                               | Ruth Wang, APAF                                          |                            |
| Prashanth Gouda, UWA(Student)                                                  | Michela Mitchell, WCHN                                   |                            |
| Kristina Gagalova, Curtin University                                           | Hossein V Kahrood, Monash Proteomics                     |                            |
| Nikeisha Caruana, Unimelb                                                      | Ben Goudey, BioCommons                                   |                            |
| Nicholas DeBono (Institute for Biomedicine and Glycomics, Griffith University) | Joel Steele, Monash Proteomics and Metabolomics Platform |                            |
|                                                                                |                                                          |                            |

### Agenda + Minutes

| Item                                                       | Item / Description                                                                                                                                                                      |
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| <b>Welcome to meeting &amp; intros</b><br>Johan Gustafsson | An introduction to the <a href="#">Australian BioCommons</a><br>The <a href="#">Proteomics bioinformatics community</a><br><br>Community leadership and invitation to join the effort 😊 |

## Presentation

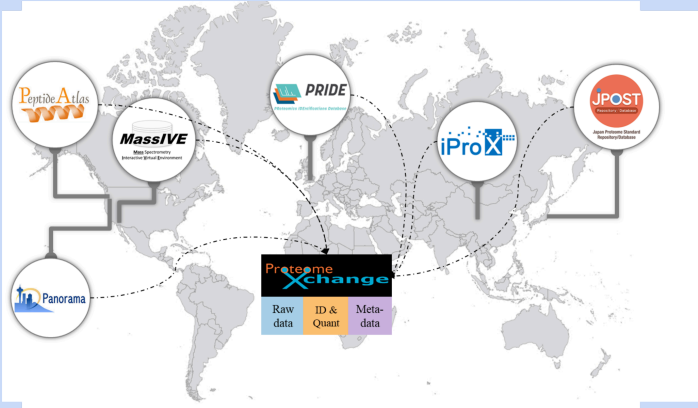
### “From APAF to CSIRO, life as a proteomics enjoyer in an epigenetics group”

Dr Dana Pascovici, CSIRO, Macquarie University

- Group: Cell and Molecular Health
- Proteomics @ CSIRO
  - MS capability in proteomics / metabolomics (Canberra, Brisbane, Melbourne)
  - Leverage internal expertise + connections to external Astral, Olink, Somascan etc.
- Multiomics - why?
  - Samples can be precious
  - De-risk by having alternatives
  - Proteomics looks good / moves quickly - ‘golden age of plasma proteomics’
  - Boosting sensitivity of methylation assays with proteins?
- Case studies presented
  - Oesophageal cancer multiomics - tissue and plasma cross-facility work (Monash, ProCan, AGRF)
  - Detection of disease in plasma
  - Saliva Alzheimer’s diagnostics <https://doi.org/10.1002/alz.14420>
- Multiomics - how?
  - Still working on that one
  - Analysis side
    - Combining (i.e. mixOmics)
    - Side-by-side (e.g. WGCNA)
    - Data reduction and ML
    - 2 omics is more than twice as difficult as 1
  - Translation side
    - Validation / assay dev is expensive
    - Multiple techs in clinic is expensive
    - Makes sense to combine tech (e.g. proteomics, metabolomics)
- ML
  - SWATH opened door to ML for low level analysis (library gen, protein ID)
  - Diagnostics panels
    - Traditional ML (LASSO, elastic net, boosted trees, SVM) in variable selection / biomarker ranking
  - Multiple cohorts, filtering / normalisation, variable selection, small panels + model dev
- BioCommons have a multi-omics community group, you can join this group here: <https://groups.google.com/a/biocommons.org.au/g/multi-omics>
  - We meet quarterly with our next meeting scheduled for Wednesday, 19th March, 13:00 - 14:30 AEDT, [see in your timezone](#), [add to google calendar](#), [add to calendar via .ics file](#). Join the google group to be invited.
  - Our recent meeting saw a presentation from Dr Ignatius Pang (also here at this meeting!) covering *Integrative multi-omics analysis for exploring rare disease mechanisms and biomarker discovery: a case study with Rett Syndrome*. You can [watch the recording here](#).

### Questions

- Are we able to work as a group to define the term Multi-Omics? May be able to publish an opinion/definition article on this.
  - More than one omics?
  - Less about the omics, and more about the question? What are you hoping to get from a multiomics approach?
- Step change for proteomics as a result of ML / DL?
  - Might still be coming, not here yet
  - Can invite others working in this space as well to get their perspective
  - Maybe someone from ProCan?

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|                       | <p><b>Community resources &amp; Open discussion</b></p> <ul style="list-style-type: none"> <li>• Join the <a href="#">new Slack group</a></li> <li>• GitHub organisation <a href="https://github.com/Australian-Computational-Proteomics">https://github.com/Australian-Computational-Proteomics</a></li> <li>• Proteomics Learning Library Collection <ul style="list-style-type: none"> <li>◦ Example <a href="https://australianbiocommons.github.io/Learning-Library/structural_biology">https://australianbiocommons.github.io/Learning-Library/structural_biology</a></li> <li>◦ You can add resources to <a href="#">this spreadsheet</a></li> </ul> </li> <li>• Databases <ul style="list-style-type: none"> <li>◦ Standardisation?</li> <li>◦ ProteomicsDB (<a href="https://www.proteomicsdb.org/about">https://www.proteomicsdb.org/about</a>)</li> <li>◦ PRIDE (<a href="https://www.ebi.ac.uk/pride/">https://www.ebi.ac.uk/pride/</a>)</li> <li>◦ ProteomeXchange (<a href="https://proteomecentral.proteomexchange.org/">https://proteomecentral.proteomexchange.org/</a>)</li> <li>◦ MassIVE (<a href="https://massive.ucsd.edu/ProteoSAFe/static/massive.jsp">https://massive.ucsd.edu/ProteoSAFe/static/massive.jsp</a>)</li> <li>◦ PanoramaWeb ( <a href="https://panoramaweb.org/home/project-begin.view?">https://panoramaweb.org/home/project-begin.view?</a>)</li> <li>◦ Chorus ( <a href="https://chorusproject.org/pages/index.html">https://chorusproject.org/pages/index.html</a>)</li> <li>◦ JPostDb (<a href="https://repository.jpostdb.org/entry/JPST002257">https://repository.jpostdb.org/entry/JPST002257</a>)</li> <li>◦ <a href="https://gen3.org/">https://gen3.org/</a></li> <li>◦ MediaFlux</li> </ul> </li> </ul>  |
|                       | <p><b>Community feedback</b></p> <ul style="list-style-type: none"> <li>• <a href="#">2022 Roadmap</a> and <a href="#">2024 forum report</a></li> <li>• 📅 2025-03-04 Revisiting proteomics roadmaps</li> <li>• Resources required, and other challenges?</li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| <p><b>Updates</b></p> | <ul style="list-style-type: none"> <li>• <a href="#">Other BioCommons events</a>, including webinars, workshops and community meetings</li> <li>• AusOMICS 2025: <a href="https://www.ausomics.com/">https://www.ausomics.com/</a></li> <li>• ACF: <a href="https://australasiancorefacilities.org/">https://australasiancorefacilities.org/</a></li> <li>• AusOmics Workshops (including multi-omics R workshop), in-person booking full, online places still available: <a href="https://www.ausomics.com/pre-conference-workshops">https://www.ausomics.com/pre-conference-workshops</a></li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |

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|-----------------------------------------------------------------------------|-------------------------------------------------------------------------|
|                                                                             | <ul style="list-style-type: none"> <li>Next meeting 13th May</li> </ul> |
| <b>Add your item(s) for discussion here</b><br>Anyone can add an item here! | <ul style="list-style-type: none"> <li></li> </ul>                      |
| Next meeting is on 13th May 2025                                            |                                                                         |

## Monday 2nd of December 2024

10:30 am (AWST), 11:30 pm (AEST), 12:00 pm (ACST), 12:30 pm (AEDT)

### [Zoom link](#)

**Chair:** Johan Gustafsson (Australian BioCommons)

**Minutes:** Collectively recorded

### In attendance

| Please add your name and affiliation here       |                                                  |  |
|-------------------------------------------------|--------------------------------------------------|--|
| Johan Gustafsson, BioCommons                    | Tiff Nelson, Australian BioCommons               |  |
| Ziad Al Bkhetan, BioCommons                     | Giorgia Mori, Australian BioCommons              |  |
| Matt Padula, UTS.                               | Keiran Rowell, Structural Biology Facility, UNSW |  |
| Will Klare, APAF, MQ                            | Georgie Samaha, SIH, USyd                        |  |
| Nikeisha Caruana, Unimelb                       |                                                  |  |
| Michela Mitchell, Womens and Childrens Hospital |                                                  |  |
| Muhammad Zenaidee, APAF, MQ                     |                                                  |  |
| Joel Steele, Monash, MPMP                       | Monash Proteomics and Metabolomics Platform      |  |
| Stephanie Town, UTS                             |                                                  |  |

### Agenda + Minutes

| Item | Item / Description |
|------|--------------------|
|------|--------------------|

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| <p><b>Welcome to meeting &amp; intros</b><br/>Johan Gustafsson</p> | <p>An introduction to the <a href="#">Australian BioCommons Proteomics bioinformatics community</a></p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| <p><b>Presentation</b></p>                                         | <p><b>“Folding entire proteomes - get a molecular inventory of your organism”</b><br/>Dr. Keiran Rowell, Structural Biology Facility UNSW</p> <ul style="list-style-type: none"> <li>• Alphafold2</li> <li>• Using the tools, not necessarily how they work</li> <li>• Novel organism -&gt; sequencing -&gt; folding / prediction</li> <li>• Models in chemical biology - function follows chemical form</li> <li>• Calculated structures are increasing and are now predominant in databases (i.e. PDB)</li> <li>• The “XFold” programs (not just AlphaFold) <ul style="list-style-type: none"> <li>◦ Does not include physics</li> <li>◦ Co-evolutionary correlations (i.e. residues that mutate together are likely closely associated structurally)</li> </ul> </li> <li>• Evoformers: AlphaFold, OpenFold, RoseTTAfold, AbFold, and others!</li> <li>• Protein-LMs: ESMFold, ProtTrans</li> <li>• Structural alignment: FoldSeek, Foldmason</li> <li>• Need GPUs to run this software / code <ul style="list-style-type: none"> <li>◦ NVIDIA and AMD</li> </ul> </li> <li>• Folding proteomes <ul style="list-style-type: none"> <li>◦ N = 613 proteins -&gt; 8 hours using ESMFold on GPU (22 days using AlphaFold)</li> <li>◦ N = 4622 proteins -&gt; 10 days using ESMFold on GPU (estimate of 2 years using AlphaFold)</li> </ul> </li> <li>• Different entry points for folding: <ul style="list-style-type: none"> <li>◦ Australian AlphaFold service <a href="https://www.biocommons.org.au/alphafold">https://www.biocommons.org.au/alphafold</a></li> <li>◦ At UNSW: dev / using nf-core proteinfold workflow: <a href="https://nf-co.re/proteinfold/1.0.0/">https://nf-co.re/proteinfold/1.0.0/</a></li> <li>◦ Open On Demand (OOD) for proteinfold workflow</li> </ul> </li> <li>• ESMFold <ul style="list-style-type: none"> <li>◦ Use website (<a href="https://esmatlas.com/resources?action=fold">esmatlas.com/resources?action=fold</a>)</li> <li>◦ Command line</li> <li>◦ Install on GPU server</li> </ul> </li> <li>• Folding a proteome <ul style="list-style-type: none"> <li>◦ 4378 proteins (&lt; 900 residues)) using ESMFold (10.5 hours)</li> <li>◦ 160 proteins (900-3000 residues)) using AlphaFold 2.3 (10.5 hours)</li> <li>◦ 6 proteins (3000 + residues) using AlphaFold 3 (pretty quick!)</li> </ul> </li> <li>• What then? <ul style="list-style-type: none"> <li>◦ Structures in PDB -&gt; go to <a href="https://search.foldseek.com">search.foldseek.com</a></li> <li>◦ Pull up homologues</li> <li>◦ What functions do these proteins have, based on other databases?</li> <li>◦ Compare with MS, including cross-linking efforts <ul style="list-style-type: none"> <li>■ Bartolec et al. 2023 <i>BioChemistry</i> Cross-linking mass spectrometry discovers, evaluates, and corroborates structures and protein-protein interactions in the human cell <a href="https://doi.org/10.1073/pnas.2219418120">https://doi.org/10.1073/pnas.2219418120</a></li> </ul> </li> </ul> </li> <li>• Community effort: <a href="https://australian-structural-biology-computing.github.io/website/">https://australian-structural-biology-computing.github.io/website/</a> <ul style="list-style-type: none"> <li>◦ Including How-to Guides and links to other resources</li> <li>◦ Also: <ul style="list-style-type: none"> <li>■ VSC-AlphaFold community (Belgium)</li> <li>■ SciLifeLab, Berzelius cluster (Sweden)</li> <li>■ Stanford University (US)</li> </ul> </li> </ul> </li> </ul> |

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|                                                                     | <p><b>Questions</b></p> <ul style="list-style-type: none"> <li>• How do you see this scaling in future? Given areas like proteo-genomics and the thousands of organisms being sequenced</li> <li>• How do you determine if the structures are bioactive? Possible? <ul style="list-style-type: none"> <li>◦ Depends on the structure</li> <li>◦ Annotations tell you what it's related to</li> <li>◦ Will often be a variant of an existing protein</li> </ul> </li> <li>• Full tertiary structures with AlphaFold? Yes! <ul style="list-style-type: none"> <li>◦ AlphaFold doesn't work well with point mutations</li> </ul> </li> <li>• DBs for non-model organisms and structures - to begin working out structure-function relationships? <ul style="list-style-type: none"> <li>◦ Single point mutations example - AlphaMissense for Human only (training on highly curated human and primate data)</li> <li>◦ Not for non-model organisms</li> </ul> </li> </ul> |
| Presentation                                                        | <p><b>"ABLeS and proteomics"</b></p> <p>Dr. Johan Gustafsson, Dr. Ziad Al Bkhetan, Australian BioCommons</p> <ul style="list-style-type: none"> <li>• <a href="https://www.biocommons.org.au/ables">https://www.biocommons.org.au/ables</a></li> <li>• Main motivation: difficulty of accessing high end compute for bioinformatics</li> <li>• 3 aspects: <ul style="list-style-type: none"> <li>◦ Reference data generation,</li> <li>◦ Production bioinformatics,</li> <li>◦ Software accelerator</li> </ul> </li> </ul> <p><b>Questions</b></p> <ul style="list-style-type: none"> <li>•</li> </ul>                                                                                                                                                                                                                                                                                                                                                                 |
| Proteomics Learning Library Collection                              | <ul style="list-style-type: none"> <li>• Example <a href="https://australianbiocommons.github.io/Learning-Library/data_management">https://australianbiocommons.github.io/Learning-Library/data_management</a></li> <li>• You can add resources to <a href="#">this spreadsheet</a></li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| Updates                                                             | <ul style="list-style-type: none"> <li>• <a href="#">Join the Slack group</a></li> <li>• <a href="#">Other events</a>, including webinars, workshops and community meetings</li> <li>• AUS-oMicS 2025 abstract submission open <a href="https://www.ausomics.com/abstracts">https://www.ausomics.com/abstracts</a></li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| Add your item(s) for discussion here                                | <ul style="list-style-type: none"> <li>• AusOMICS event? Discuss offline</li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| <p><b>Next meeting is in 2025</b></p> <p><b>Happy Holidays!</b></p> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |

# Friday 16th of August 2024

10:30 am (AWST)

12:00 pm (ACST)

12:30 pm (AEST)

## Zoom link

**Chair:** Johan Gustafsson (Australian BioCommons)

**Minutes:** Collectively recorded

### In attendance

| Please add your name and affiliation here |                                                   |                                        |
|-------------------------------------------|---------------------------------------------------|----------------------------------------|
| Johan Gustafsson, BioCommons              | Will Klare, APAF, Macquarie University            | Ziad Al-Bkhetan, Australian BioCommons |
| Murtada D. Naser                          | University of Basra, Iraq                         | nasergriffith@gmail.com                |
| Amaal Gh. Yasser                          | University of Basra, Iraq                         | a.ghaziyasser@gmail.com                |
| ELA HAVARY                                | ISTANBUL BILGI UNIVERSITY                         | alaa.bilgi@gmail.com                   |
| James Chan                                | SA Health                                         | james.chan@sa.gov.au                   |
| Dr Michela Mitchell, CF                   | Women's and Children's Health Network, SA         | michela.mitchell@sa.gov.au             |
| Magnus Palmblad                           | Leiden University Medical Center, The Netherlands | n.m.palmblad@lumc.nl                   |
| Jeff Christiansen                         | Australian BioCommons                             |                                        |
| Ignatius Pang                             | APAF, Macq U                                      | ignatius.pang@mq.edu.au                |
| Andrew Isaac                              | Metabolomics Australia                            | aisaac@unimelb.edu.au                  |
| Harry Wang                                | Metabolomics Australia                            | harry.wang2@unimelb.edu.au             |
| Nigel Ward                                | Australian BioCommons                             |                                        |
| Alex Ip                                   | AARNet                                            | alex.ip@aarnet.edu.au                  |
| Melissa Burke                             | Australian BioCommons                             | melissa@biocommons.org.au              |
| Matthew Downton                           | NCI                                               | matthew.downton@anu.edu.au             |
| Joel Steele                               | Monash Proteomics and Metabolomics Platform       | joel.steele@monash.edu                 |

| Please add your name and affiliation here |                                        |                                        |
|-------------------------------------------|----------------------------------------|----------------------------------------|
| Johan Gustafsson, BioCommons              | Will Klare, APAF, Macquarie University | Ziad Al-Bkhetan, Australian BioCommons |
| Murtada D. Naser                          | University of Basra, Iraq              | nasergriffith@gmail.com                |
| Amaal Gh. Yasser                          | University of Basra, Iraq              | a.ghaziyasser@gmail.com                |
| Georgie Samaha                            | SIH, University of Sydney              | georgina.samaha@sydney.edu.au          |
| Cali Willet                               | SIH, University of Sydney              | cali.willet@sydney.edu.au              |
| Samitha Amarapathy                        | Australian BioCommons                  | samitha@biocommons.org.au              |
| Ben Crossett                              | SydneyMS, USyd                         | ben.crossett@sydney.edu.au             |
| Conrad Leonard                            | Australian BioCommons                  |                                        |
| Jerry li                                  |                                        | qiyerensheng@gmail.com                 |
| Riya Shrestha                             | UNSW Sydney                            | riya.shrestha@unsw.edu.au              |

## Agenda + Minutes

| Item                                                       | Item / Description                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
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| <b>Welcome to meeting &amp; intros</b><br>Johan Gustafsson | An introduction to the <a href="#">Australian BioCommons Proteomics bioinformatics community</a><br>Welcome to the other communities joining today's meeting.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| <b>Presentation</b>                                        | <p><b>"Workflomics"</b><br/>Magnus Palmblad, Leiden University Medical Center, Netherlands</p> <p>Presenting Workflomics, "a platform used to help bioinformaticians to automatically generate and compare computational workflows." One of the key use cases for this platform is proteomics, and in this presentation you will have the opportunity to hear more about this platform and how it can be used to streamline workflow creation and benchmarking.</p>                                                                                                                                                                                                                                                                 |
| <b>Questions</b>                                           | <ul style="list-style-type: none"> <li>• What would be really great is to "close the loop" after benchmarking by storing the scores of the generated workflows so that next time someone wants to evaluate the parameter space they can see what worked well before <ul style="list-style-type: none"> <li>◦ Public benchmarks increasing efficiency - reducing random walk through parameter space</li> </ul> </li> <li>• Working with the OpenEBench team, including literature mining etc.</li> <li>• What about the individual parameter choices within each tool chosen for the workflows? <ul style="list-style-type: none"> <li>◦ Domain knowledge critical</li> <li>◦ Reasonably good default inputs</li> </ul> </li> </ul> |



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|            | <ul style="list-style-type: none"> <li>○ Comparing default settings at the moment</li> <li>● Click on the 2 "best looking" workflows and compare a few parameter changes</li> <li>● Can the workflows be exported and run locally? <ul style="list-style-type: none"> <li>○ Yes, download Docker containers, in future also HPC compatible (maybe Singularity)</li> </ul> </li> <li>● Which data is being used? <ul style="list-style-type: none"> <li>○ User provides data for benchmarking, so this is tailored to your use case</li> <li>○ Some standard data available (i.e. ground truth)</li> <li>○ Also working on generating synthetic data for evaluating workflows</li> </ul> </li> <li>● What is the infrastructure behind the benchmarking? Eg a handful of thermos raw files can be a few GB, or in the genomics space, very large fastq pairs. <ul style="list-style-type: none"> <li>○ Can run on national HPC in NL</li> <li>○ Benchmarking on big data - need bigger compute resources</li> <li>○ Should only benchmark on enough data</li> </ul> </li> <li>● Thinking about a link to Galaxy</li> <li>● Workflomics available to use now? Yes!</li> <li>●</li> </ul>       |
| Updates    | <p><b>General</b></p> <ul style="list-style-type: none"> <li>● <a href="#">Join the Slack group</a></li> <li>● <a href="#">Join the community (for updates)</a></li> <li>● <a href="#">Other events</a>, including webinars, workshops and community meetings <ul style="list-style-type: none"> <li>○ <a href="#">WORKSHOP: Online data analysis for biologists</a></li> <li>○ <a href="#">Top Tips from Galaxy Australia</a></li> <li>○ <a href="#">WORKSHOP: Hello Nextflow!</a></li> </ul> </li> </ul> <p><b>Proteomics Lab update</b> <a href="https://proteomics.usegalaxy.org.au/">https://proteomics.usegalaxy.org.au/</a></p> <ul style="list-style-type: none"> <li>●  Proteomics Lab community working group</li> <li>● Proteomics Lab being presented at IMSC2024 next week!</li> </ul> <p><b>Tools and workflows</b></p> <ul style="list-style-type: none"> <li>● Fragpipe on Galaxy</li> <li>● DIA-NN on Galaxy - if you have feedback, or something isn't working, please let us know <a href="https://site.usegalaxy.org.au/request">https://site.usegalaxy.org.au/request</a></li> </ul> |
| Co-working | <p><b>Proteomics training</b></p> <p>All</p> <p>We'll continue working together to collate a list of proteomics-themed learning resources that explain a concept or demonstrate how to perform a task. These should be resources that we already know about and would recommend to a friend or colleague. If you're extra keen or you can't join us you can add resources to <a href="#">this spreadsheet</a>.</p> <p>This collection will ultimately be included in the Australian BioCommons' Learning Library.</p> <ul style="list-style-type: none"> <li>● <a href="#">Discussion notes</a></li> <li>● Example <a href="https://australianbiocommons.github.io/Learning-Library/data_management">https://australianbiocommons.github.io/Learning-Library/data_management</a></li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                  |

|                                    |                                        |
|------------------------------------|----------------------------------------|
| Action(s)                          | •                                      |
| AOB?                               | • Add your item(s) for discussion here |
| Next meeting is 18th November 2024 |                                        |

## Monday 3rd of June 2024

10:30 am (AWST)

12:00 pm (ACST)

12:30 pm (AEST)

### In attendance

| Please add your name and affiliation here |                                    |                                        |
|-------------------------------------------|------------------------------------|----------------------------------------|
| Johan Gustafsson, BioCommons              | Lisa Phippard, BioCommons          | Melissa Burke, BioCommons              |
| Asif Ahmed, CSIRO ACDP                    | Will Klare, APAF, Macquarie Uni    | Uwe Winter, BioCommons                 |
| Maz Ali, VCCRI, UNSW                      | Cali Willet, USyd                  | Ilgnatius Pang, APAF Macquarie U       |
| Joel Steele, Monash, MPMP                 | Georgie Samaha, USyd               | Muhammad Zenaidee, APAF, Macquarie Uni |
| Denise Tran, USyd                         | Chingyu Lu, USyd                   | Adam Carroll, JMSF, ANU                |
| Matthew Downton, NCI                      | Ziad Al-Bkhetan, BioCommons        | Ben Crossett, SydneyMS, USyd           |
| Hossein Valipour, Monash, MPMP            | Fozia Masood, Macquarie University |                                        |

### Agenda + Minutes

| Item                                                       | Item / Description                                                                                                                                                                                                                                                                                                               |
|------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Welcome to meeting &amp; intros</b><br>Johan Gustafsson | An introduction to the Australian BioCommons<br>The context for these meetings <ul style="list-style-type: none"> <li>• <a href="#">Australian BioCommons</a></li> <li>• <a href="#">Proteomics bioinformatics community page</a></li> <li>• <a href="#">Proteomics Analysis Infrastructure Roadmap for Australia</a></li> </ul> |
| <b>Presentation</b>                                        | <b>"Scaling DIA-NN to HPC for accelerated large-scale proteomics"</b><br>Cali Willet, Sydney Informatics Hub                                                                                                                                                                                                                     |

|           |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
|-----------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|           | Dr. Cali Willet (Sydney Informatics Hub) will present her work to speed up DIA-NN analyses using high performance computing (HPC) at the National Computational Infrastructure (NCI), reducing processing time for large proteomics experiments from days / weeks to just hours.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| Questions | <ul style="list-style-type: none"> <li>• What were the hardware specifications i.e. Core count, Ram, Storage space and speed ? <ul style="list-style-type: none"> <li>◦ Gadi normal nodes ~ 150,000 cores</li> <li>◦ Could run with fewer cores as well</li> </ul> </li> <li>• mzML effect - closer look at spectra? Do they look different after conversion? Explanation for the difference in results? <ul style="list-style-type: none"> <li>◦ Dev for ProteoWizard - <a href="#">issue</a></li> <li>◦ Recommended software to check converted mzML files: SeeMS</li> <li>◦ Converted mzML had same values as wiff EXCEPT for Number of data points: this was much lower for mzML than wiff</li> <li>◦ Suggested that DIA-NN might be doing peak picking differently to ProteoWizard (issue available on GitHub repository) <ul style="list-style-type: none"> <li>■ <a href="https://github.com/vdemichev/DiaNN/issues/777">https://github.com/vdemichev/DiaNN/issues/777</a></li> </ul> </li> <li>◦ ProteoWizard conversion was ok, but observations different</li> </ul> </li> <li>• GPUs ? <ul style="list-style-type: none"> <li>◦ Might need DIA-NN to be modified - would need discussion with Vadim (dev for DIA-NN) as this may need a source code change</li> </ul> </li> <li>•</li> </ul>                                                                                                       |
| Updates   | <p><b>General</b></p> <ul style="list-style-type: none"> <li>• <a href="#">Join the Slack group</a></li> <li>• <a href="#">Join the community (for updates)</a></li> <li>• <a href="#">Other events</a>, including webinars, workshops and community meetings</li> <li>• Gustafsson, O. J. R. (2024). FORUM Report: Connections in Computational Proteomics. Zenodo. <a href="https://doi.org/10.5281/zenodo.10929402">https://doi.org/10.5281/zenodo.10929402</a></li> <li>•</li> </ul> <p><b>Proteomics Lab update</b> <a href="https://proteomics.usegalaxy.org.au/">https://proteomics.usegalaxy.org.au/</a></p> <ul style="list-style-type: none"> <li>•  Proteomics Lab community working group</li> </ul> <p><b>Tools and workflows</b></p> <ul style="list-style-type: none"> <li>• Fragpipe on Galaxy - major elements are being merged at the moment - JG will keep the group up-to-date <ul style="list-style-type: none"> <li>◦ MSFragger part of this work: <a href="https://github.com/bioconda/bioconda-recipes/pull/45127">https://github.com/bioconda/bioconda-recipes/pull/45127</a></li> </ul> </li> <li>• DIA-NN on Galaxy - if you have feedback, or something isn't working, please let us know <a href="https://site.usegalaxy.org.au/request">https://site.usegalaxy.org.au/request</a></li> </ul> |
| Workshop  | <p><b>Proteomics training</b><br/>Melissa Burke, Australian BioCommons</p> <p>The proteomics bioinformatics community recognises the need to train more life scientists in proteomics. Collating and sharing collections of recommended training resources is one way that we might address this as a community. Melissa Burke, Australian BioCommons Training</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |

|                                  |                                                                                                                                                                                                                                                                                                                                                                               |
|----------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                                  | <p>and Communications Officer will join us to facilitate a discussion on how we might create a collection of recommended proteomics training resources and share them with Australian life scientists. Everyone is welcome to join the discussion. No training experience is needed.</p> <ul style="list-style-type: none"> <li>• <a href="#">Discussion notes</a></li> </ul> |
| Action(s)                        | <ul style="list-style-type: none"> <li>•</li> </ul>                                                                                                                                                                                                                                                                                                                           |
| AOB?                             | <ul style="list-style-type: none"> <li>• Add your item(s) for discussion here</li> </ul>                                                                                                                                                                                                                                                                                      |
| Next meeting is 16th August 2024 |                                                                                                                                                                                                                                                                                                                                                                               |

## Monday 11th of March 2024

10:30 am (AWST)

12:30 pm (AEST)

13:00 pm (ACDT)

13:30 pm (AEDT)

### In attendance

| Please add your name and affiliation here |  |  |  |
|-------------------------------------------|--|--|--|
| Johan Gustafsson<br>Australian BioCommons |  |  |  |
| Winnie Mok<br>Australian Biocommons       |  |  |  |
| Joel Steele<br>Monash (MPMP)              |  |  |  |

### Agenda + Minutes

| Item                                                       | Item / Description                                                                                                                                                                                                                                                                                                                          | Action(s) |
|------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|
| <b>Welcome to meeting &amp; intros</b><br>Johan Gustafsson | <p>An introduction to the Australian BioCommons</p> <p>The context for these meetings</p> <ul style="list-style-type: none"> <li>• <a href="#">Australian BioCommons</a></li> <li>• <a href="#">Proteomics bioinformatics community page</a></li> <li>• <a href="#">Proteomics Analysis Infrastructure Roadmap for Australia</a></li> </ul> |           |
| Presentation                                               | "A summary of the FORUM: Connections in computational proteomics"                                                                                                                                                                                                                                                                           |           |

|                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |  |
|----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|
| Johan Gustafsson     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |  |
| Questions            | <ul style="list-style-type: none"> <li>•</li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |  |
| General updates      | <ul style="list-style-type: none"> <li>• <a href="#">Join the Slack group</a></li> <li>• <a href="#">Join the community (for updates)</a></li> <li>• <a href="#">Other events</a>, including webinars, workshops and community meetings <ul style="list-style-type: none"> <li>◦ <a href="https://zenodo.org/communities/australianbiocommons-training/records?q=&amp;l=list&amp;p=1&amp;s=10&amp;sort=newest">https://zenodo.org/communities/australianbiocommons-training/records?q=&amp;l=list&amp;p=1&amp;s=10&amp;sort=newest</a></li> <li>◦ <a href="https://www.youtube.com/c/AustralianBioCommonsChannel">https://www.youtube.com/c/AustralianBioCommonsChannel</a></li> </ul> </li> <li>• UniProt survey <ul style="list-style-type: none"> <li>◦ <i>Are you using Uniprot in your work?</i></li> <li>◦ <i>If yes, we would love to hear your thoughts as part of this survey designed by economists to assess its value:</i><br/> <a href="https://ec.europa.eu/eusurvey/runner/use_value_assessment_of_UniProt">https://ec.europa.eu/eusurvey/runner/use_value_assessment_of_UniProt</a></li> <li>◦ <i>If you have industry contacts who use Uniprot, we would be delighted if you could forward the opportunity to them!</i></li> </ul> </li> <li>• Add your item for discussion here</li> <li>•</li> </ul> |  |
| Services             | ABLeS: <a href="https://www.biocommons.org.au/ables">https://www.biocommons.org.au/ables</a><br>Alphafold2: <a href="https://www.biocommons.org.au/alphafold">https://www.biocommons.org.au/alphafold</a><br>Training infrastructure:<br><a href="https://www.biocommons.org.au/training-infrastructure">https://www.biocommons.org.au/training-infrastructure</a><br>Galaxy Australia: <a href="https://www.biocommons.org.au/galaxy-australia">https://www.biocommons.org.au/galaxy-australia</a>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |  |
| Community activities | <b>Proteomics Lab update</b> <a href="https://proteomics.usegalaxy.org.au/">https://proteomics.usegalaxy.org.au/</a> <ul style="list-style-type: none"> <li>•  Proteomics Lab community working group</li> </ul> <b>Tools and workflows</b> <ul style="list-style-type: none"> <li>• DIA-NN on NCI</li> <li>• Fragpipe on Galaxy - major elements are being merged at the moment - JG will keep the group up-to-date <ul style="list-style-type: none"> <li>◦ MSFragger part of this work:<br/> <a href="https://github.com/bioconda/bioconda-recipes/pull/45127">https://github.com/bioconda/bioconda-recipes/pull/45127</a></li> </ul> </li> <li>• DIA-NN on Galaxy - if you have feedback, or something isn't working, please let us know</li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |  |

|                                                        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |  |
|--------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|
|                                                        | <a href="https://site.usegalaxy.org.au/request">https://site.usegalaxy.org.au/request</a> <ul style="list-style-type: none"> <li>Pathway mapping - this work will continue early next year<br/><a href="https://australianbiocommons.github.io/pathway_mapping_to_ols/">https://australianbiocommons.github.io/pathway_mapping_to_ols/</a></li> </ul>                                                                                                                                                                                                                                                                                          |  |
| <b>Next meeting topic - sharing training resources</b> | <p>The proteomics bioinformatics community recognises the need to train more life scientists in proteomics. Collating and sharing recommended training resources is one way that we might address this as a community.</p> <p>Our next community meeting will focus on how we might collectively address this challenge, and help make high quality proteomics training resources more visible to the Australian life scientists. Melissa Burke, Australian BioCommons Training and Communications Officer will join us to facilitate the discussion.</p> <p>Everyone is welcome to join the discussion. No training experience is needed.</p> |  |
| <b>Add your item here!</b>                             |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |  |
| <b>AOB?</b>                                            | <ul style="list-style-type: none"> <li></li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |  |
| Next meeting is 3rd June 2024                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |  |

## Monday 13th of November 2023

10:30 am (AWST)

13:00 pm (ACDT)

13:30 pm (AEDT)

### In attendance

| Please add your name and affiliation here   |                                       |                            |  |
|---------------------------------------------|---------------------------------------|----------------------------|--|
| Johan Gustafsson<br>Australian BioCommons   | Luke Carroll<br>APAF                  | Pawel Sadowski<br>QUT-CARF |  |
| Jairo A. Pinzon-Cortes<br>Monash University | Matthew Downton<br>NCI                |                            |  |
| Michael Dausmann<br>Children's Medical      | Cali Willet<br>Sydney Informatics Hub |                            |  |

|                                                             |                                                    |  |  |
|-------------------------------------------------------------|----------------------------------------------------|--|--|
| Research Institute                                          | University of Sydney                               |  |  |
| Joel Steele (MPMP)<br>Monash University                     | Ben Crossett<br>SydneyMS, USyd                     |  |  |
| Ignatius Pang<br>Children's Medical<br>Research Institute   | Matt Padula<br>UTS                                 |  |  |
| Dorothy Loo Oey<br>Translational Research<br>Institute, Qld | Clifford Young<br>University of South<br>Australia |  |  |
|                                                             |                                                    |  |  |

### Agenda + Minutes

| Item                                                       | Item / Description                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | Action(s) |
|------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|
| <b>Welcome to meeting &amp; intros</b><br>Johan Gustafsson | An introduction to the Australian BioCommons<br>The context for these meetings <ul style="list-style-type: none"> <li>• <a href="#">Australian BioCommons</a></li> <li>• <a href="#">Proteomics bioinformatics community page</a></li> <li>• <a href="#">Proteomics Analysis Infrastructure Roadmap for Australia</a></li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |           |
| <b>Presentation</b><br>Ori Livson<br>ProCan / CMRI         | <b>Scaling DIA-NN and Cross Cohort Data Exploration</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |           |
| <b>Questions</b>                                           | <ul style="list-style-type: none"> <li>• <b>SWON vs. Nextflow?</b> <ul style="list-style-type: none"> <li>○ Could Nextflow achieve the same thing as SWON?</li> <li>○ Running of workflows - yes</li> <li>○ Producing same DB - no <ul style="list-style-type: none"> <li>■ If you have graph like requirements for exploring data, you won't get this with nextflow</li> <li>■ <b>OL:</b> It turns out Nextflow has SQL plugins now for managing workflow metadata but that didn't exist at the time ProCan developed swon.</li> </ul> </li> <li>○ For QC, we hash files</li> <li>○ Bespoke system at the moment</li> </ul> </li> <li>• POCKET aspect run in house - clinical data</li> <li>• Possible to replicate the workflow approach? <ul style="list-style-type: none"> <li>○ Not straightforward</li> <li>○ Not easy to set up, but technically feasible</li> </ul> </li> </ul> |           |

|                                                                                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |  |
|--------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|
|                                                                                            | <ul style="list-style-type: none"> <li>Visualisation tools - compute heavy? What are they doing? <ul style="list-style-type: none"> <li>Visualising data</li> <li>Example, high quality read access - large csv or MS data</li> <li>POCKET query engine - 100s of GB or RAM</li> <li>Lightweight, but high mem available</li> <li>Visualisation platforms lightweight in principle, with post-processing completed before hand if possible</li> <li>K8 with unrestricted resources are helpful for heavier jobs</li> </ul> </li> </ul>                                                                                                                                                                                                                                                                                                                                                   |  |
| General updates                                                                            | <ul style="list-style-type: none"> <li><a href="#">Join the Slack group</a></li> <li><a href="#">Join the community (for updates)</a></li> <li><a href="#">Other events</a>, including webinars, workshops and community meetings</li> <li>Add your item for discussion here</li> <li></li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |  |
| Community activities                                                                       | <p><b>Proteomics Lab update</b> <a href="https://proteomics.usegalaxy.org.au/">https://proteomics.usegalaxy.org.au/</a></p> <ul style="list-style-type: none"> <li>Tools list update (in progress)</li> <li>Centre page update (in progress)</li> <li> Proteomics Lab community working group</li> </ul> <p><b>Tools and workflows</b></p> <ul style="list-style-type: none"> <li>DIA-NN on Galaxy - if you have feedback, or something isn't working, please let us know<br/><a href="https://site.usegalaxy.org.au/request">https://site.usegalaxy.org.au/request</a></li> <li>Pathway mapping - this work will continue early next year<br/><a href="https://australianbiocommons.github.io/pathway_mapping_to_ols/">https://australianbiocommons.github.io/pathway_mapping_to_ols/</a></li> </ul> |  |
| <b>FORUM:</b><br><a href="#">Connections in computational proteomics</a><br>30-31 Jan 2024 | <p>Computational proteomics forum in Melbourne on 30th and 31st of January - right before Lorne Proteomics 2024</p> <p>If you would like to attend, please register 😊</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |  |
| Plan for 2024                                                                              | <ul style="list-style-type: none"> <li>Quarterly meetings will continue</li> <li>Will continue working on Proteomics Lab - if you would like to join the working group, let Johan know<br/> Proteomics Lab community working group</li> <li></li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |  |



|                                              |   |  |
|----------------------------------------------|---|--|
| Add your item here!                          |   |  |
| AOB?                                         | • |  |
| Next meeting is in 2024<br>Happy Holidays!!! |   |  |

## Monday 21st of August 2023

11:30 am (AWST)

13:00 pm (ACDT)

13:30 pm (AEST)

### In attendance

| Please add your name and affiliation here |                           |  |  |
|-------------------------------------------|---------------------------|--|--|
| Johan Gustafsson<br>Australian BioCommons | Matt Padula<br>UTS        |  |  |
| Matthew Downton NCI                       | Nikeisha Caruana, Unimelb |  |  |
| Luke Carrol APAF                          |                           |  |  |
| Rohan Lowe, La Trobe U                    |                           |  |  |
| Clifford Young, UniSA                     |                           |  |  |

### Agenda + Minutes

| Item                                                       | Item / Description                                                                                                                                                                                                                                                                                                               | Action(s) |
|------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|
| <b>Welcome to meeting &amp; intros</b><br>Johan Gustafsson | An introduction to the Australian BioCommons<br>The context for these meetings <ul style="list-style-type: none"> <li>• <a href="#">Australian BioCommons</a></li> <li>• <a href="#">Proteomics bioinformatics community page</a></li> <li>• <a href="#">Proteomics Analysis Infrastructure Roadmap for Australia</a></li> </ul> |           |
| <b>Presentation #1</b><br>Nikeisha Caruana                 | “RDMassSpec Explorer: An online platform for the interrogation of rare disease proteomics data.”                                                                                                                                                                                                                                 |           |
| <b>Questions</b>                                           | •                                                                                                                                                                                                                                                                                                                                |           |

|                                           |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                                                         |
|-------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------|
| <b>Proteomics Lab</b><br>Johan Gustafsson | <p>“Proteomics Lab: <a href="https://proteomics.usegalaxy.org.au/">https://proteomics.usegalaxy.org.au/</a>”</p> <p>Also inviting community members to join a working group that will direct and co-create content for Proteomics Lab.</p> <ul style="list-style-type: none"> <li></li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |                                                                                         |
| <b>General updates</b>                    | <ul style="list-style-type: none"> <li>Proteomics BoF outcome <a href="#">Galaxy Community Conference 2023 (Brisbane)</a> <ul style="list-style-type: none"> <li> GCC 2023 Global Galaxy MS planning</li> </ul> </li> <li>Survey on MS imaging standards being conducted by <a href="https://www.imagingmssociety.org/">https://www.imagingmssociety.org/</a></li> <li><a href="#">Other events</a>, including webinars, workshops and community meetings</li> <li>PMV conference: 25th October 2023 <ul style="list-style-type: none"> <li>Together with ECR conference</li> <li>Free event</li> <li>Registration open until close to conference</li> </ul> </li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                                                                         |
| <b>Community activities</b>               | <p><b>Training</b></p> <ul style="list-style-type: none"> <li>WEBINAR: <a href="#">Getting started with proteomics</a></li> </ul> <p><b>Event possibilities before Lorne 2024</b></p> <ul style="list-style-type: none"> <li>First community F2F meeting in Melbourne?</li> <li>Open discussion about this idea</li> </ul> <p><b>Tools and workflows</b></p> <ul style="list-style-type: none"> <li>Pathway mapping<br/><a href="https://australianbiocommons.github.io/pathway_mapping_to_ols/">https://australianbiocommons.github.io/pathway_mapping_to_ols/</a> <ul style="list-style-type: none"> <li> 2023 Evaluation of pathway mapping software ...</li> </ul> </li> <li>Fragpipe workflows</li> <li><a href="#">DIA-NN installed on Galaxy Australia</a></li> <li>Has anyone used the following tools? <ul style="list-style-type: none"> <li>Prolfqua<br/><a href="https://doi.org/10.1021/acs.jproteome.2c00441">https://doi.org/10.1021/acs.jproteome.2c00441</a></li> <li>Einprot <a href="https://doi.org/10.1101/2023.07.27.550821">https://doi.org/10.1101/2023.07.27.550821</a></li> </ul> </li> </ul> | <p><b>Action Johan:</b><br/>summarise plan for Lorne and send to group for feedback</p> |
| <b>Add your item here!</b>                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                                                         |
| <b>AOB?</b>                               | <ul style="list-style-type: none"> <li></li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |                                                                                         |
| Next meeting is 13th November 2023        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                                                         |

# Monday 29th of May 2023

10:30 am (AWST)

12:30 pm (AEST)

13:00 pm (ACDT)

13:30 pm (AEDT)

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## In attendance

| Please add your name and affiliation here |  |  |
|-------------------------------------------|--|--|
| Johan Gustafsson<br>Australian BioCommons |  |  |
| Joel Steele,<br>Monash (MPMP)             |  |  |
| Matt Padula - UTS.                        |  |  |
| Keiran Rowell - MQ                        |  |  |
| Clifford Young (UniSA)                    |  |  |
| Dorothy Loo-Oey (TRI)                     |  |  |
|                                           |  |  |

## Chair

Johan Gustafsson (Australian BioCommons)

## Minutes

Collectively recorded

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## Agenda + Minutes

| Item                                                       | Item / Description                                                                                                                                                                                                                                                                                                                                                                                                                   | Action(s) |
|------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|
| <b>Welcome to meeting &amp; intros</b><br>Johan Gustafsson | <b><i>An introduction to the Australian BioCommons</i></b><br>The context for these meetings <ul style="list-style-type: none"><li>BioCommons: <a href="https://www.biocommons.org.au/">https://www.biocommons.org.au/</a></li><li>Proteomics community: <a href="https://www.biocommons.org.au/proteomics">https://www.biocommons.org.au/proteomics</a></li><li>Proteomics Analysis Infrastructure Roadmap for Australia:</li></ul> |           |

|                                                   |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |  |
|---------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|
|                                                   | <a href="https://doi.org/10.5281/zenodo.7460248">https://doi.org/10.5281/zenodo.7460248</a>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |  |
| Questions                                         | <ul style="list-style-type: none"> <li>Please add questions here 😊</li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |  |
| <b>Presentation</b><br>Gareth Price<br>Rohan Lowe | <i>Introducing TlaaS – Training Infrastructure as a Service - for proteomics</i>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |  |
| Questions / open discussion                       | <ul style="list-style-type: none"> <li>Pre-computed results for environmental computing</li> <li>Reducing the unnecessary expenditure of compute cycles</li> <li>How to teach based on mistakes, when pre-computed results are available?</li> <li></li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |  |
| Updates                                           | <ul style="list-style-type: none"> <li><b>Community activities</b> <ul style="list-style-type: none"> <li>WEBINAR: <a href="#">Getting started with proteomics</a></li> <li> 2023 Evaluation of pathway mapping softw...</li> <li><a href="https://proteomics.usegalaxy.au">Proteomics.usegalaxy.au</a></li> <li>Fragpipe workflows</li> </ul> </li> <li><b>CONFERENCE:</b> <a href="#">Galaxy Community Conference 2023 (Brisbane)</a> <ul style="list-style-type: none"> <li>Proteomics BoF together with Galaxy-Proteomics from US</li> </ul> </li> <li><b>TRAINING:</b> <a href="#">Galaxy Training Network Smorgasbord 2023 (Online)</a></li> <li><b>MEETING:</b> <a href="#">Australian metabolomics community</a></li> <li><b>Other events</b>, including webinars, workshops and community meetings</li> </ul> |  |
| Add your item here!                               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |  |
| AOB?                                              | <ul style="list-style-type: none"> <li>Pre Conference workshop possibilities? For Lorne 2024?</li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |  |
| Next meeting is 29th May 2023                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |  |

## Monday 6th of March 2023

10:30 am (AWST)

12:30 pm (AEST)

13:00 pm (ACDT)

13:30 pm (AEDT)

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## In attendance

| Please add your name and affiliation here |                |                   |
|-------------------------------------------|----------------|-------------------|
| Johan Gustafsson<br>Australian BioCommons | Ali Raza       | Ralf Schittenhelm |
| Jeff Christiansen                         | Luke Carroll   | Dorothy Loo-Oey   |
| Harry Wang                                | Igy Pang       | Rob Goode         |
| Hailey Zhang                              | Ben Crossett   | Amar Inder        |
| Clifford Young                            | Pawel Sadowski | Matt Padula       |
| Shanice                                   | Tara Pukala    |                   |
|                                           |                |                   |

## Chair

Johan Gustafsson (Australian BioCommons)

## Minutes

Collectively recorded

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## Agenda + Minutes

| Item                                                       | Item / Description                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | Action(s) |
|------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|
| <b>Welcome to meeting &amp; intros</b><br>Johan Gustafsson | <b><i>An introduction to the Australian BioCommons</i></b><br>The context for these meetings <ul style="list-style-type: none"><li>• BioCommons: <a href="https://www.biocommons.org.au/">https://www.biocommons.org.au/</a></li><li>• Proteomics community: <a href="https://www.biocommons.org.au/proteomics">https://www.biocommons.org.au/proteomics</a></li><li>• Proteomics Analysis Infrastructure Roadmap for Australia: <a href="https://doi.org/10.5281/zenodo.7460248">https://doi.org/10.5281/zenodo.7460248</a></li></ul> |           |
| <b>Questions</b>                                           | <ul style="list-style-type: none"><li>• Please add questions here 😊</li></ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                          |           |
| <b>Presentation</b><br>Hailey Zhang                        | <b><i>Phospho-Analyst: visualising and analysing phosphoproteomics data with "one-click"</i></b>                                                                                                                                                                                                                                                                                                                                                                                                                                       |           |

|                               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |  |
|-------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|
|                               | <a href="https://analyst-suites.org/apps/phospho-analyst/">https://analyst-suites.org/apps/phospho-analyst/</a>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |  |
| Questions / open discussion   | <ul style="list-style-type: none"> <li>When will PathwayAnalyst be available? <ul style="list-style-type: none"> <li>Being integrated with Rshiny now</li> </ul> </li> <li>Is it available on Galaxy? <ul style="list-style-type: none"> <li>Not yet, hopefully it will be</li> </ul> </li> <li></li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |  |
| Updates                       | <ul style="list-style-type: none"> <li><b>Looking for speakers</b> for the next community meeting (29th May 2023)!</li> <li><b>We need your help!</b> Help us improve the <a href="#">ToolFinder service</a> by chatting with us about your experience: <a href="http://tinyurl.com/finding-tools">http://tinyurl.com/finding-tools</a></li> <li><b>Do you struggle to obtain data from international repositories?</b> <a href="#">Let us know what infrastructure would make your life easier</a></li> <li><b>WORKSHOP:</b> <a href="#">Make your bioinformatics workflows findable and citable</a></li> <li><b>CONFERENCE:</b> <a href="#">Galaxy Community Conference 2023 (Brisbane)</a></li> <li><b>TRAINING:</b> <a href="#">Galaxy Training Network Smorgasbord 2023 (Online)</a></li> <li><b>Other events</b>, including webinars, workshops and community meetings <ul style="list-style-type: none"> <li>MaxQuant training</li> </ul> </li> </ul> |  |
| Tool availability             | <ul style="list-style-type: none"> <li><a href="#">MSfragger on Galaxy</a></li> <li>Meeting with Fragpipe Galaxy dev team soon</li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |  |
| Add your item here!           |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |  |
| AOB?                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |  |
| Next meeting is 29th May 2023 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |  |

## Other Relevant Information

### More information

- Visible Research Software Interest Group
  - <https://sites.google.com/ardc.edu.au/visible-research-software>
  - <https://github.com/au-research/Visible-Research-Software/discussions>
- International Workflows Community Initiative: <https://workflows.community/>

- Research Software Engineer (RSE) Association of Australia and New Zealand
  - <https://rse-aunz.github.io/>

## Australian BioCommons Community Engagement

- This community is one of several research community groups within the Australian BioCommons that we're engaging to understand the community-scale bioinformatics infrastructure challenges. It's our mission over the next few years to deliver a more coherent national infrastructure for Bioinformatics that will allow researchers in these communities to spend more time doing their research and less time on that bioinformatics infrastructure set up and management.
- The [Australian BioCommons Project](#).
- The [Australian BioCommons Code of Conduct](#)
- Other [Communities](#) in the Australian BioCommons.
- BioCommons strategy documents:
  - Nelson, T. et al, March 2021, [The Australian BioCommons Community Engagement Strategy: Understanding community-scale challenges to inform solution delivery](#), conference presentation, eResearch New Zealand.
  - Lonie, A. and Francis, R. 2020, [Australian BioCommons Strategic Plan 2021-2023](#)
- Example Infrastructure Roadmaps from other communities:
  - Nelson, T., Griffin, P. and Christiansen, J. 2020, [Genome Annotation Infrastructure Roadmap for Australia](#).
  - Nelson, T. and Christiansen, J. 2020, [Genome Assembly Infrastructure Roadmap for Australia](#).
- Hall, C. et al, 2021, [Application of a bioinformatics training delivery method for reaching dispersed and distant trainees](#), PLoS Computational Biology, <https://doi.org/10.1371/journal.pcbi.1008715>
- Have something to say but didn't get the chance? Please contact us at [communities@biocommons.org.au](mailto:communities@biocommons.org.au).