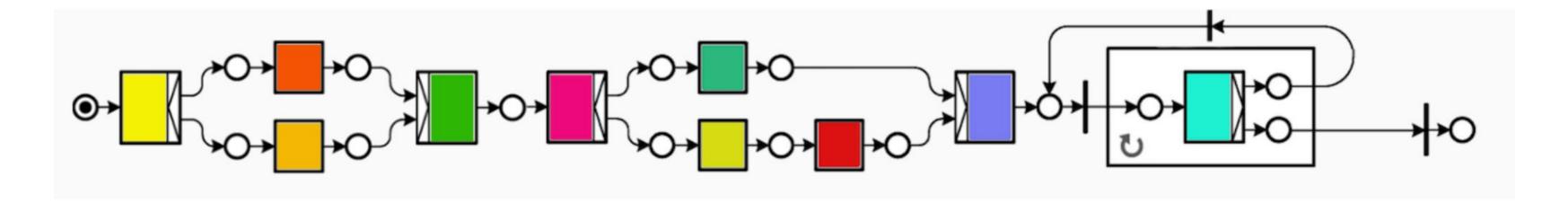
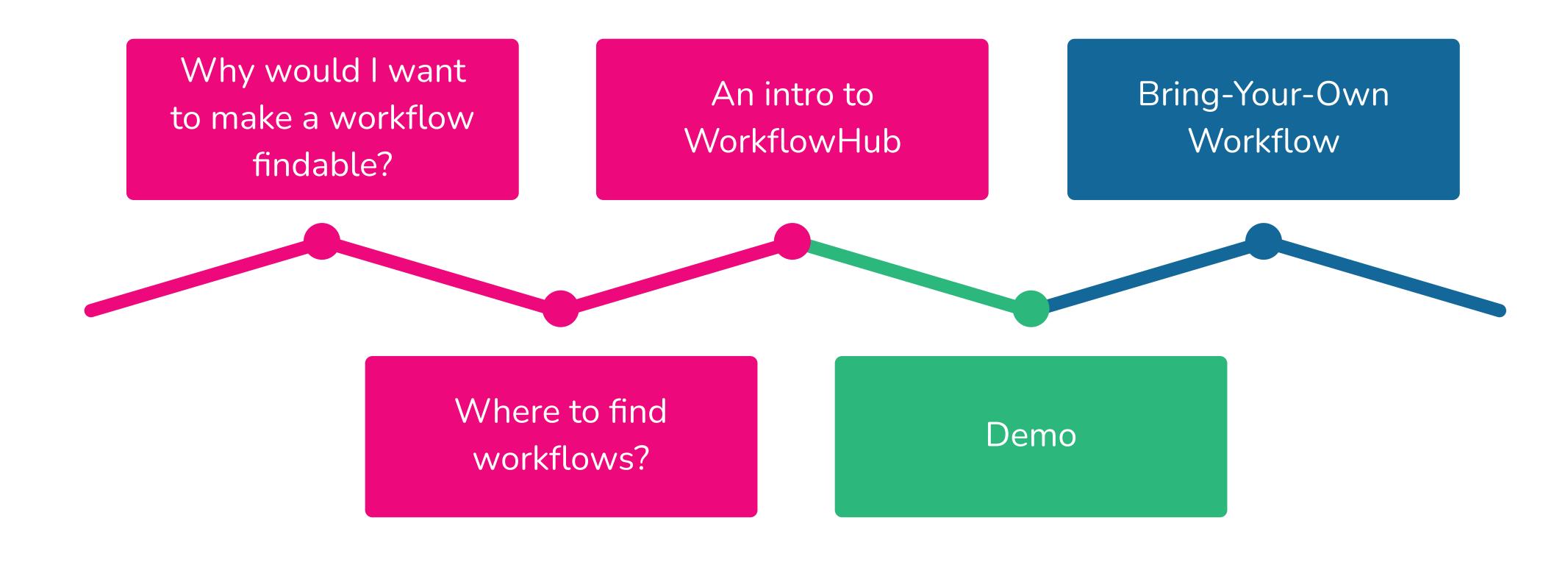
Make your bioinformatics workflows findable and citable



Johan Gustafsson, Australian BioCommons Georgina Samaha, Sydney Informatics Hub

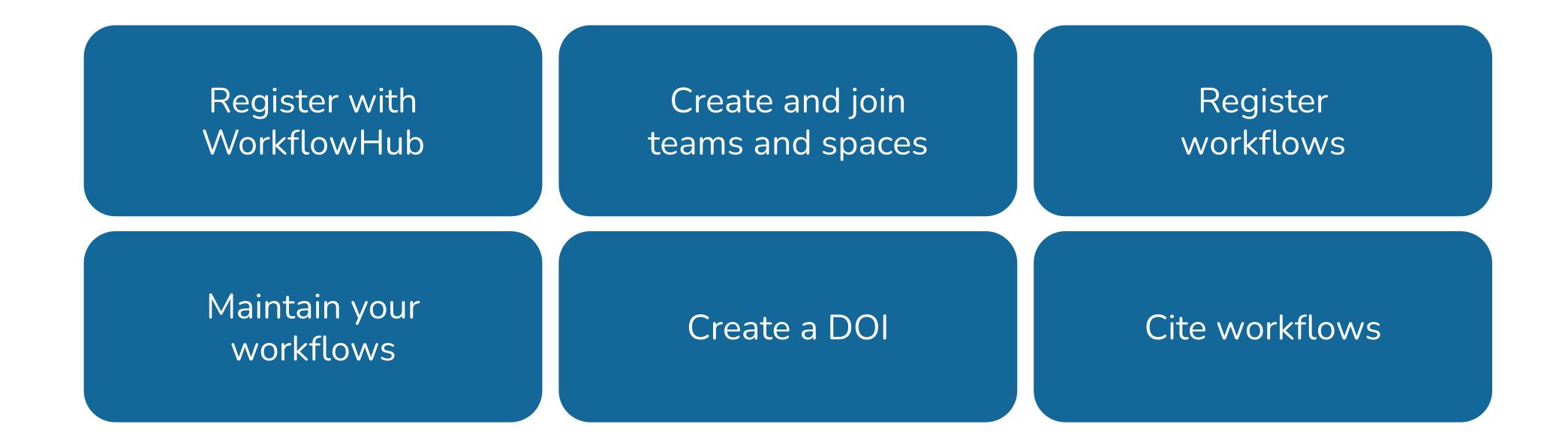


Today

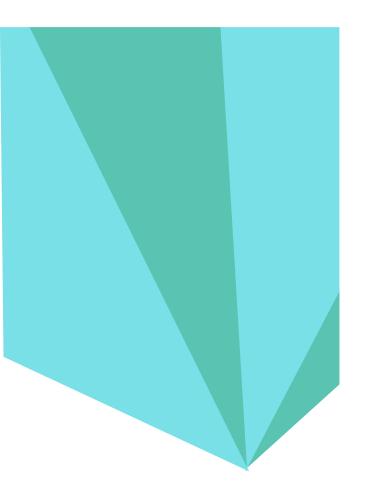




Learning outcomes







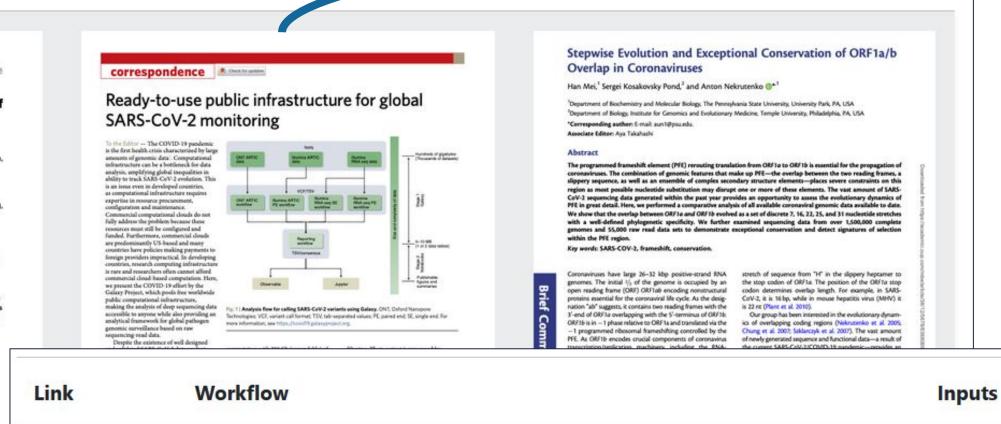
Why make workflows findable?

Workflows are important

GalaxyProject SARS-CoV-2 analysis effort

https://galaxyproject.org/projects/covid19/

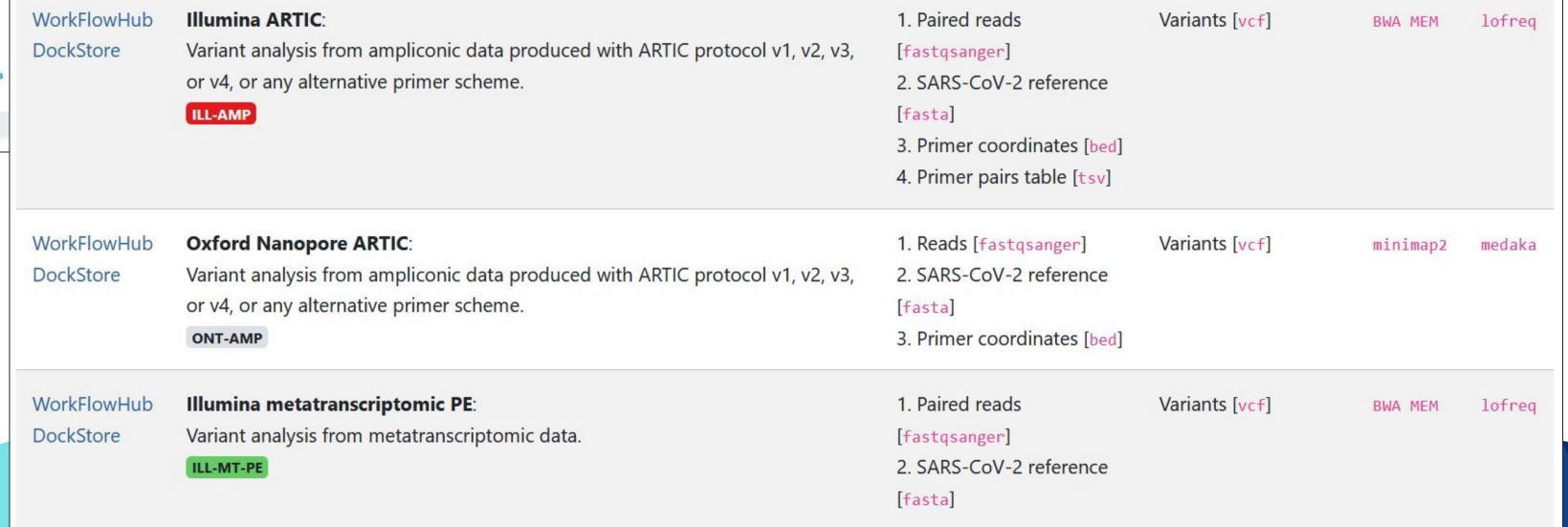




Maier W, Bray S, et al. Ready-to-use public infrastructure for global SARS-CoV-2 monitoring. 10.1038/s41587-021-01069-1

Outputs

Caller





Workflows are important

326

workflow languages

https://s.apache.org/existing-workfl ow-systems

1.34 M

clones for nf-core workflows

https://nf-co.re/stats



Workflows are important

326

workflow languages

https://s.apache.org/existing-workfl ow-systems

1.34 M

clones for nf-core workflows

https://nf-co.re/stats

2,262

workflows in Dockstore (WDL, CWL, NextFlow, Galaxy)

https://dockstore.org/search?entryT
ype=workflows&searchMode=files

298

workflows in WorkflowHub (all public)

https://workflowhub.eu/workflows

874

of workflows on Galaxy Europe instance

https://usegalaxy.eu/api/workflows

329

of workflows on Galaxy Australia instance

https://usegalaxy.org.au/api/workflows



Workflows can also be ...

- **Time consuming**
- Maintenance heavy
- O Difficult to find
- O Difficult to redeploy
- O Duplicated by many

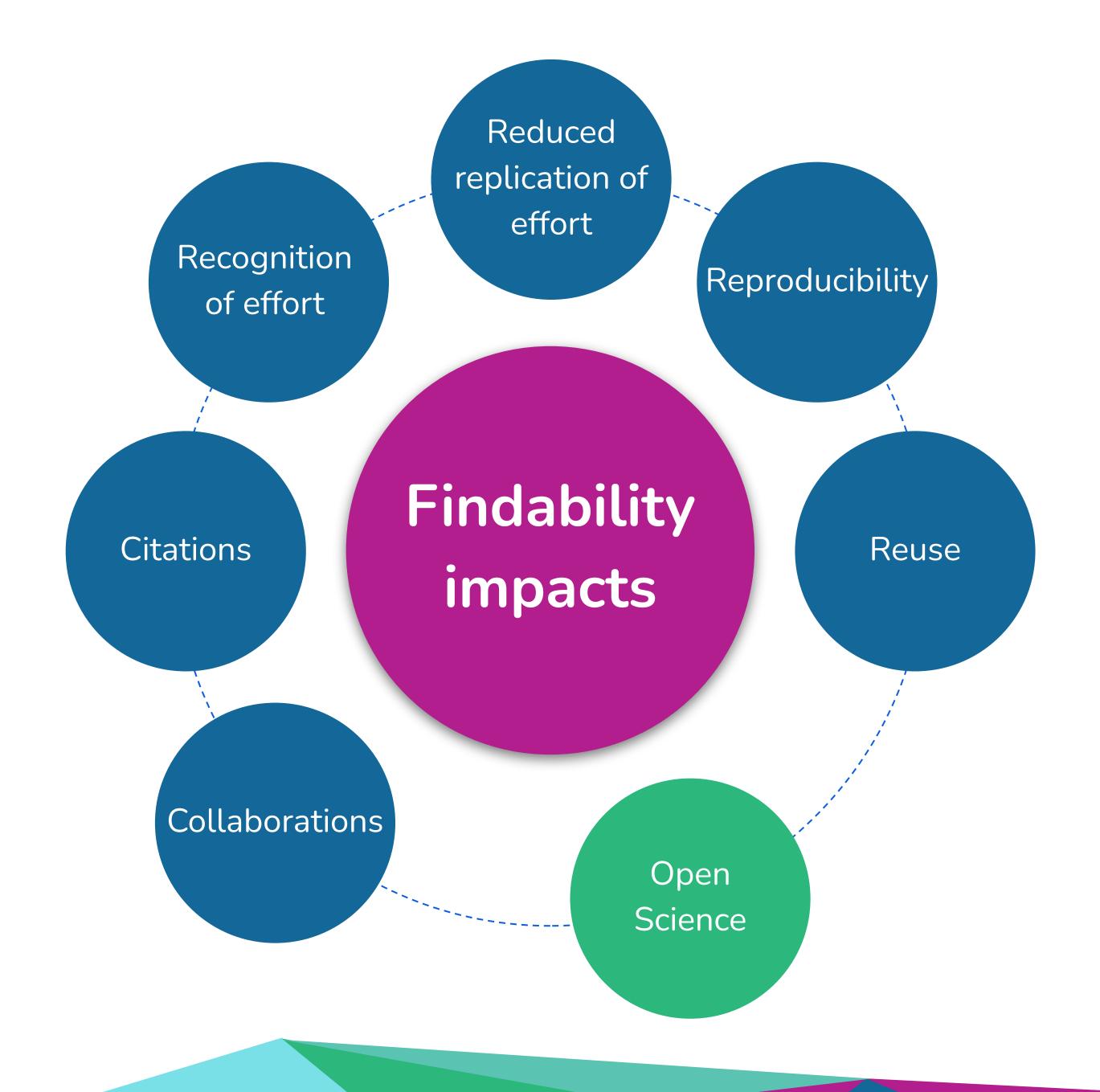


... and should be ...

- Difficult to find
- Difficult to redeploy
- Duplicated by many

- **Solution** Findable
- Reusable
- **©** Citable



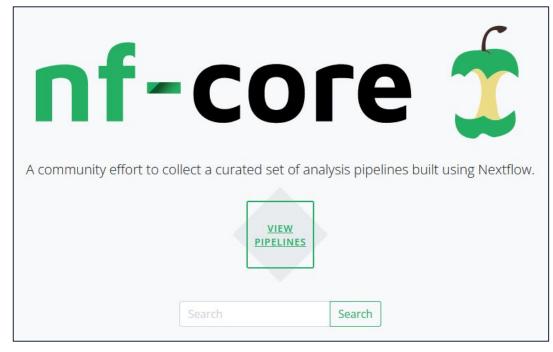




So where can I 2 find workflows?

Platforms / community repositories

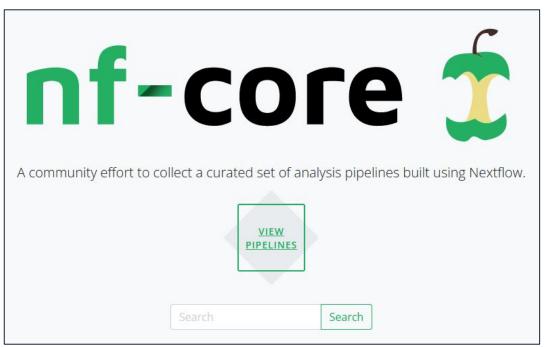




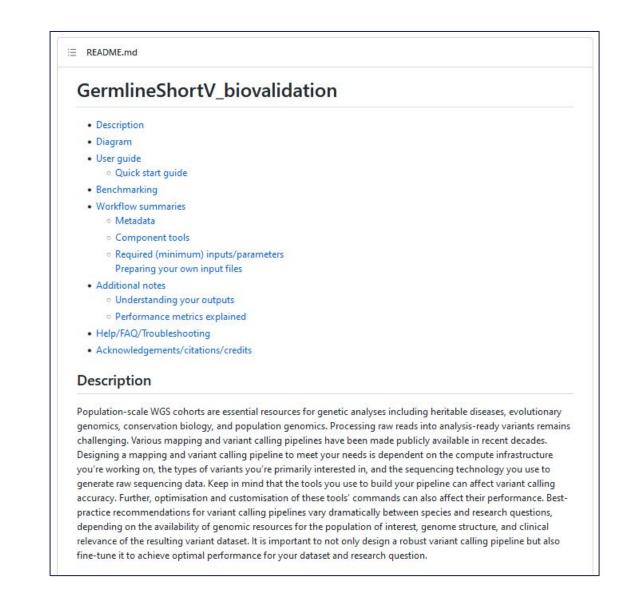


Platforms / community repositories





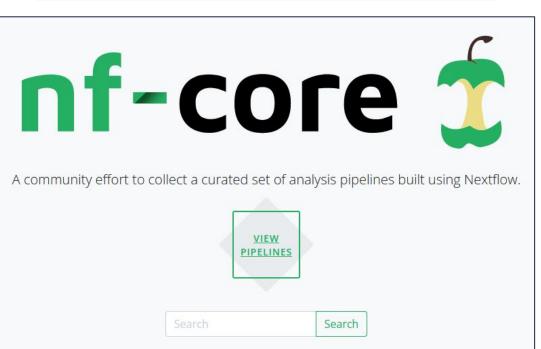
GitHub



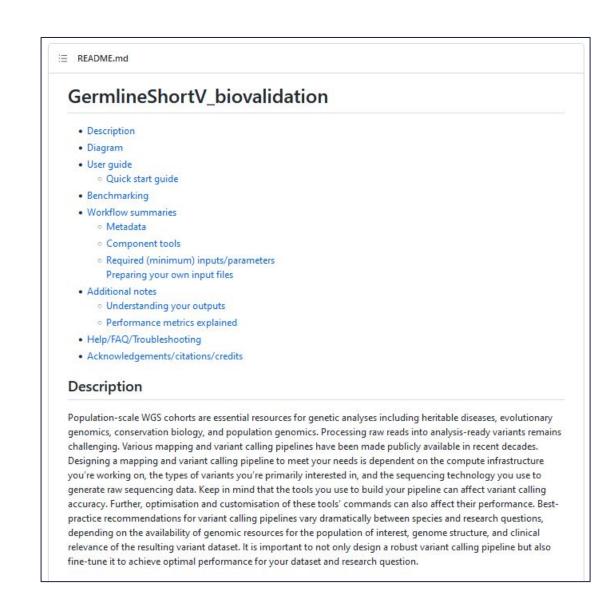


Platforms / community repositories





GitHub



Publications

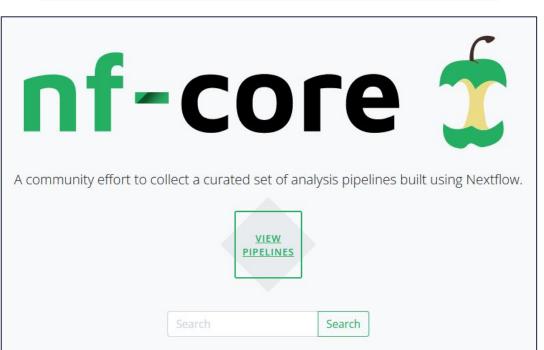
Murigneux, V., Roberts, L.W., Forde, B.M. *et al.* MicroPIPE: validating an end-to-end workflow for high-quality complete bacterial genome construction. *BMC Genomics* **22**, 474 (2021). https://doi.org/10.1186/s12864-021-07767-z

Lott, M. J., Wright, B. R., Neaves, L. E., Frankham, G. J., Dennison, S., Eldridge, M. D. B., Potter, S., Alquezar-Planas, D. E., Hogg, C. J., Belov, K., & Johnson, R. N. (2022). Future-proofing the koala: Synergising genomic and environmental data for effective species management. Molecular Ecology, 31, 3035–3055. https://doi.org/10.1111/mec.16446

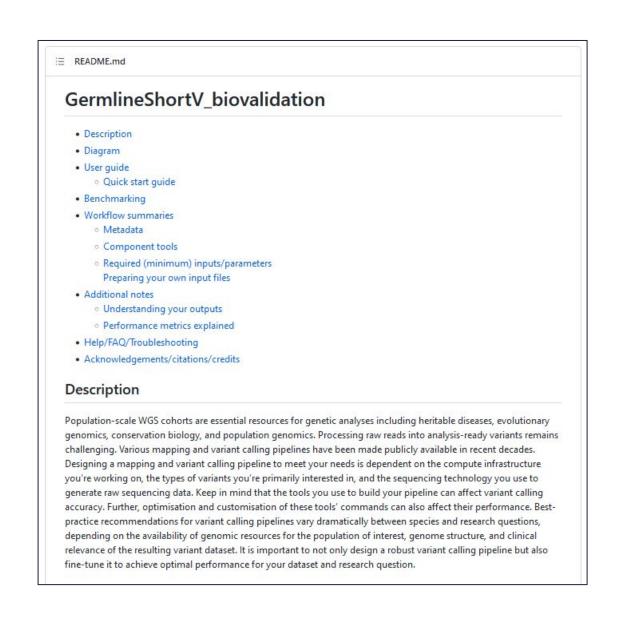


Platforms / community repositories





GitHub



Publications

Murigneux, V., Roberts, L.W., Forde, B.M. *et al.* MicroPIPE: validating an end-to-end workflow for high-quality complete bacterial genome construction. *BMC Genomics* **22**, 474 (2021). https://doi.org/10.1186/s12864-021-07767-z

Lott, M. J., Wright, B. R., Neaves, L. E., Frankham, G. J., Dennison, S., Eldridge, M. D. B., Potter, S., Alquezar-Planas, D. E., Hogg, C. J., Belov, K., & Johnson, R. N. (2022). Future-proofing the koala: Synergising genomic and environmental data for effective species management. Molecular Ecology, 31, 3035–3055. https://doi.org/10.1111/mec.16446

Google



Consider a registry

- searchable
- integrated
- standardised
- interoperable



Infrastructure efforts

Publications

Workflow organisations



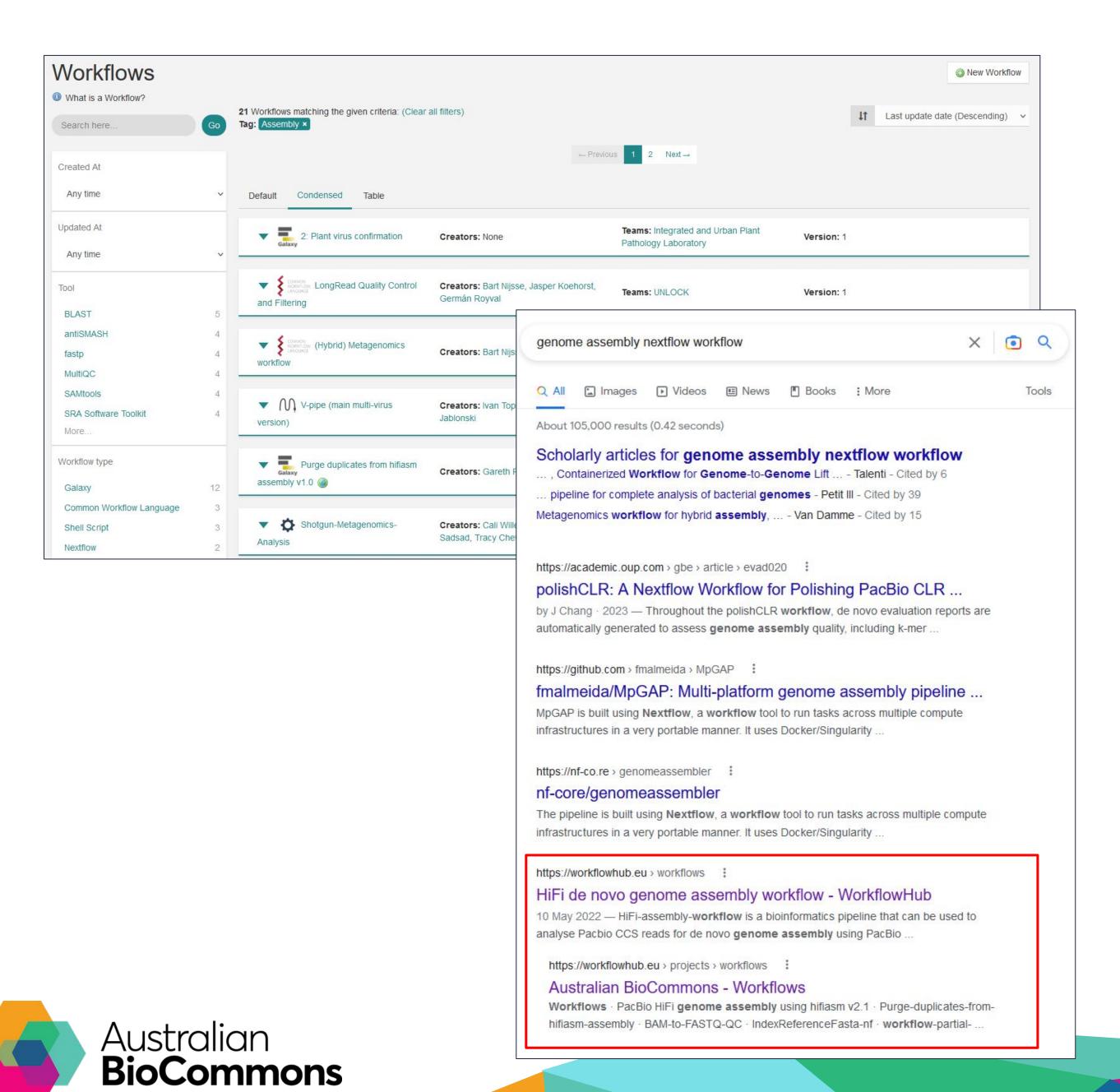


Single GitHub repositories

Workflow language specific registries

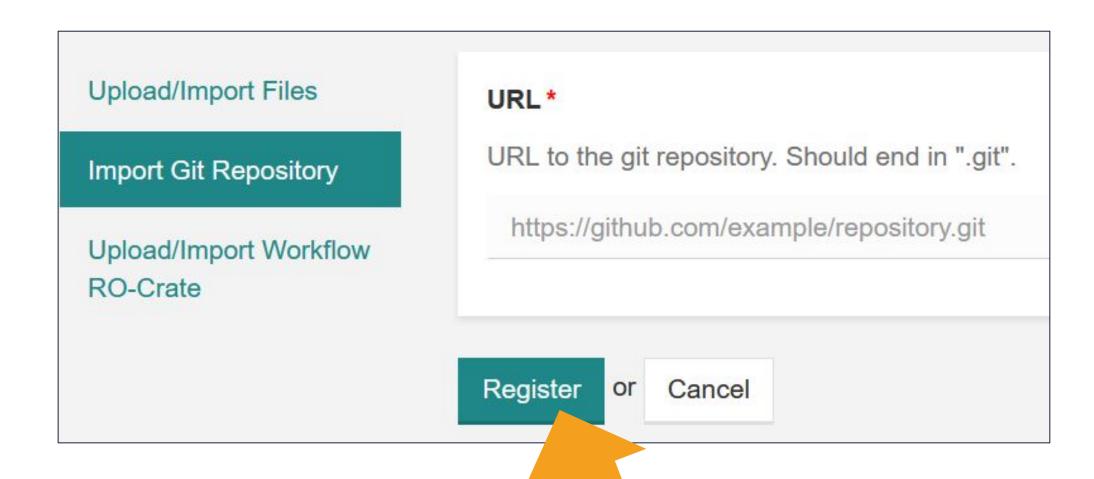
Research consortia

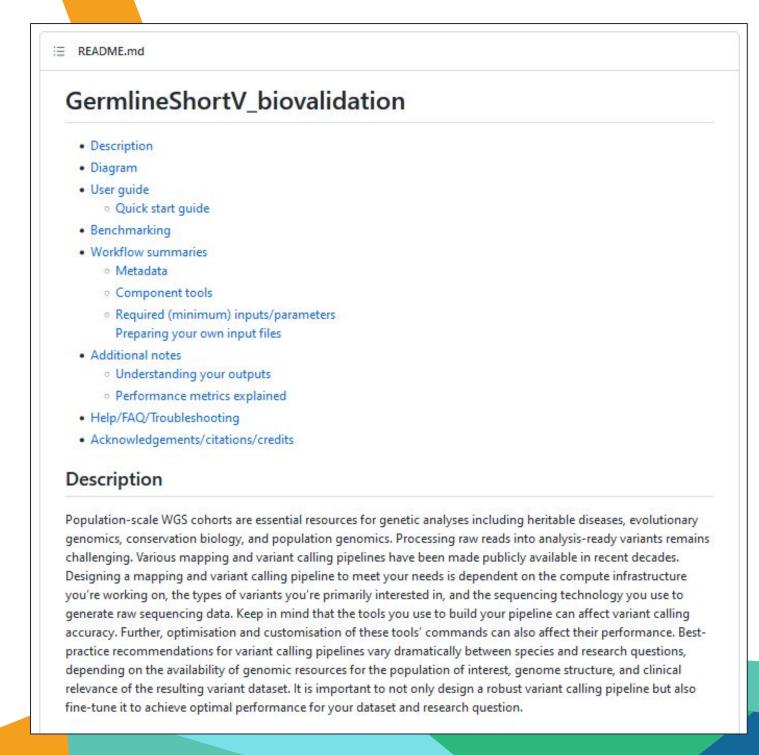












- **o** integrated



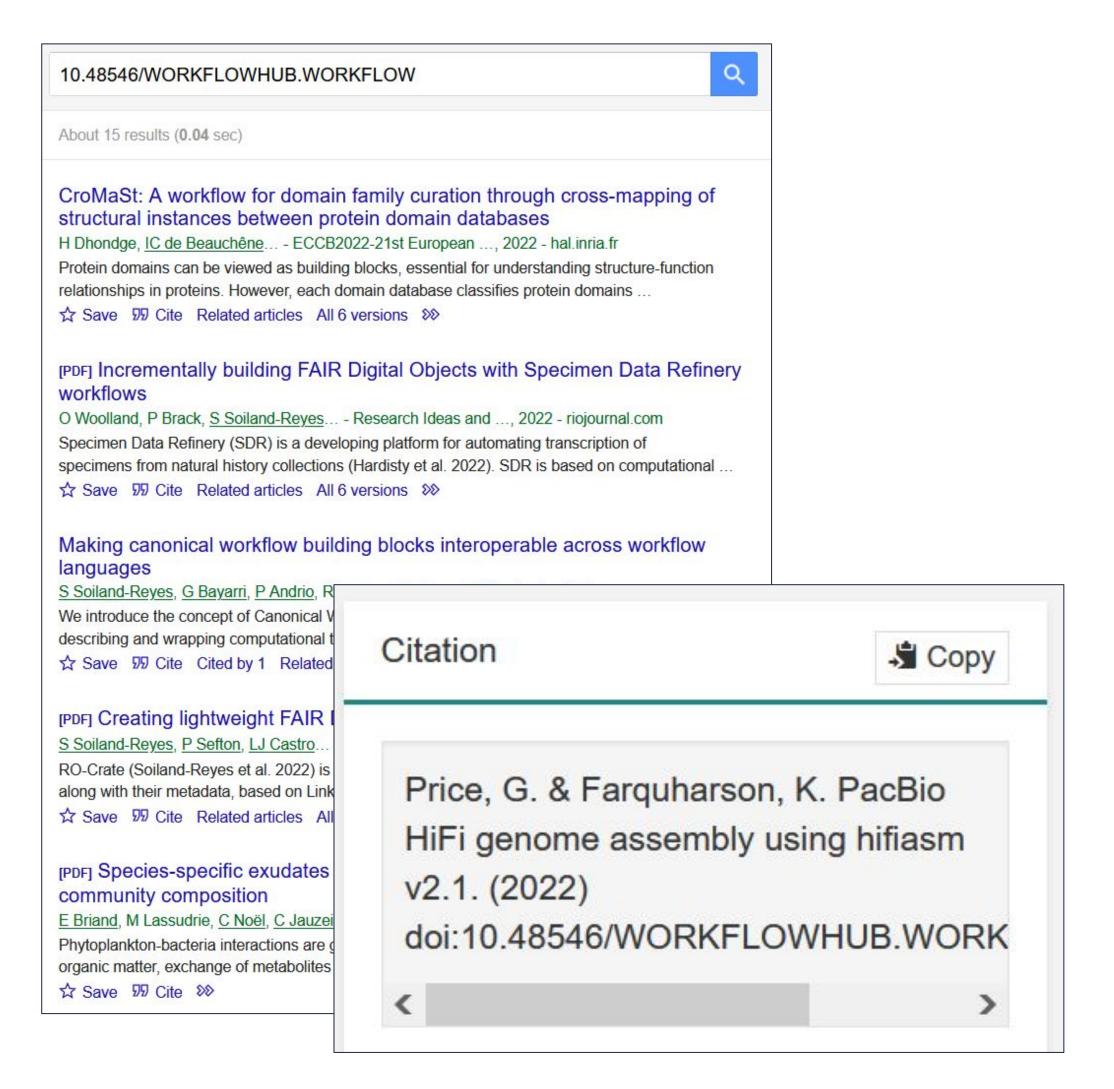
Name	Description	Mandatory
Title*	This field is mandatory and is with some workflow types pre-filled with the title of the workflow.	Yes
Description	If a CWL (abstract) file is given, the description will be parsed automatically out of the doc attribute. In any other case this field can be used to write some documentation that will be shown on the workflow page.	No
Source	If the workflow came from an external repository (i.e. GitHub), you can include its original URL here.	No
Maturity	This field can be used to specify in which maturity state the workflow is. The two available options are: • work-in-progress • stable	No
Teams*	Every workflow registration is linked to one or more teams. If you can not select the correct team, please go to Joining a team.	Yes
Licence	The standard licence is Apache Software Licence 2.0. If you did not make the workflow yourself, be sure that the licence corresponds to the licence where you took the workflow from (for example github licences).	No
Sharing	Specify who can view the summary, get access to the content, and edit the Workflow. This is possibly already filled in according to the selected project.	No
Tags	Choose an appropriate tag for your workflow. Please check if your tag is already available and use the existing one if so. If you make a new tag, keep it simple without capitals or spaces. For example all new covid-19 workflows need to be tagged with covid-19.	No
Creators	This is an important section where all the people that were involved in making / publishing this workflow are listed. These creators will be added to the metadata in the RO-crate. 3 sections are used to specify the contributors or creators of the workflow. So far you have specified the following creators	No

Based on computational workflow profile for BioSchemas

https://bioschemas.org/profiles/ComputationalWorkflow/1.0-RELEASE



Standardised



- **standardised**
- **⊘** citable

Price, G. & Farquharson, K. PacBio HiFi genome assembly using hifiasm v2.1. (2022)

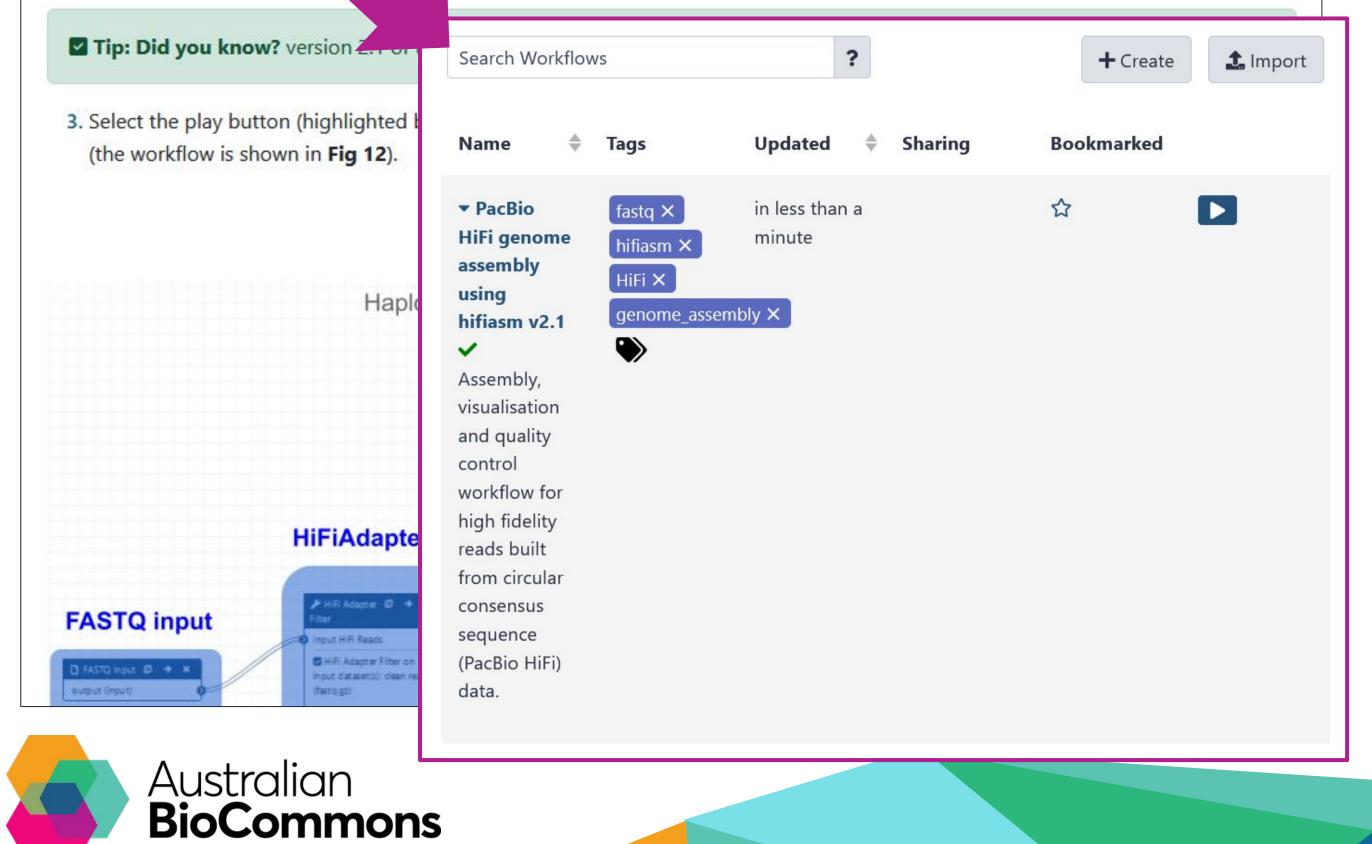
doi: https://doi.org/10.48546/WORKFLOWHUB.WORKFLOW.221.3





▲ Important: This workflow includes an adapter filtering step that makes use of HiFiAdapterFilt. Adapter contamination in the reads could cause misassemblies, and will result in NCBI rejecting the upload of affected genome assemblies. HiFiAdapterFilt identifies .ccs reads containing adapter sequences using the same method as NCBI and removes the entire read prior to genome assembly to avoid such misassemblies.

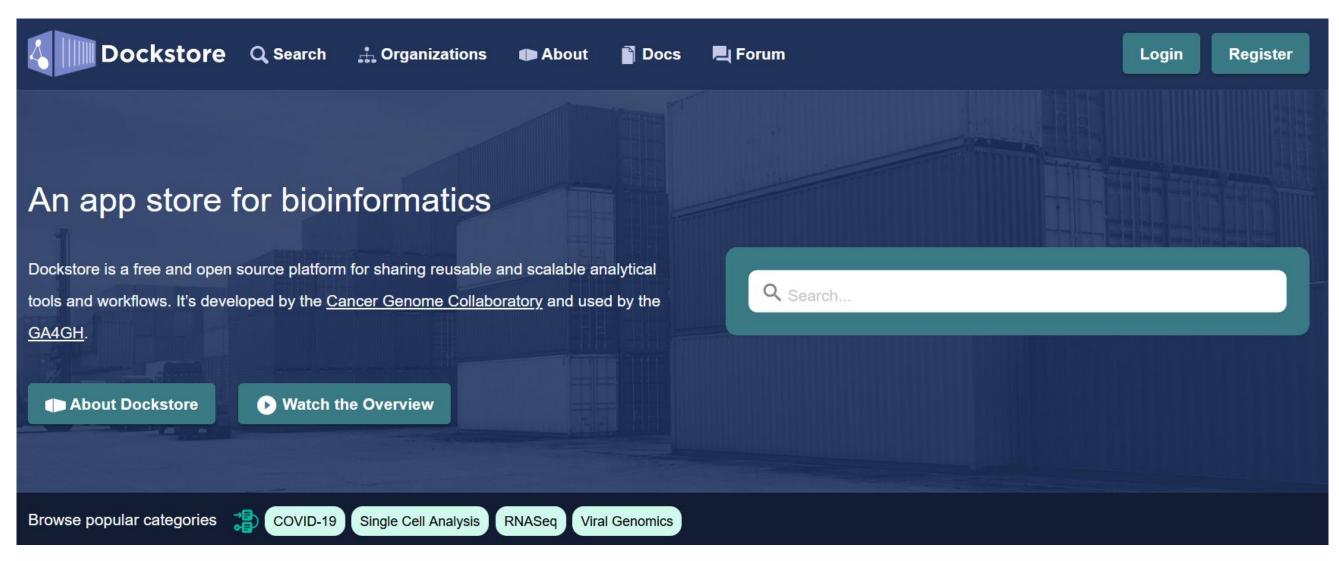
- 1 Make sure you are logged into Galaxy Australia
- 2. Visit this link to:
 - o retrieve v2 e assembly workflow,
 - o add it to you ustralia workflows list, and
 - open your workfile hich can also be reached by clicking the Workflow tab [highlighted by a red box in Fig 6] in the Galaxy interface)



- **standardised**
- **⊘** interoperable

Two key options

Dockstore



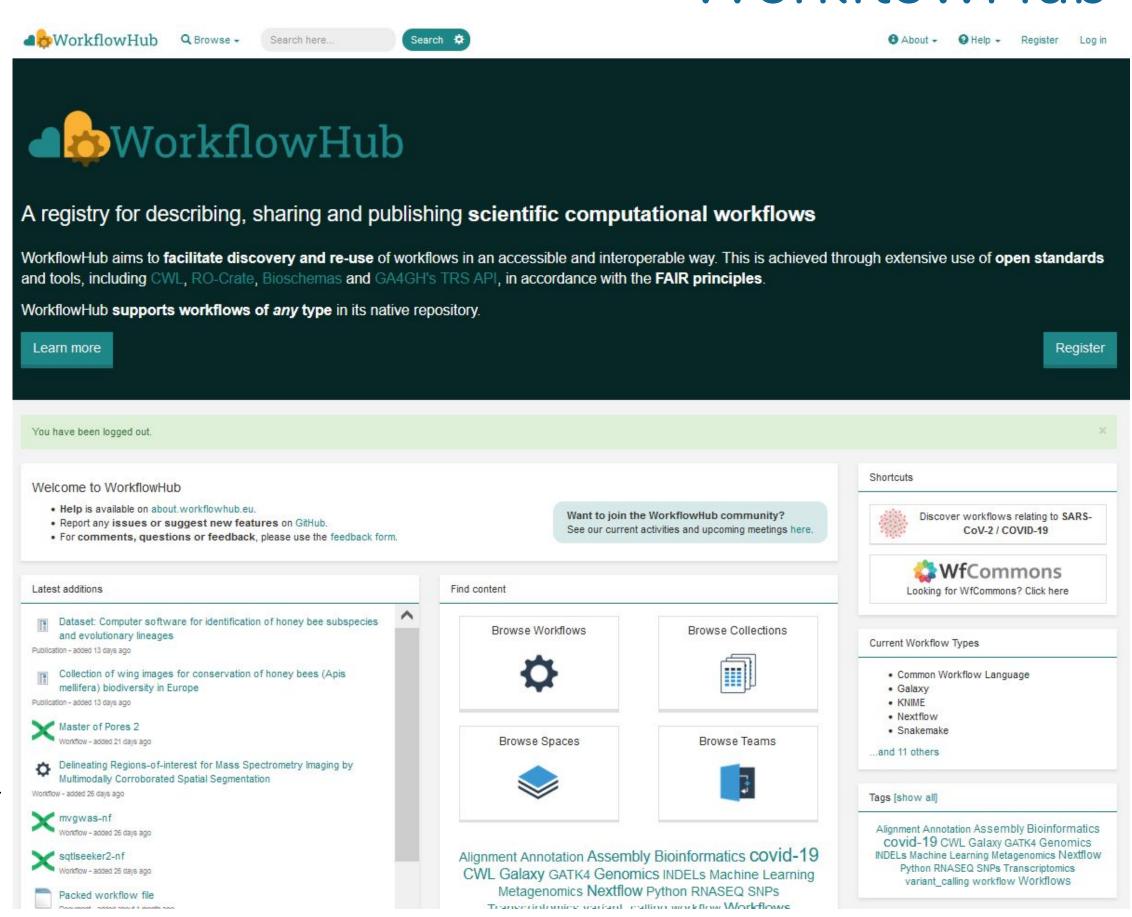
https://dockstore.org/

O'Connor BD, Yuen D, Chung V et al. The Dockstore: enabling modular, community-focused sharing of Docker-based genomics tools and workflows [version 1; peer review: 2 approved]. F1000Research 2017, 6:52 (https://doi.org/10.12688/f1000research.10137.1)



Two key options

WorkflowHub



https://workflowhub.eu/

Carole Goble, Stian Soiland-Reyes, Finn Bacall, Stuart Owen, Alan Williams, Ignacio Eguinoa, Bert Droesbeke, Simone Leo, Luca Pireddu, Laura Rodríguez-Navas, José Mª Fernández, Salvador Capella-Gutierrez, Hervé Ménager, Björn Grüning, Beatriz Serrano-Solano, Philip Ewels, & Frederik Coppens. (2021). Implementing FAIR Digital Objects in the EOSC-Life Workflow Collaboratory. Zenodo. https://doi.org/10.5281/zenodo.4605654



Two key options

Dockstore WorkflowHub

Register tools and workflows

Register workflows

Standard metadata

Standard metadata

Git integration

Git integration

DOI minting capability

DOI minting capability

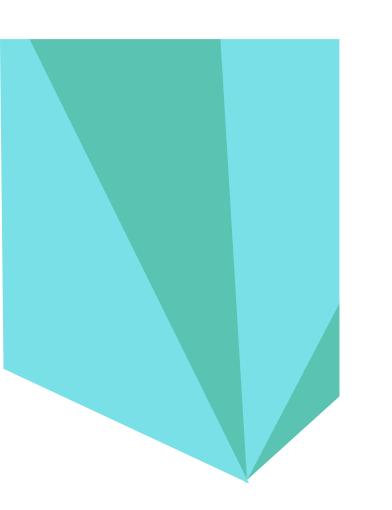
Organisations

Spaces & teams

WDL, CWL, Nextflow, Galaxy

All workflow types





WorkflowHub step-by-step

3

Shortcuts



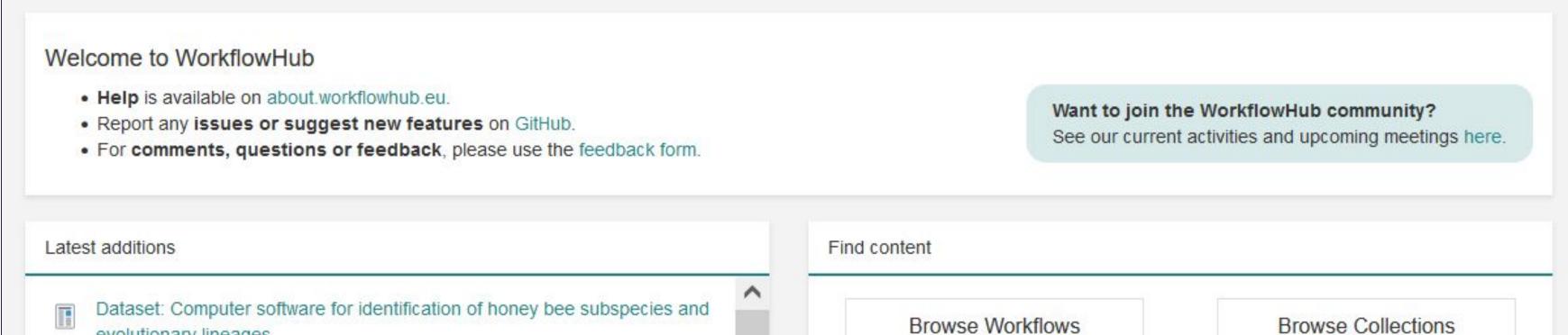
A registry for describing, sharing and publishing scientific computational workflows

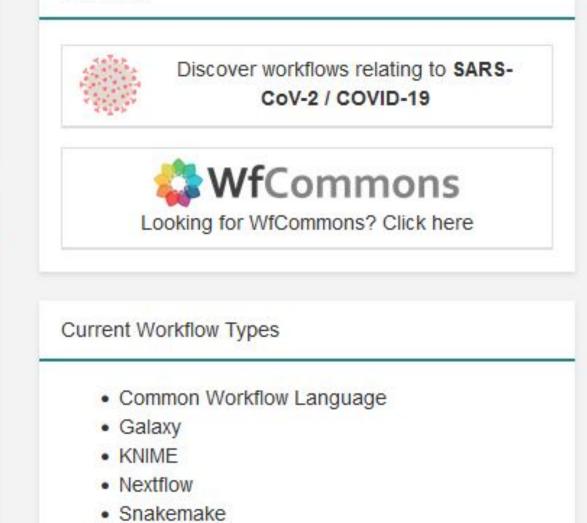
WorkflowHub aims to facilitate discovery and re-use of workflows in an accessible and interoperable way. This is achieved through extensive use of open standards and tools, including CWL, RO-Crate, Bioschemas and GA4GH's TRS API, in accordance with the FAIR principles.

WorkflowHub supports workflows of any type in its native repository.

Learn more

Register





Collection of wing images for conservation of honey bees (Apis mellifera) biodiversity in Europe

Publication - added 20 days ago

Publication - added 20 days ago

evolutionary lineages

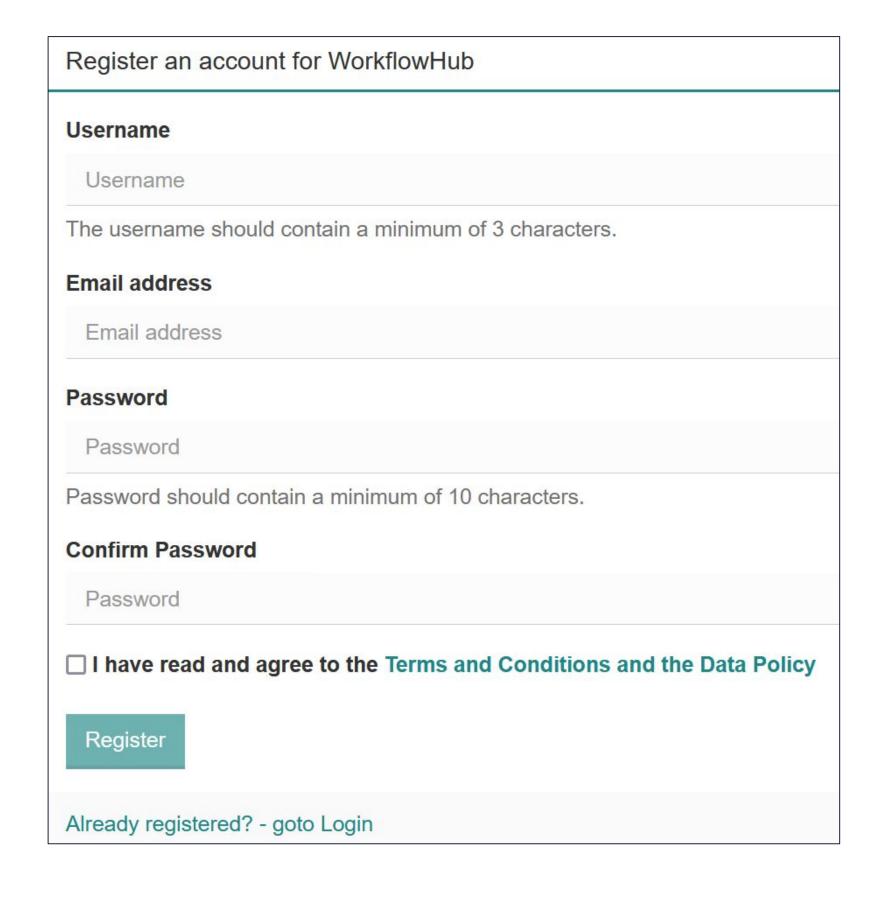


Browse Spaces

Browse Teams

Register







Log in using GitHub



Choose a space

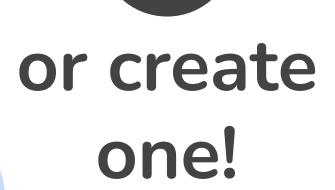






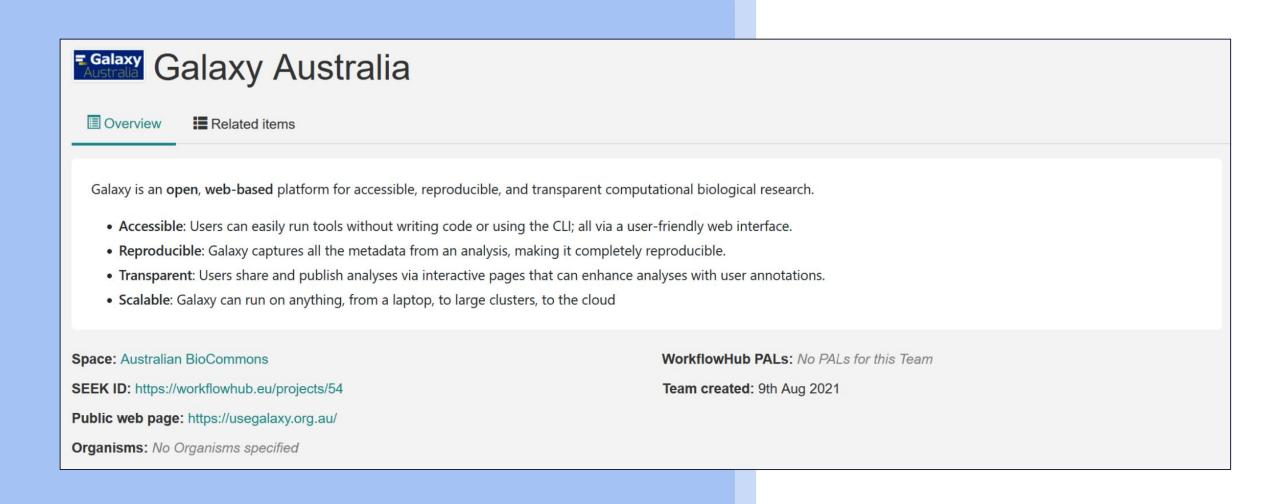


Join a team



Space

Team



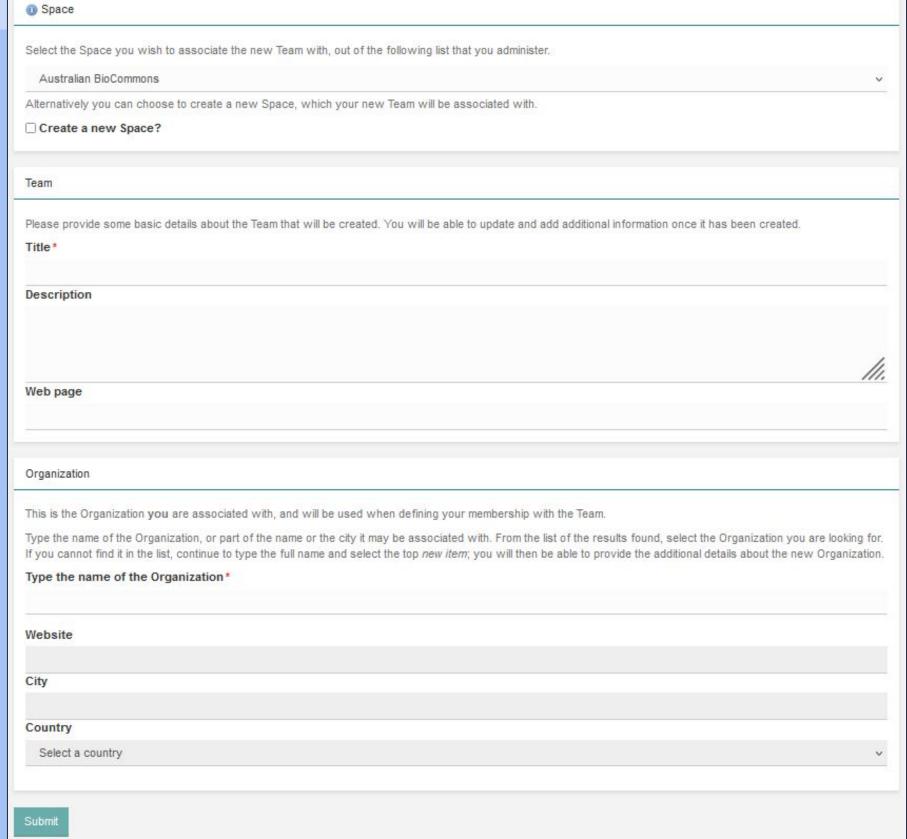


Join a team

or create one!

Space

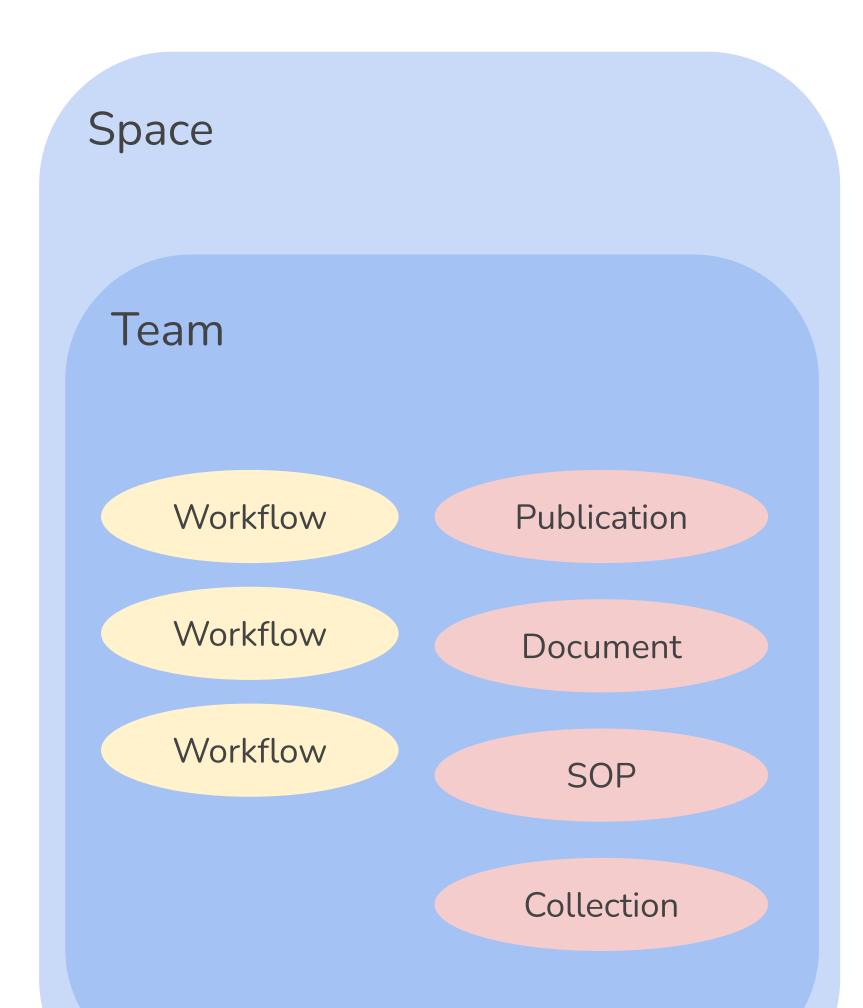
Τ	e	a	Ϋ́	1	



One wizard accommodates these processes

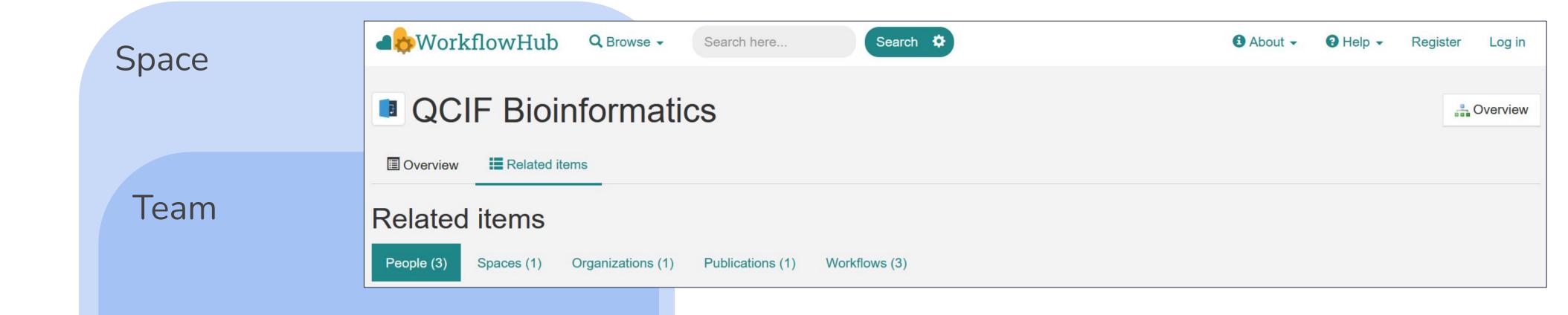


Add items



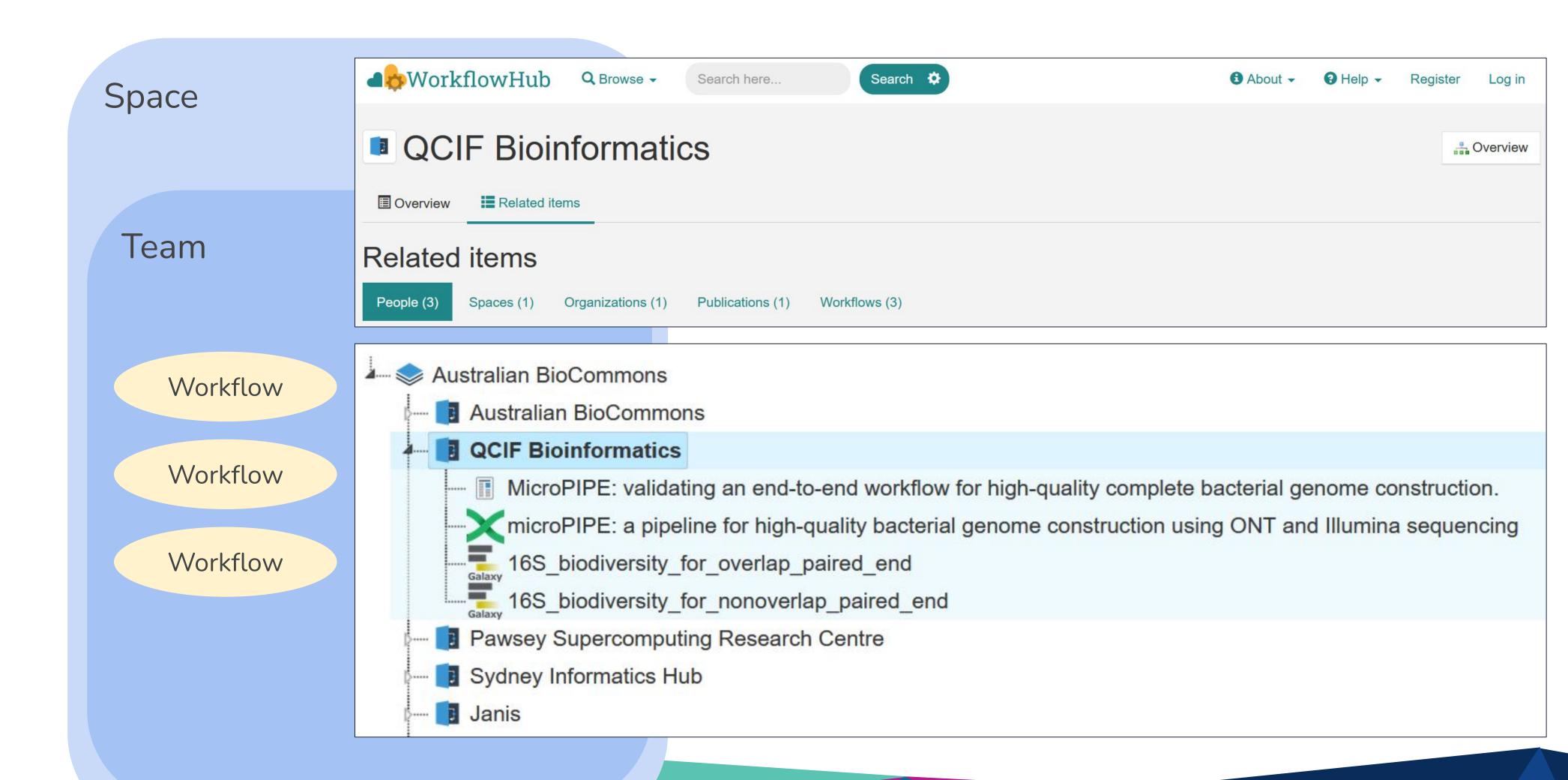


Add items





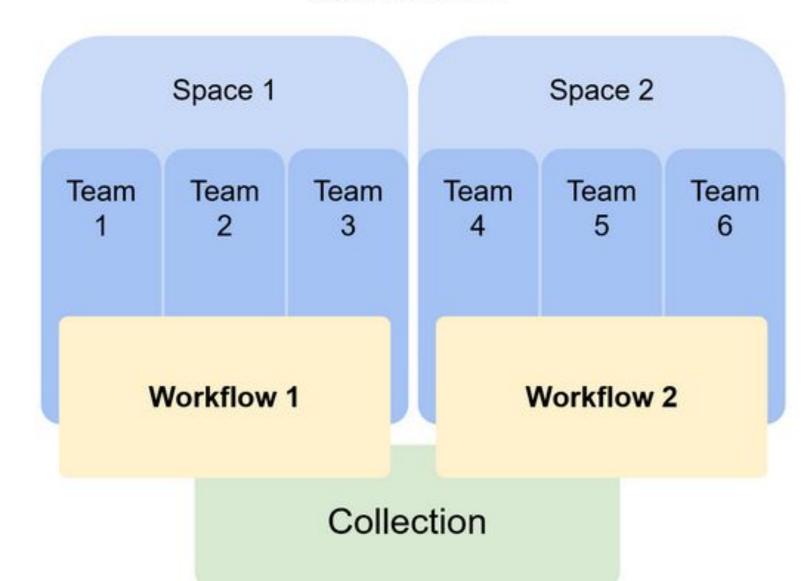
Add items





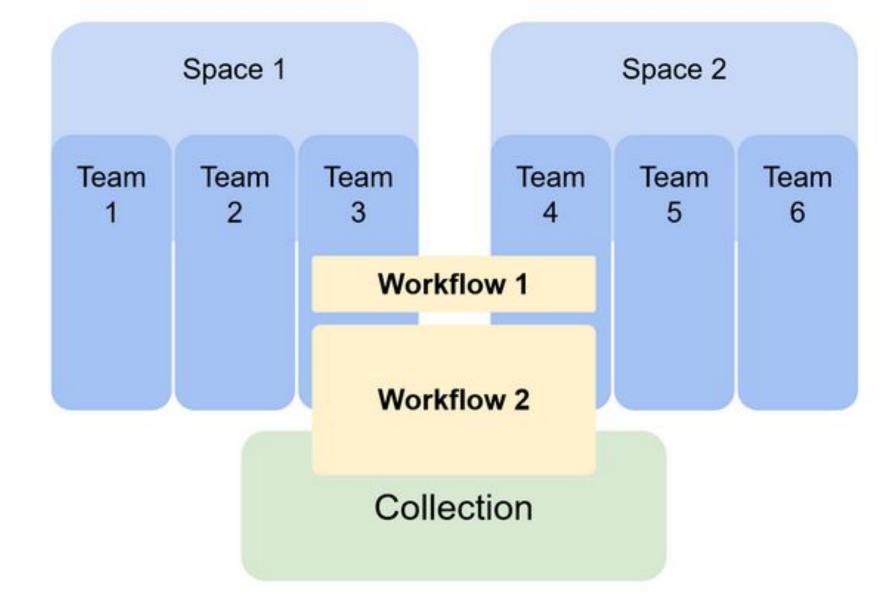
Note: these structures are flexible

Scenario A



- 3 Teams from space one, and 3 Teams from space two have created a workflow each
- These are both part of the same collection
- Spaces are not sharing a workflow, but do contribute to the same Collection

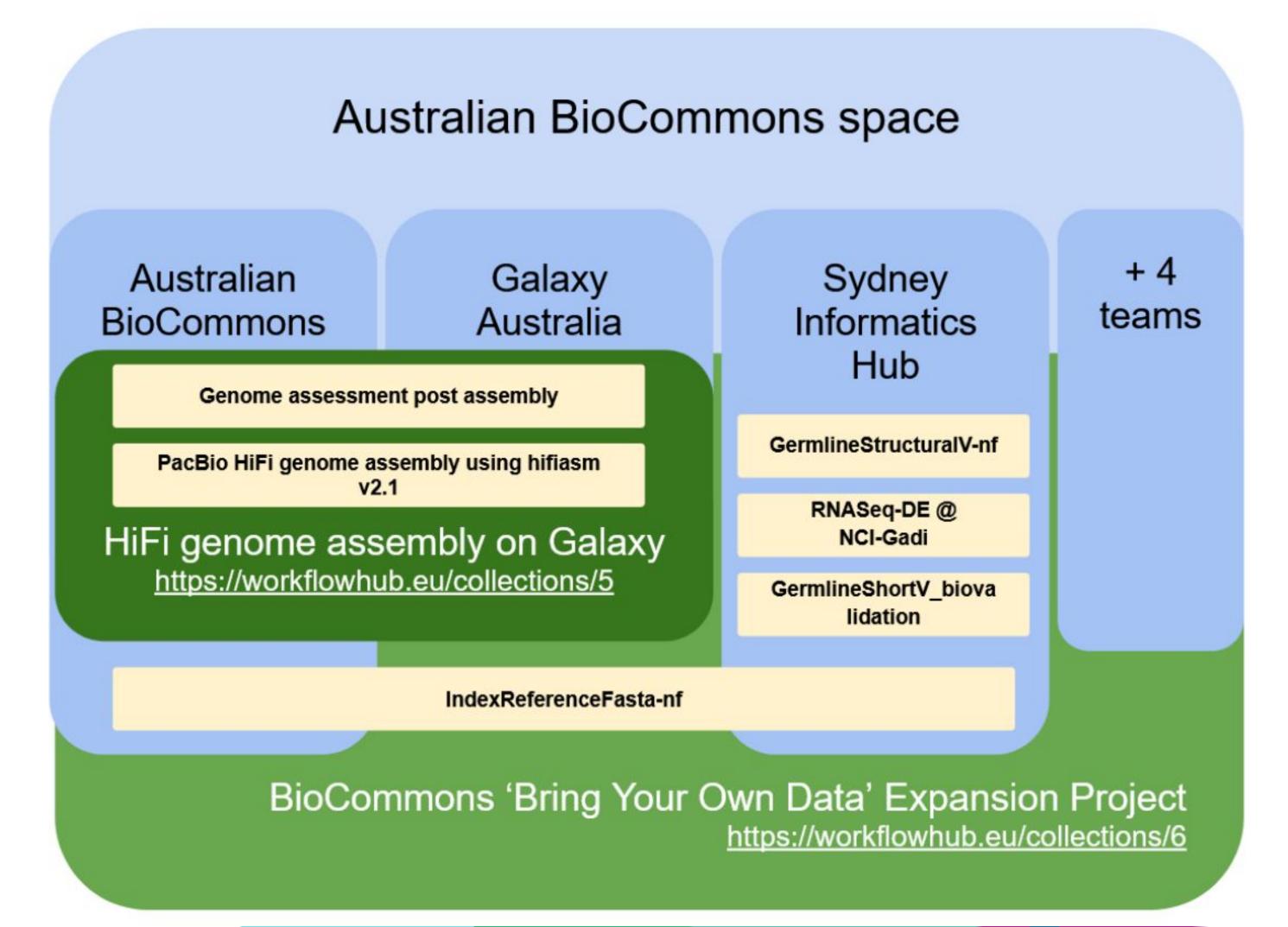
Scenario B



- Team #3 from space one, and team #4 from space two have collaborated to create 2x workflows
- Workflow 2 is contributed to a collection
- Spaces are sharing workflows via their component Teams, but do not directly share the workflows



Australian BioCommons example

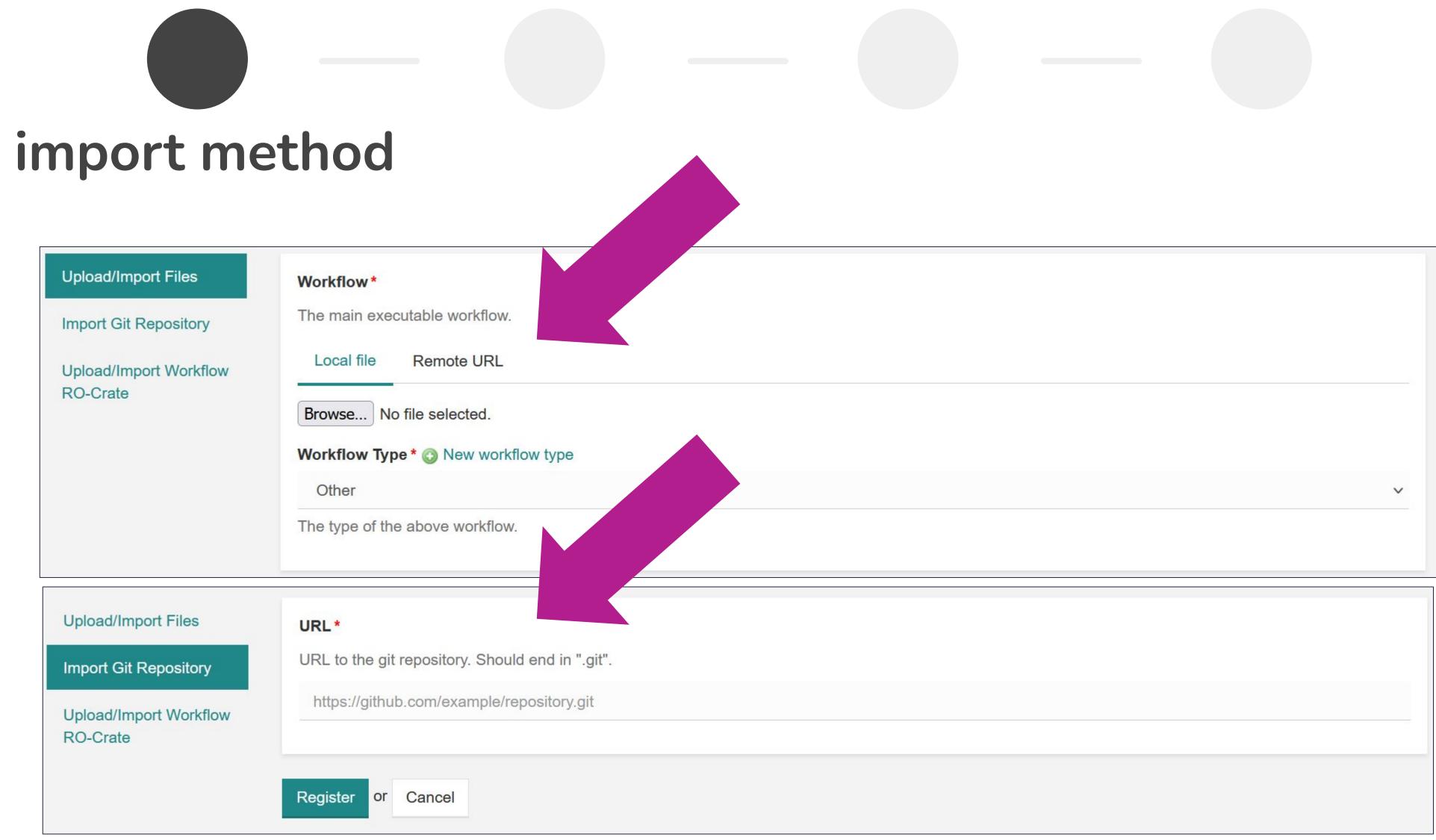




Let's register a workflow!



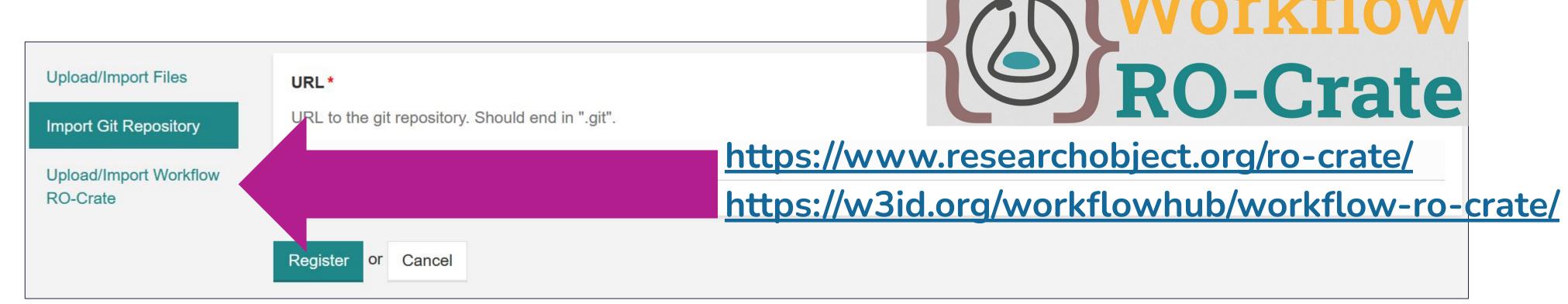
Select your file





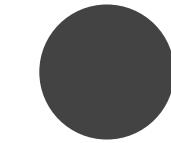
Select your file

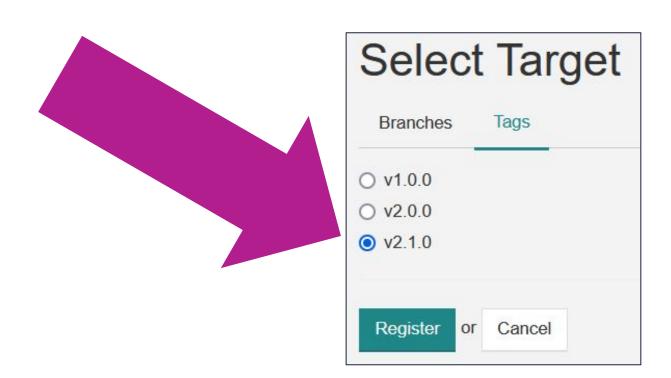






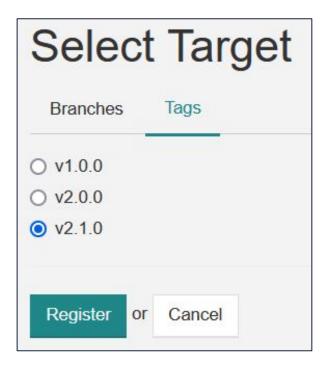
Import

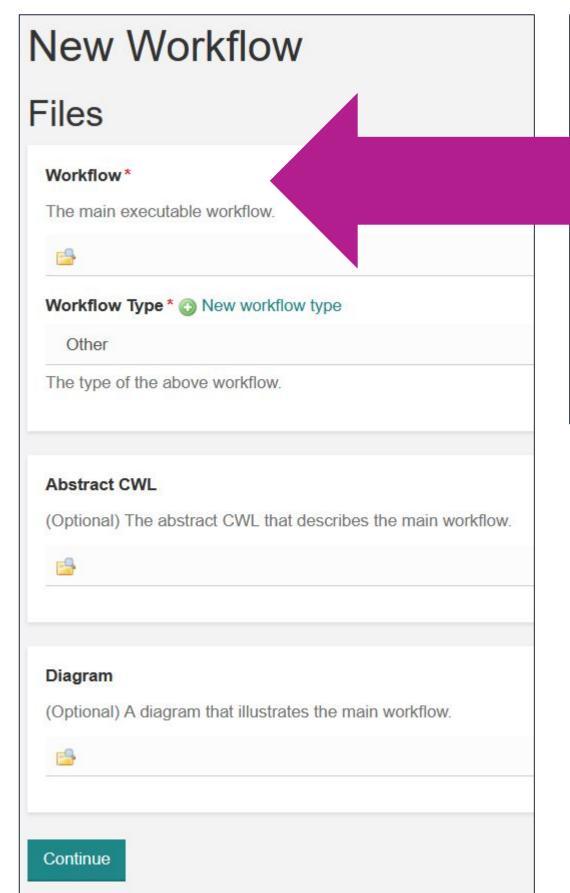


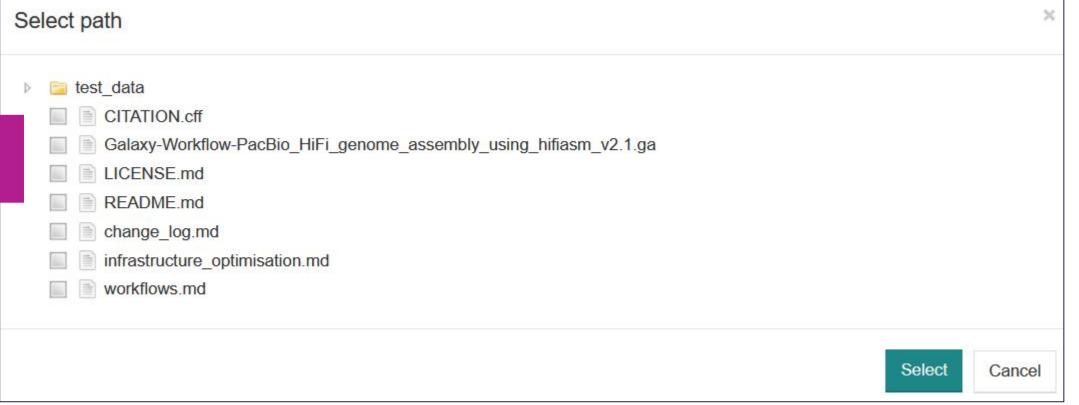




Import

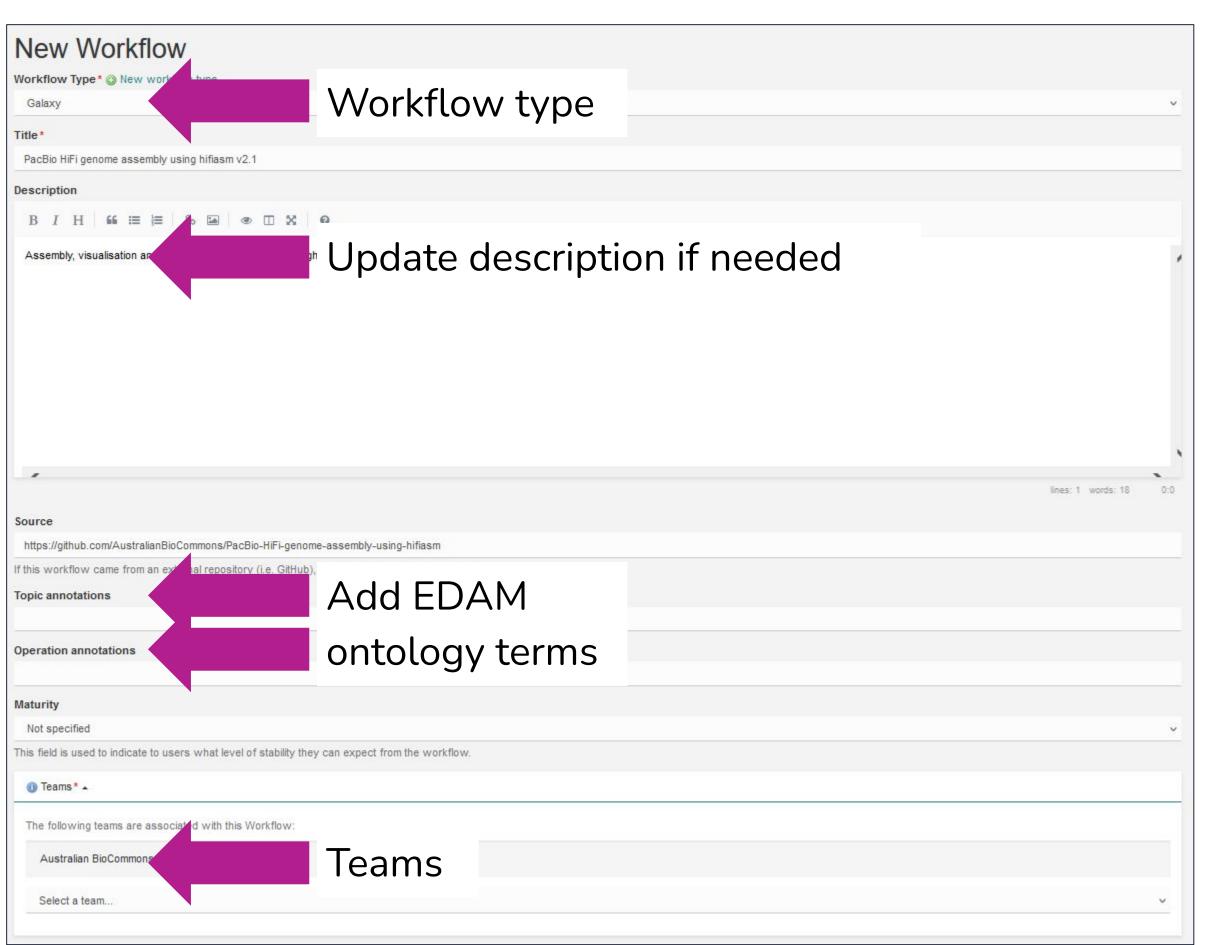


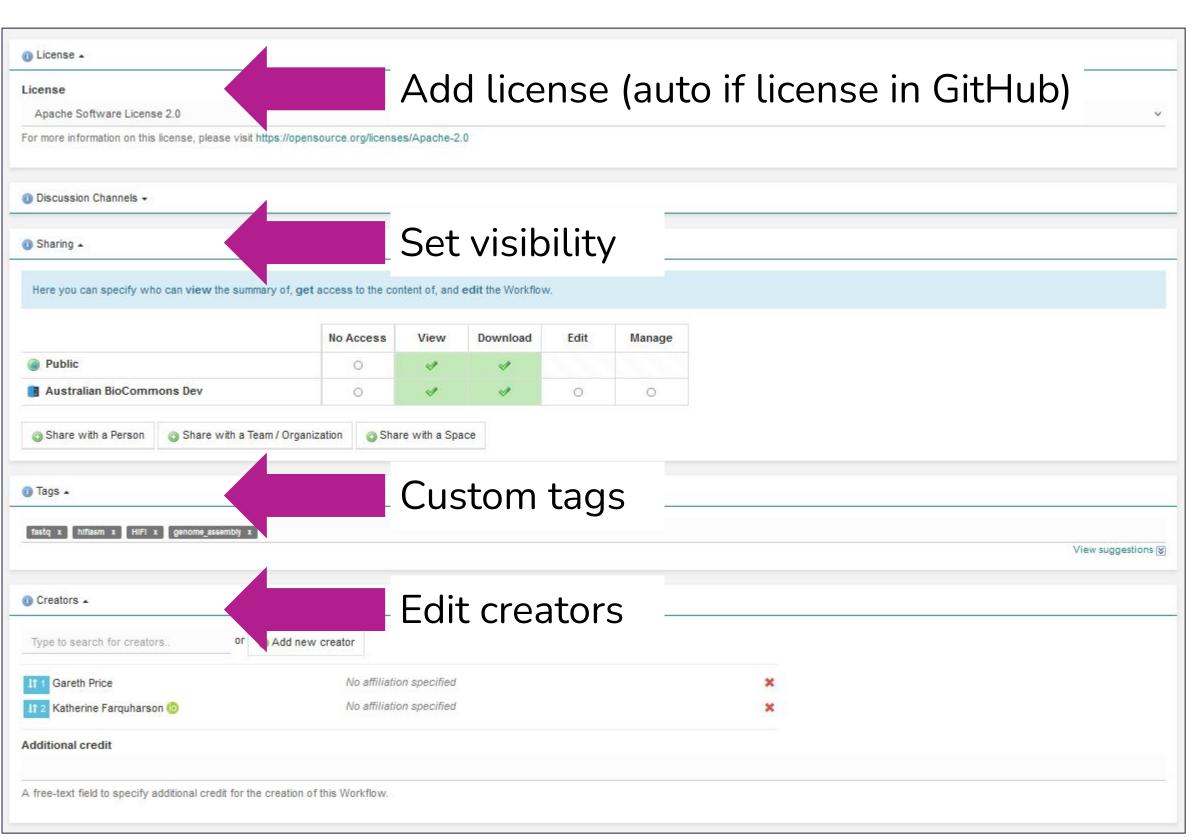






Add metadata

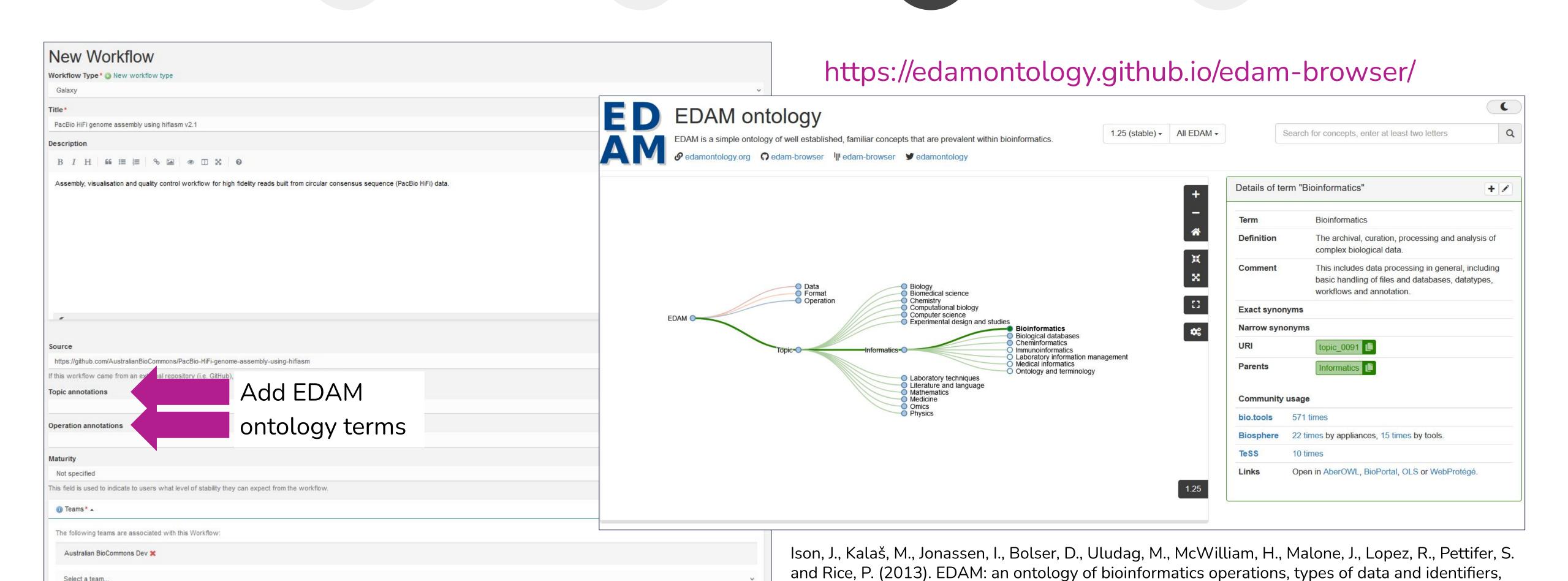






Add metadata

topics and formats. Bioinformatics, 29(10): 1325-1332. 10.1093/bioinformatics/btt113 PMID:

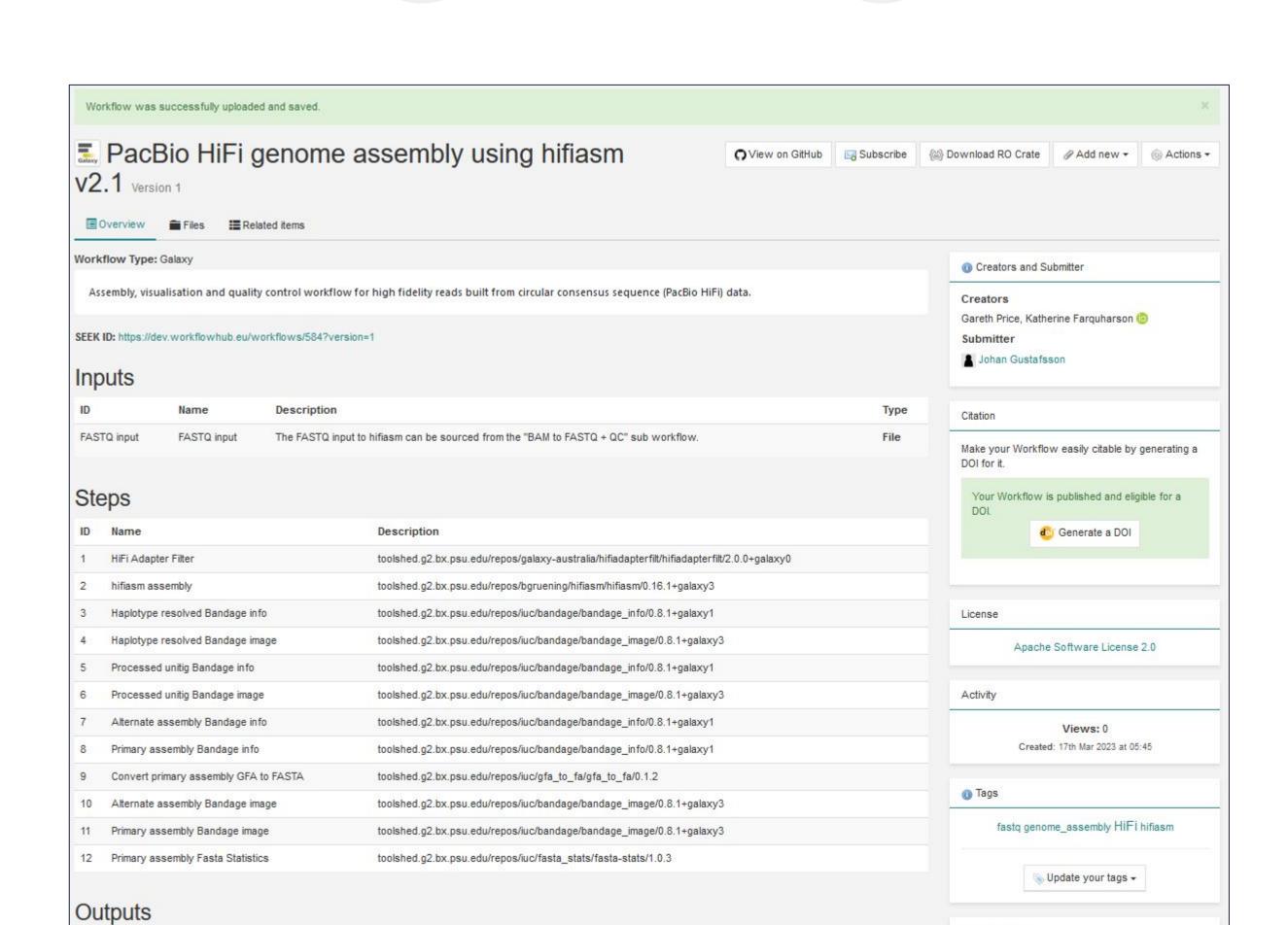


23479348 Open access



Select a team..

Review



HiFi Adapter Filter on input dataset(s): clean reads

HiFi Adapter Filter on input dataset(s): clean reads

Attributions

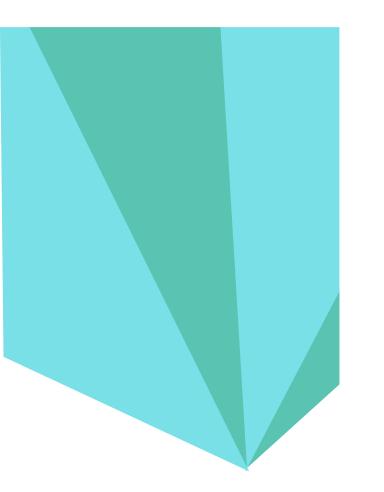


Look at a best practice example

 □ GermlineShortV biovalidation Version 1 🔾 View on GitHub 🔛 Request Contact 🔛 Unsubscribe 🔠 Download RO Crate Add to collection ▼ Overview Files Related items Structured Workflow Type: Shell Script O Creators and Submitter Creators Complete author list documentation GermlineShortV biovalidation 🜌 Georgina Samaha, 📓 Tracy Chew, 💄 Cali Willet, Nandan Deshpande (6) Description (in correct order) imported from GitHub Diagram Georgina Samaha User guide Quick start guide Benchmarking Citation **№** Сору Workflow summaries Metadata Samaha, G., Chew, T., Willet, C., & Deshpande, N. Component tools (2022). GermlineShortV_biovalidation. DOI Required (minimum) inputs/parameters WorkflowHub. https://doi.org/10.48546 Preparing your own input files /WORKFLOWHUB.WORKFLOW.339.1 Additional notes Understanding your outputs Performance metrics explained American Psychological Association 7th edition > Help/FAQ/Troubleshooting Acknowledgements/citations/credits License Description License GNU General Public License 3.0 Population-scale WGS cohorts are essential resources for genetic analyses including heritable diseases, evolutionary genomics, conservation biology, and population genomics. Processing raw reads into analysis-ready variants remains challenging. Various mapping and variant calling pipelines have been made publicly available in recent decades. Designing a mapping and variant calling pipeline to meet your needs is dependent on the compute infrastructure you're Activity Views: 1155 What type of organism are you Created: 5th May 2022 at 08:02 working with? Annotated Properties Topic annotations Non-human Annotations Non-model Genetic variation, Bioinformatics, Whole geno model organism sequencing organism Diagram Operation annotations SNP detection, Indel detection, Validation Sample-based Sample-based metrics metrics Tags This item has not yet been tagged. Variant-based Variant-based metrics vcfstat.sh Attributions



Samaha, G., Chew, T., Willet, C., & Deshpande, N. (2022). GermlineShortV_biovalidation. WorkflowHub. https://doi.org/10.48546/WORKFLOWHUB.WORKFLOW.339.1



Demo

Include a CFF file in your GitHub repository

```
1 cff-version: 2.1.0
2 message: "If you use this workflow, please cite it as below."
3 authors:
4 - family-names: "Price"
5 given-names: "Gareth"
6 orcid: "https://orcid.org/0000-0003-2439-8650"
7 - family-names: "Farquharson"
8 given-names: "Katherine"
9 orcid: "https://orcid.org/0000-0002-9009-7453"
10 title: "PacBio-HiFi-genome-assembly-using-hifiasm"
11 version: 2.1.0
12 doi: [DOI goes here]
13 date-released: 2022-10-21
```

https://citation-file-format.github.io/

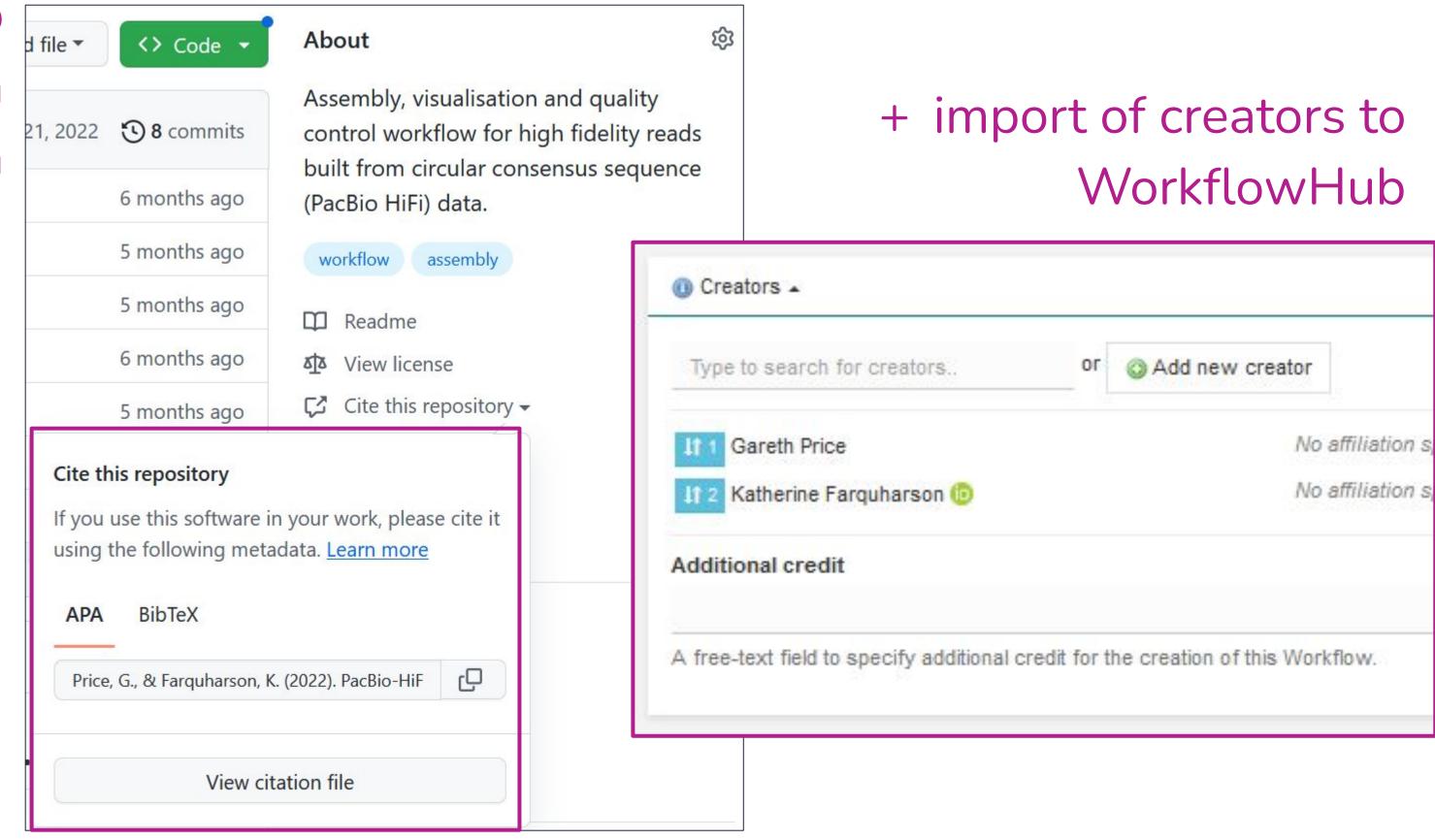
Druskat, Stephan, Spaaks, Jurriaan H., Chue Hong, Neil, Haines, Robert, Baker, James, Bliven, Spencer, Willighagen, Egon, Pérez-Suárez, David, & Konovalov, Alexander. (2021). Citation File Format (1.2.0). Zenodo. https://doi.org/10.5281/zenodo.5171937



Include a CFF file in your GitHub repository

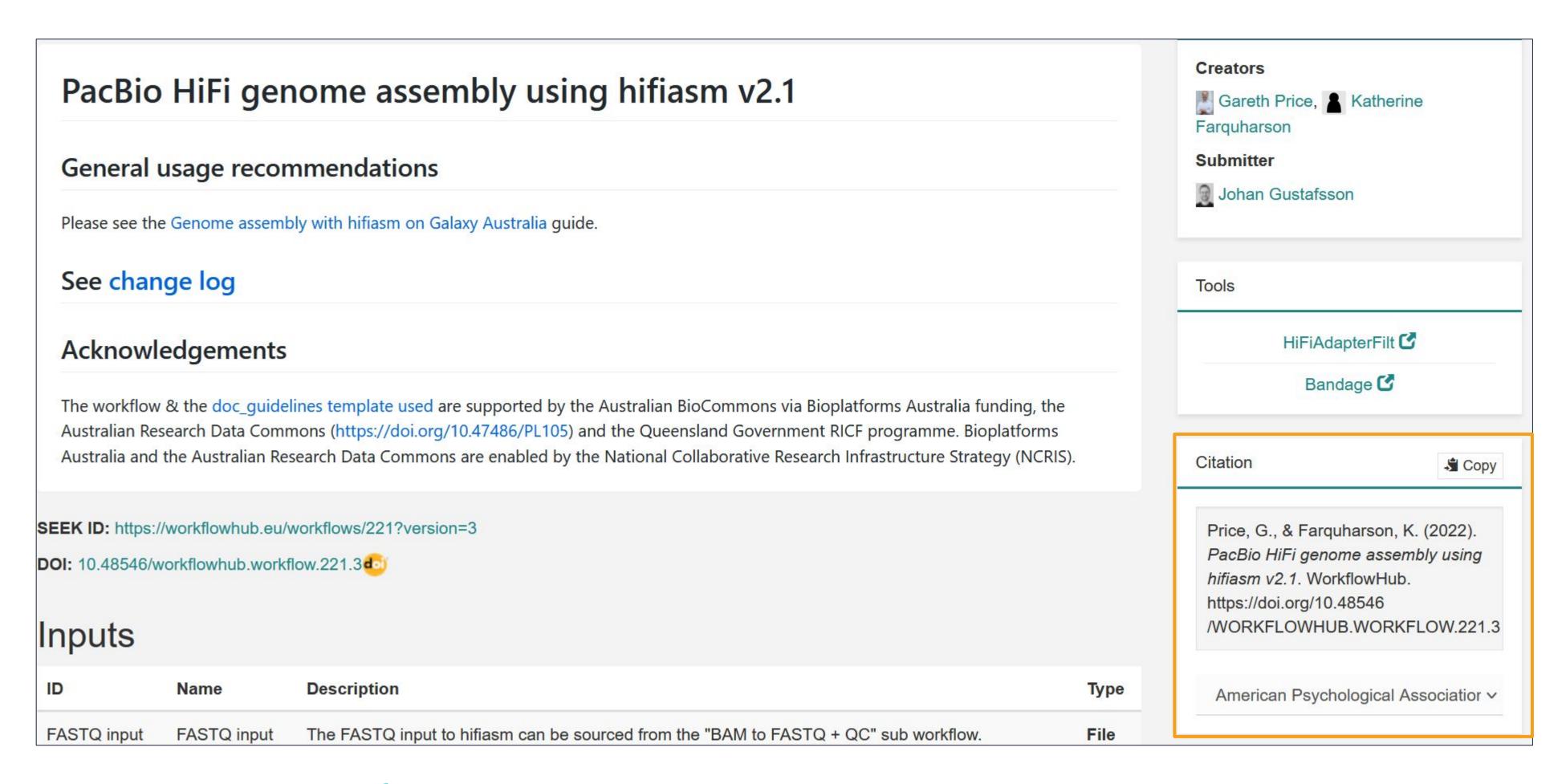
GitHub citation option

1 cff-version: 2.1.0
2 message: "If you use this workflow, please cite it as below."
3 authors:
4 - family-names: "Price"
5 given-names: "Gareth"
6 orcid: "https://orcid.org/0000-0003-2439-8650"
7 - family-names: "Farquharson"
8 given-names: "Katherine"
9 orcid: "https://orcid.org/0000-0002-9009-7453"
10 title: "PacBio-HiFi-genome-assembly-using-hifiasm"
11 version: 2.1.0
12 doi: [DOI goes here]
13 date-released: 2022-10-21





Create a DOI when metadata is completed





Create a DOI when metadata is completed

Price, G., & Farquharson, K. (2022). *PacBio HiFi genome assembly using hifiasm v2.1*. WorkflowHub. https://doi.org/10.48546/WORKFLOWHUB.WORKFLOW.221.3



Use GitHub app to automate registry updates!



GitHub App

LifeMonitor

The **LifeMonitor GitHub App** is a companion to the LifeMonitor service for supporting the sustainability and reusability of published computational scientific data analysis workflows.

The LifeMonitor GitHub App does the following things:

- Examines the repositories on which it is installed and applies a series of checks.
- Suggests pull requests to make changes or additions to bring the workflow repository closer to conforming to best practices.
- Opens issues to let you know about problems detected by the checks and to
 request new metadata.
- Registers new releases/versions of the workflow with both the LifeMonitor service and the WorkflowHub workflow registry.

Together, the LifeMonitor service and GitHub App help you keep your workflow functional over time and help you follow the community-accepted conventions for your specific workflow type, so that it may be more easily adopted and re-used by others in your scientific community.

Additional information is available in the documentation.

Useful links

Docs

API Explorer

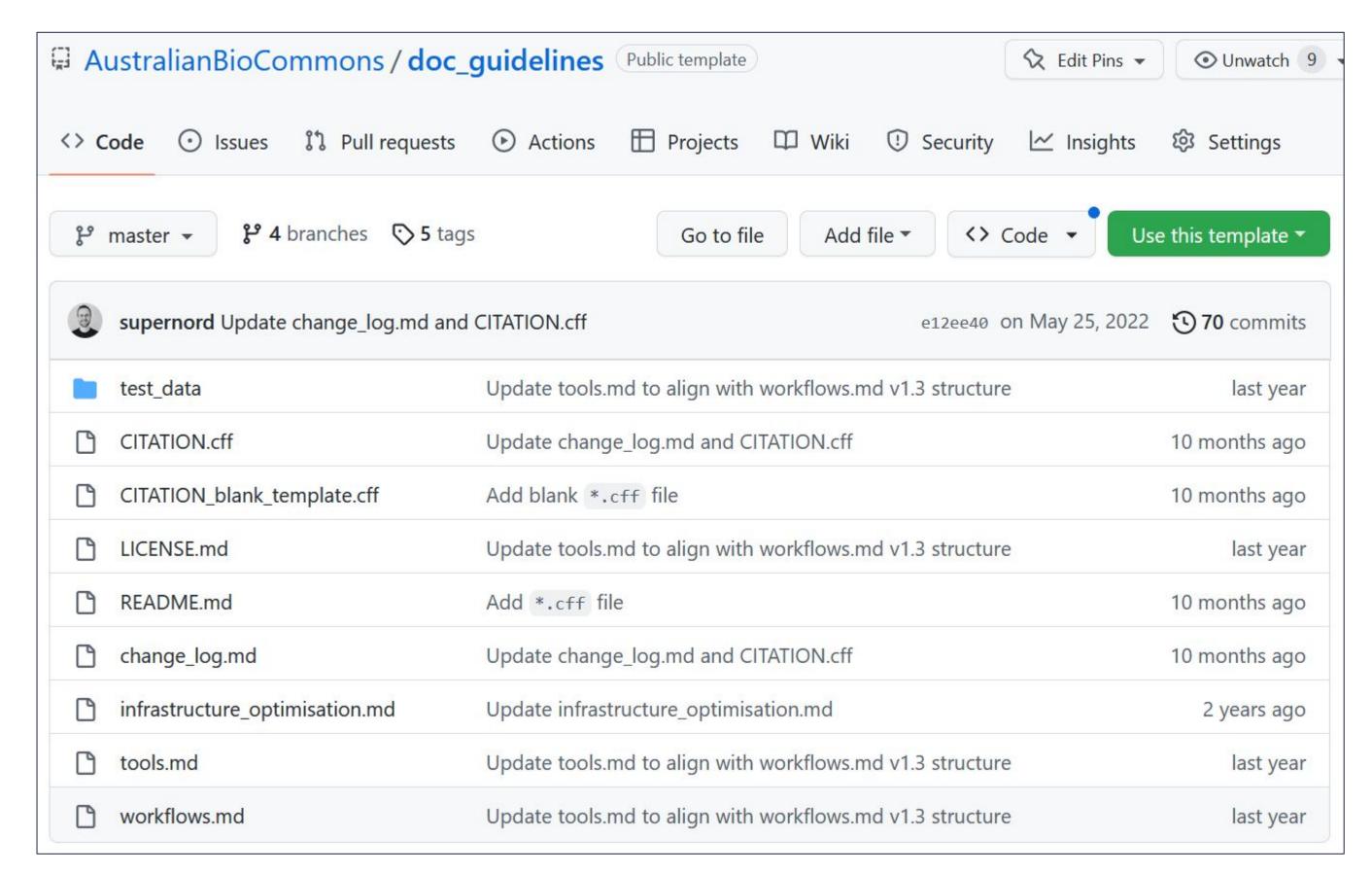
Web Application

Workflow Hub

https://crs4.github.io/life_monitor/lm_wft_best_practices_github_app#installation



Use documentation templates



https://github.com/AustralianBioCommons/doc_guidelines



Use documentation templates

Should I contribute to an existing community workflow effort instead?

The BioCommons guideline is based on learnings from multiple community efforts including the Galaxy Intergalactic Workflow Commission (IWC), nf-core and Snakemake.

If you are using Galaxy, Nextflow or Snakemake workflow languages and would like to contribute to their community workflow efforts, you could be using their specific guidelines, which are linked to below.

Community effort	Workflow language documentation	Workflow guideline information	How to create / contribute new workflows
IWC	Galaxy	IWC GitHub	IWC adding workflows
nf-core	Nextflow	nf-core developer guidelines	nf-core adding_pipelines
Snakemake	Snakemake	Snakemake-workflows guidelines	Snakemake-workflows contribute

https://australianbiocommons.github.io/how-to-guides/documentation/DocumentationGuidelines



Acknowledgements

The community of workflow developers





BioCommons 'Bring Your Own Data' Expansion Project

https://www.biocommons.org.au/byo-data-platform-expansion



























Thanks!

Any questions?

You can email me at: johan@biocommons.org.au



Tell us what you thought ...

Feedback survey

surveymonkey.com/r/findable-workflows



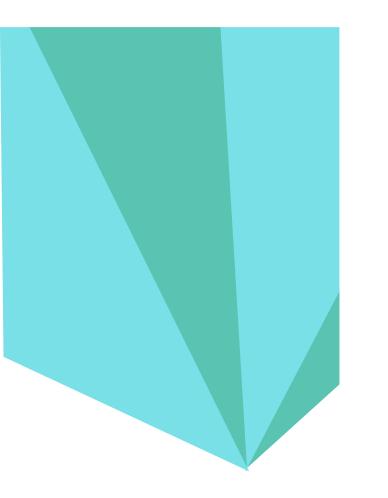
NEXT ...

Unlocking nf-core: customising workflows for your research

18-19 May 2023

biocommons.org.au/webinars-workshops





Bring-Your-Own 5 Workflow