Mass Dynamics

Automated benchmarking enables continuous confidence in scientific software development

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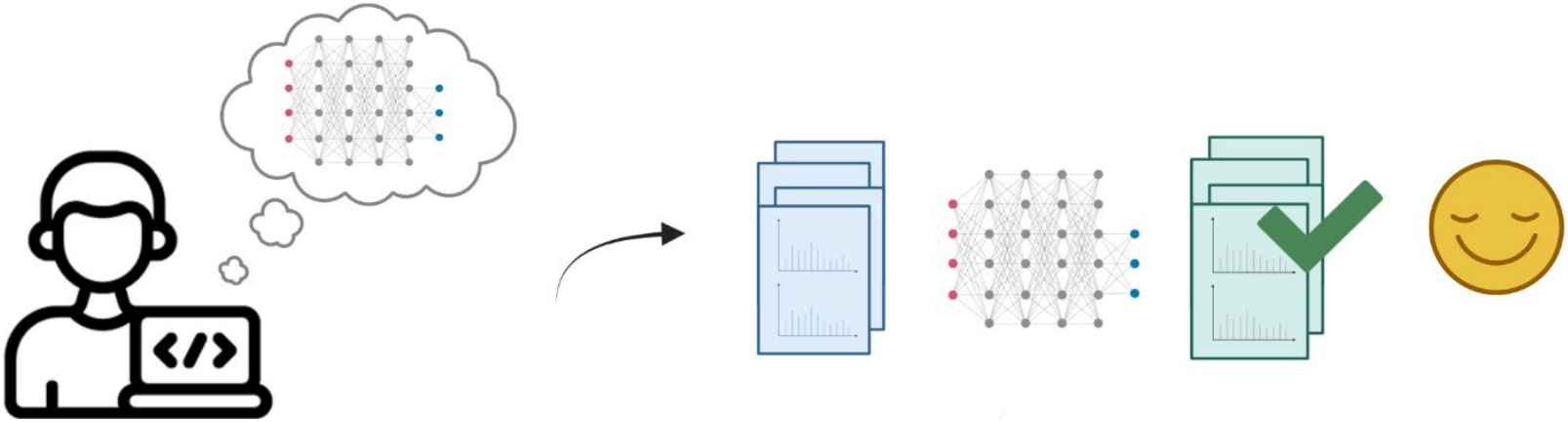
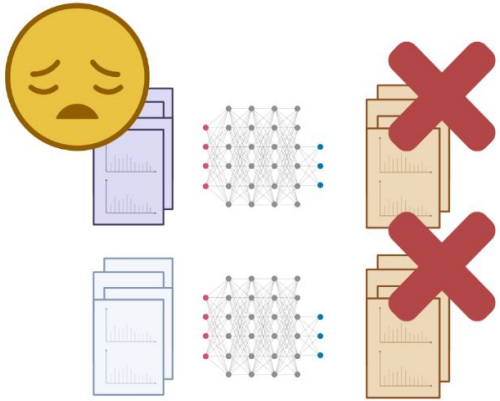
Data Scientist at Mass Dynamics

ASMS Minneapolis
7th June 2022



.....

6 months later



>8 years in Bioinformatics

Many hours spent looking for mysterious errors

- BSc, MSc in Statistics
- PhD in Statistical Genomics, WEHI Melbourne
- Since 1 year Data Scientist at Mass Dynamics, Melbourne

nature > nature human behaviour > perspectives > article

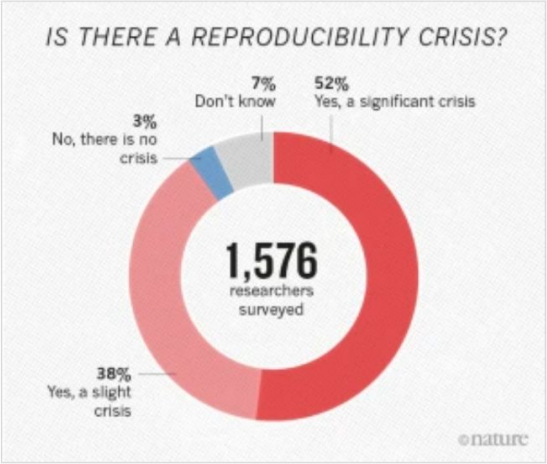
Open Access | Published: 10 January 2017

A manifesto for reproducible science

Marcus R. Munafò, Brian A. Nosek, Dorothy V. M. Bishop, Katherine S. Button, Christopher D. Chambers, Nathalie Percie du Sert, Uri Simonsohn, Eric-Jan Wagenmakers, Jennifer J. Ware & John P. A. Ioannidis

Nature Human Behaviour **1**, Article number: 0021 (2017) | Cite this article

*"… one analysis estimates that **85% of biomedical research efforts are wasted**"*



Published: 25 May 2016

1,500 scientists lift the lid on reproducibility

Monya Baker

Nature **533**, 452–454 (2016) | Cite this article

What I would like you to get from my talk

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- How at Mass Dynamics we get **quick** and **regular confidence** about the scientific software that we develop

What I would like you to get from my talk

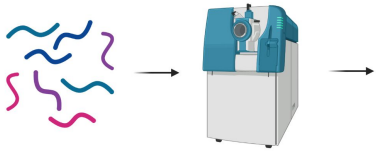
- How at Mass Dynamics we get **quick** and **regular confidence** about the scientific software that we develop

- **Learn ideas and methods** that you can apply to your own scientific development or processes

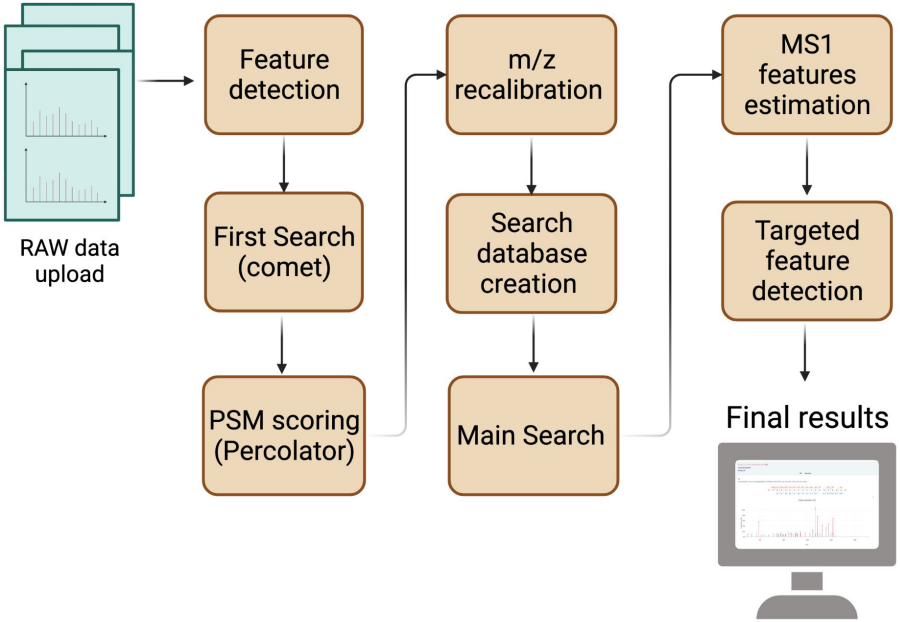
The problem in the proteomics context

Workflows in proteomics are often **Complex** and **computationally intensive**

Before Getting to Mass Dynamics



Example: Mass Dynamics Peptide Mapping workflow

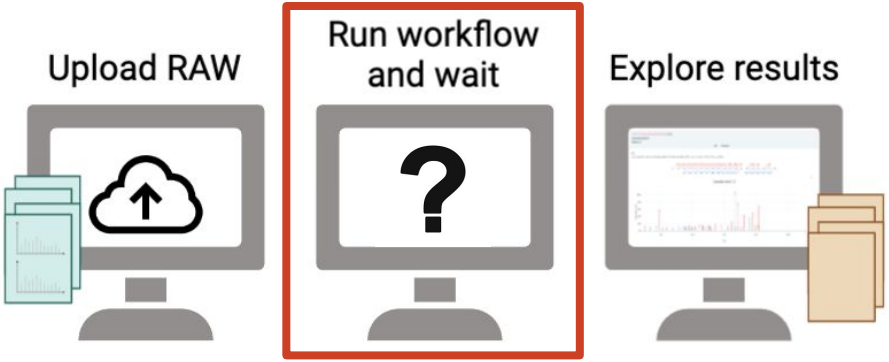


Automation overcomes complexity

Automation overcomes complexity

A complex automated workflow can feel like a black box for:

- Who uses it
- Who develops it



Benchmarking to maintain confidence

- Against ground truth before and after making changes to the code

Benchmarking to maintain confidence

- Against ground truth before and after making changes to the code
- Usually time consuming and performed manually
  - Benchmarking scripts across different folders and projects
  - To be run manually every time there is a new change

Imagine if…

We could all have a **quick development feedback**…

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To maintain results **accuracy** after changes

Minimise risk of "silent" errors

Imagine if…

We could all have a **quick development feedback**…

To maintain results **accuracy** after changes

& to maintain **transparency** of internal steps

Build trust in the black box

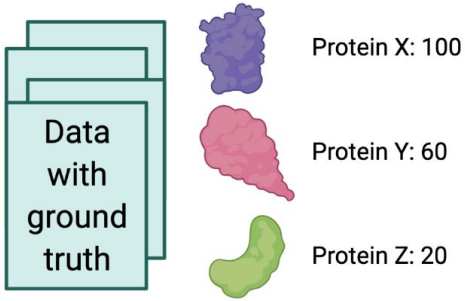
Our solution:
Automated Benchmarking System

Our solution: **Automated Benchmarking System**

Brings the CI/CD framework from software into scientific development

Produces automated reports to increase visibility of intermediate steps

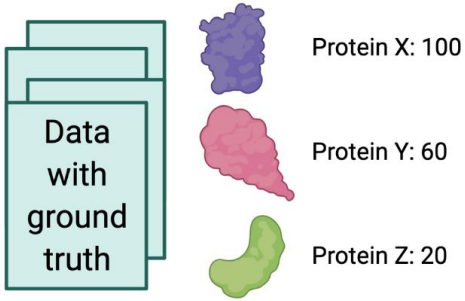
Benchmarking setup

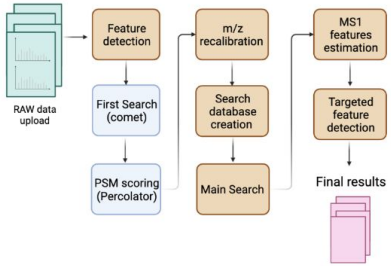


1 Data with known amounts of proteins

Public and private datasets

Benchmarking setup



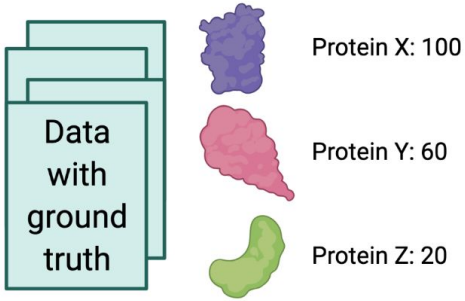


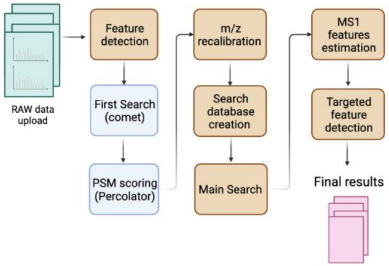
1 Data with known amounts of proteins

Public and private datasets

2 Workflow to run

Benchmarking setup





1 Data with known amounts of proteins

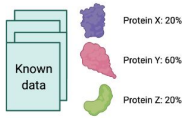
Public and private datasets

2 Workflow to run

3 Code to check results

Automated benchmarking system

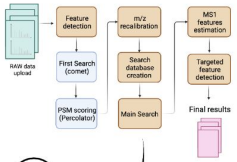
Data with ground truth



aws

1

Workflow



aws

2

Buildkite

3

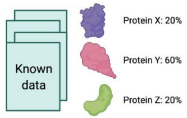
Centralised checks

GitHub

Created with BioRender.com

Automated benchmarking system

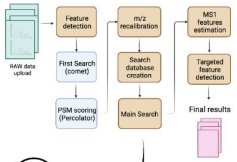
Data with ground truth



aws

1

Workflow



aws

2

Buildkite

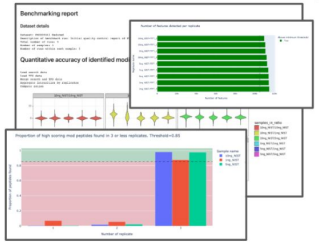
3

Centralised checks

GitHub

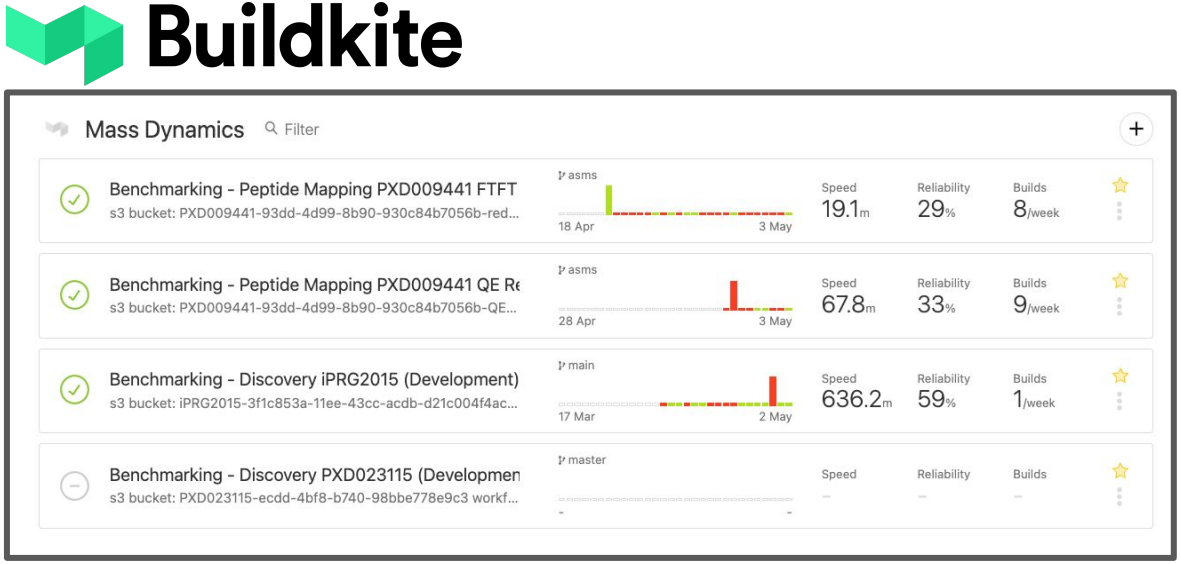
Automated tests and reports

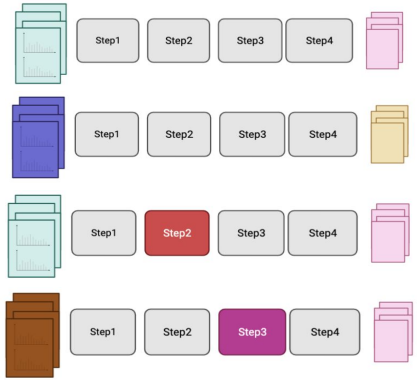
4



Created with BioRender.com

Each **dataset + workflow** has a separate pipeline

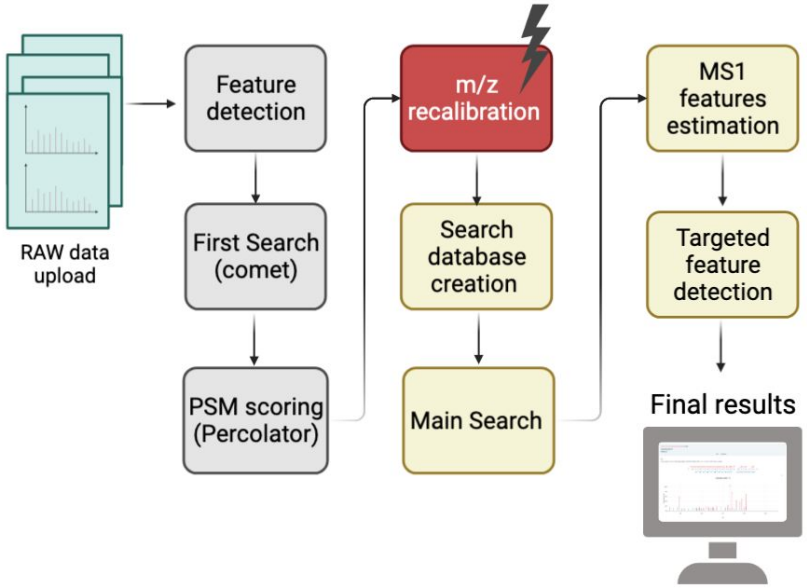




Created with BioRender.com

Automated benchmarking in action

After we make a change to a step: the underlying code changes



Created with BioRender.com

Create a new *build* for one pipeline with one click

Mass Dynamics / Benchmarking - Peptide Mapping PXD009441 / main
s3 bucket: PXD009441-93dd-4d99-8b90-930c84b7056b workflow: dcdfb159-d30c-4535-bf31...

All Builds | Edit Steps | Pipeline Settings | New Build

Test New Workflow
Build #98 | main | aa47550

Passed in 10s and blocked

buildkite-agent pi... | Be | Prepare python environ...

Remove deletable tags | Print | Rep...

Anna Quaglieri
Created today at 10:25 | Triggered

Rebuild | Cancel

buildkite-agent pipeline upl | Waited 6s | ip-172-31-18-181.ap-southeas...

New Build

Message

Test New Workflow

Description of the build. If left blank, the commit message will be used once the build starts.

Commit — Required

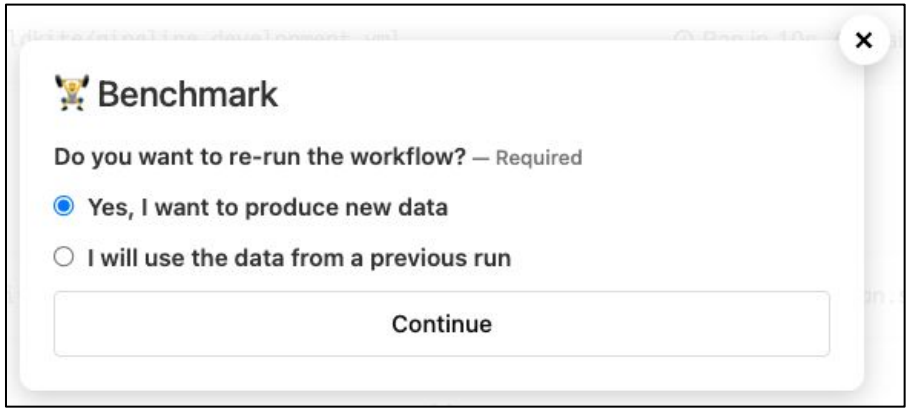
HEAD

Branch — Required

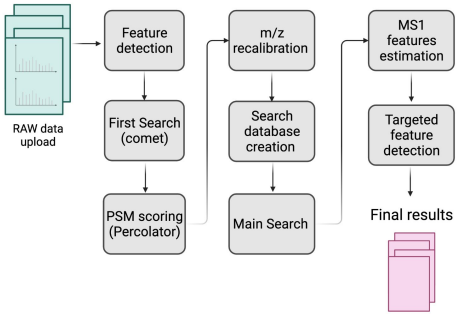
main

Options

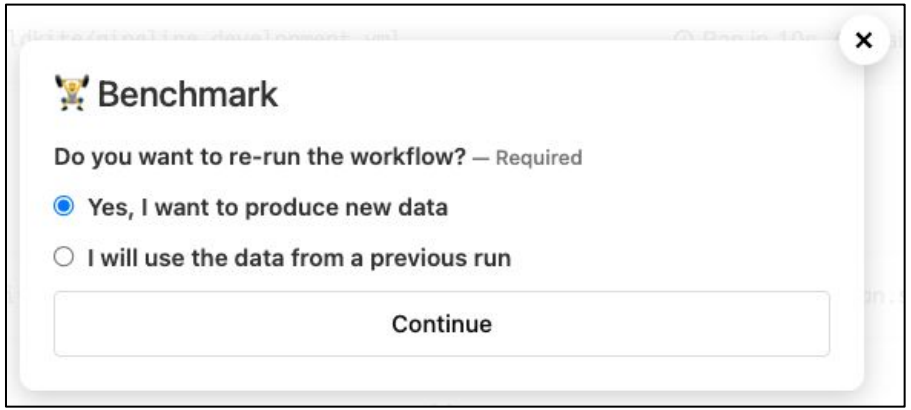
Create Build



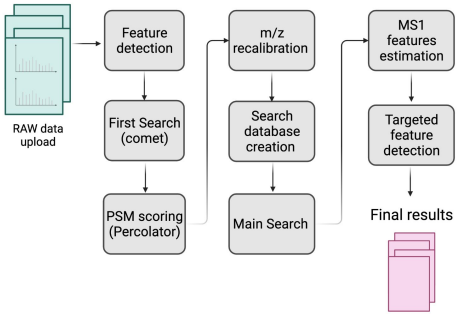
Run the Peptide Mapping Workflow end to end



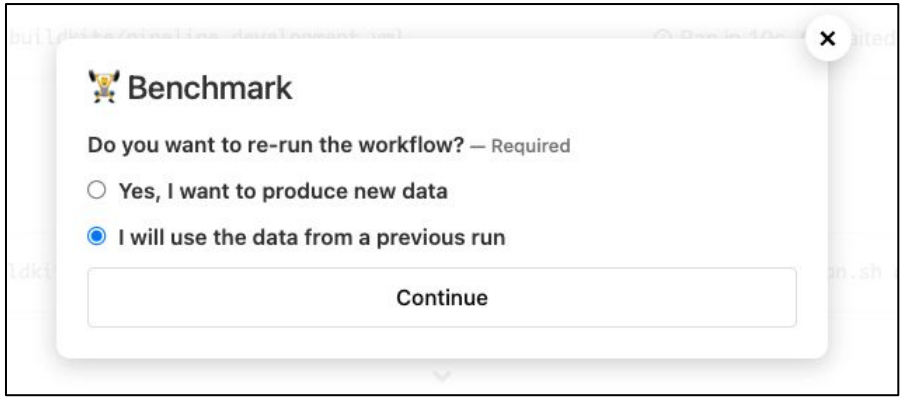
~ 2-7h



Run the Peptide Mapping Workflow end to end



~ 2-7h



Only run benchmarking code with the data already created

~ 10-15 min

If everything is good 

Mass Dynamics / Benchmarking - Peptide Mapping PXD009441 FTFT Reduce...
s3 bucket: PXD009441-93dd-4d99-8b90-930c84b7056b-reduced workflow: dcdfb159-d30c-4...

All Builds | Edit Steps | Pipeline Settings | New Build

Fix pipeline take 3
Build #27 | asms | a646cd6

Passed in 13m 3s

buildkite-agent pi... > Benchmark > Clean previous workflow > Start workflow > Wait for workflow > Prepare python environ... >
Remove deletable tags > Print AMIs > Test benchmarking code > Download + Create Rep... > Download + Test

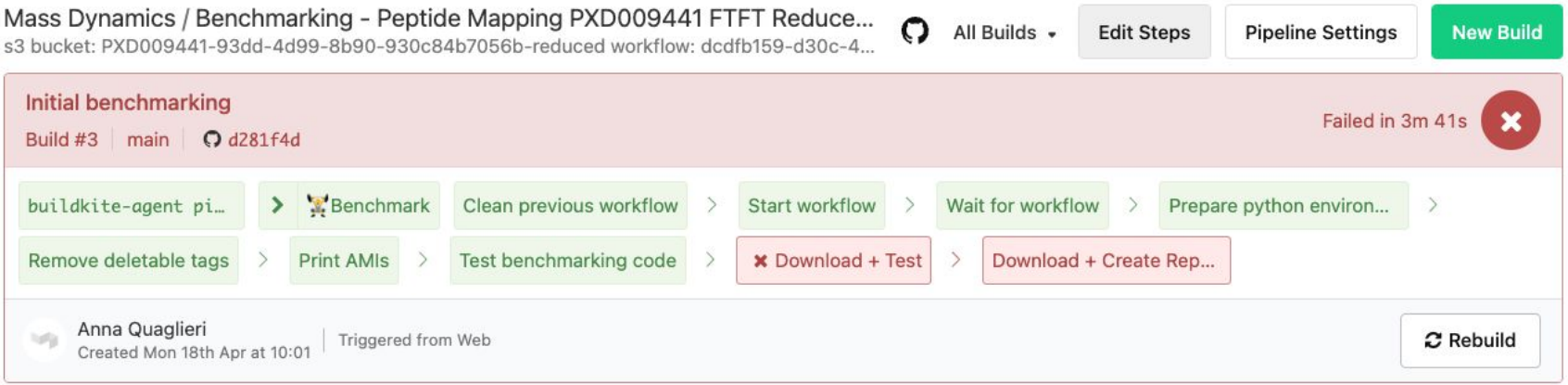
Anna Quaglieri
Created yesterday at 17:42 | Triggered from Web

Rebuild

buildkite-agent pipeline upload .buildkite/pipeline.development.yml

Ran in 6s | Waited 4s | ip-172-31-1-98.ap-southeast-...

If some tests fail

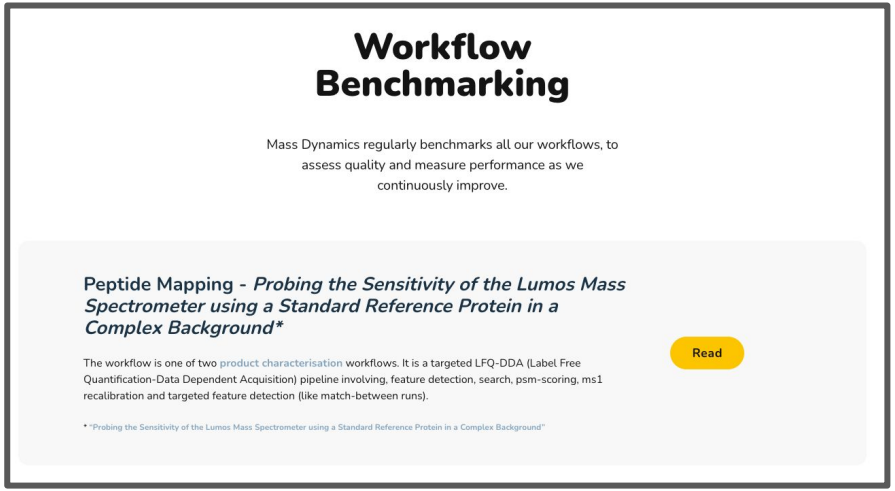


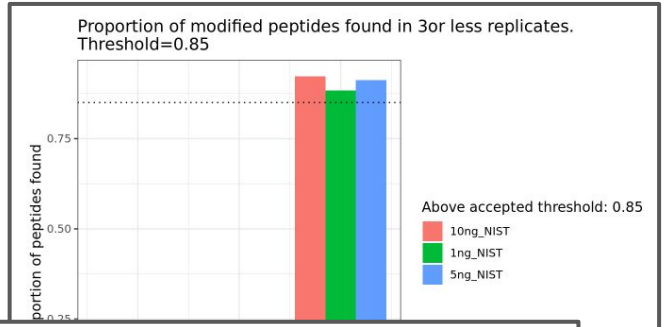
Public benchmarking report

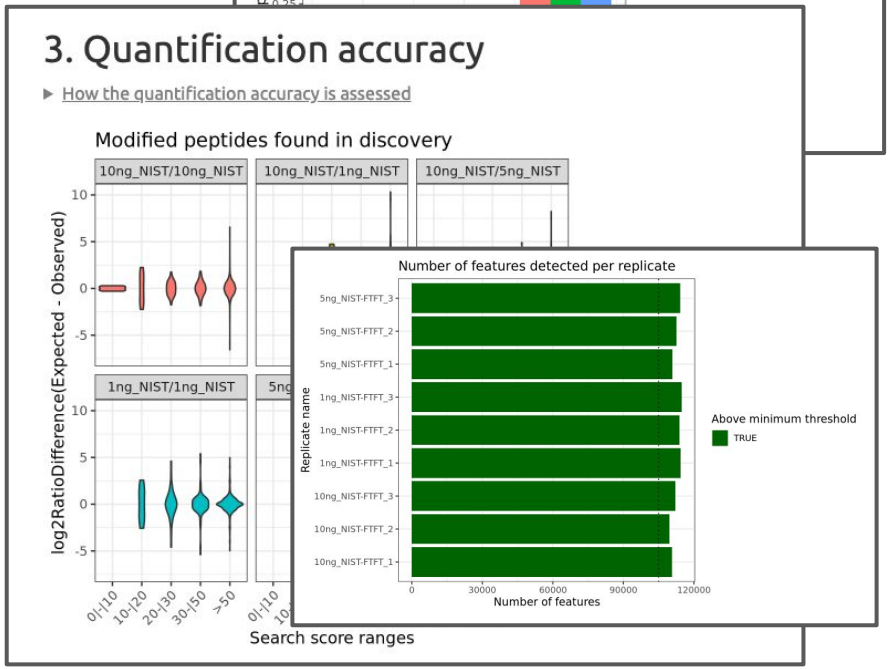
app.massdynamics.com/content/workflow/reports

Dataset with ground truth: PXD009441

Levy MG et al, 2018, JPR





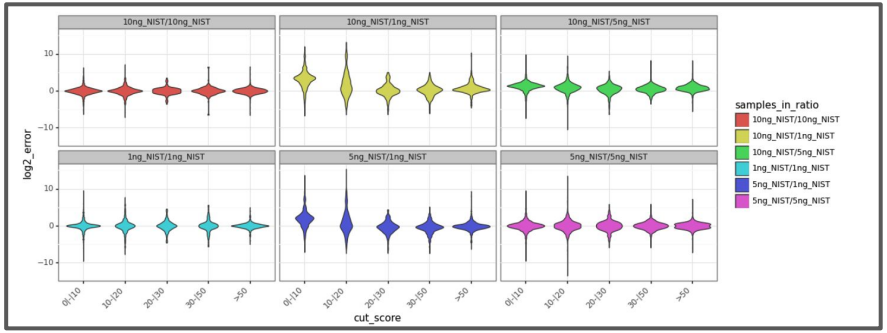


How we use the benchmarking system

Once we add a new dataset we use the results as our first benchmark

```yaml
name: PXD009441
description-benchmark: "Initial quality control report of PXD900441"
tests:
  data:
    number-of-runs: 24
    number-of-samples: 8
    replicates-per-sample: 3
  feature-detection-thermo:
    minimum-features-per-run: 100000
  protein-inference:
    expected-target-above-threshold: 0.001
    expected-decoy-below-threshold: 0.01
    q-value-threshold-psms: 0.01
    q-value-threshold-peptides: 0.01
```

Quantitative accuracy against ground truth



How we use the benchmarking setup

When the **workflow changes** we compare the results against the benchmark:

Did we improve?

Did we make it worse?

What changed?

For example: If we get a loss of identifications,

what has also changed in previous steps?

Today vs 1 year ago

- Gained quick and efficient way of getting confidence in our results
- We are more able to work concurrently than before
- Largely increased the spread of datasets that we check
- Gained a lot of knowledge about the intermediate steps and what to expect

Summary

Described the setup of Mass Dynamics **automated benchmarking framework**

To elevate the scientific development & benchmarking to the same level as the software development

Wins 🏆

- **Confidence in results Accuracy**:
  - We can make small or large changes safely
- **Transparency**:
  - Standardised quality control reports shine lights on hidden steps
  - Quality control reports and benchmarking can be accessed and explored by anyone
- **Speed**:
  - Quicker development feedback; easy to set up for new datasets; enables concurrent work
  - Unlock possibility of adding new features quicker

Suggested links

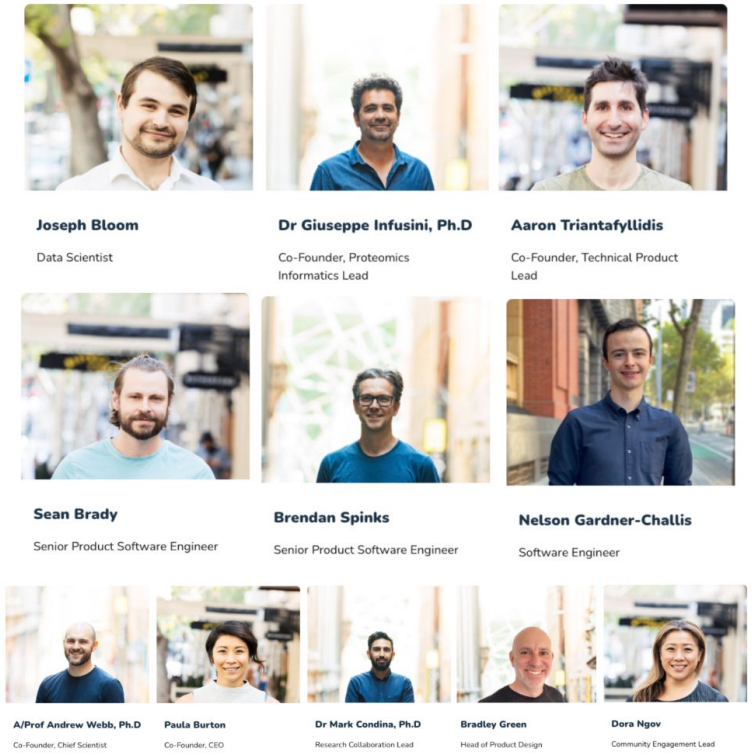
Suggested readings

- Continuous science (2021) Joseph Bloom, Towards Data Science
- DevOps and the scientific process: A perfect Pairing (2022) Christina Hupy, GitLab
- Benchmarking comes of age, (2019), Mark D. Robinson & Olga Vitek, *Genome Biology*

Examples from other fields

- Public benchmarks of robust reading methods: Robust Reading Competition
- From the AI community: Hugging Face

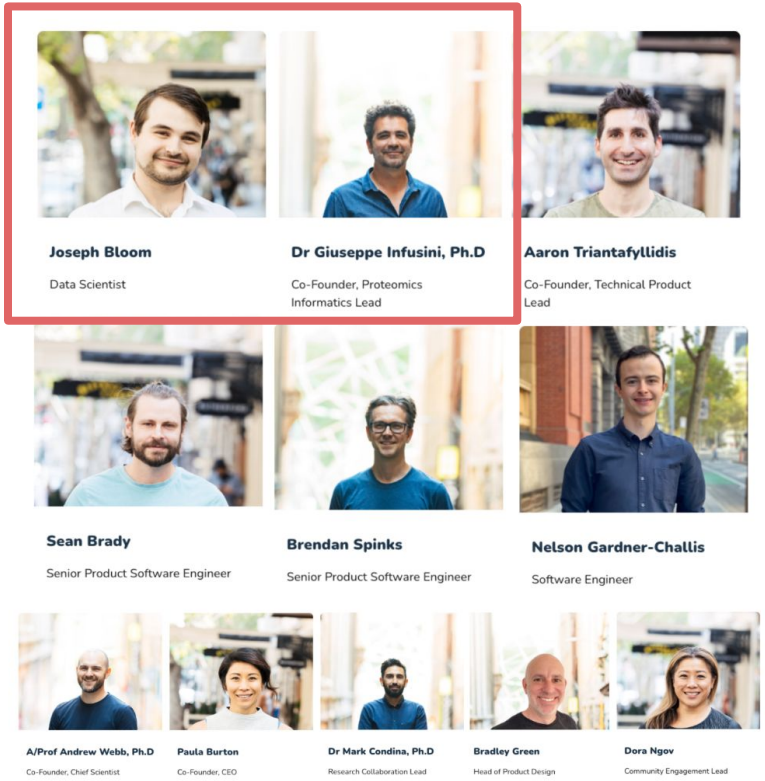
Acknowledgements



Thanks to the Mass Dynamics Team

Booth 727

Acknowledgements



Science team

Thanks to the Mass Dynamics Team

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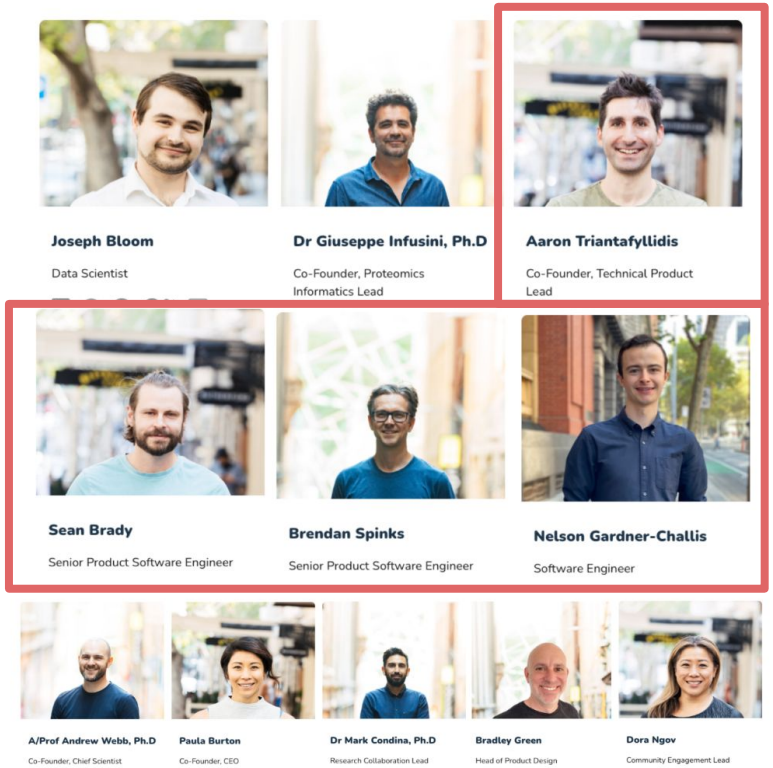
Acknowledgements



Developers team

Thanks to the Mass Dynamics Team

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Acknowledgements

PXD009441

Probing the Sensitivity of the Orbitrap Lumos Mass Spectrometer Using a Standard Reference Protein in a Complex Background

Michaella J Levy [1], Michael P Washburn [1] [2], Laurence Florens [1]

Thanks to all the scientists who created the benchmarking data

RETURN TO ISSUE | < PREV **ARTICLE** NEXT >

ABRF Proteome Informatics Research Group (iPRG) 2015 Study: Detection of Differentially Abundant Proteins in Label-Free Quantitative LC–MS/MS Experiments

Meena Choi[#†], Zeynep F. Eren-Dogu[#‡], Christopher Colangelo[§], John Cottrell[ǁ], Michael R. Hoopmann[⊥], Eugene A. Kapp[¶], Sangtae Kim[⊗], Henry Lam[□], Thomas A. Neubert[■], Magnus Palmblad[○], Brett S. Phinney[●], Susan T. Weintraub[△], Brendan MacLean[▲], and Olga Vitek[*†]