



Architecture of large projects in bioinformatics (ADP)

Lecture 10

Łukasz P. Kozłowski Warsaw, 2025

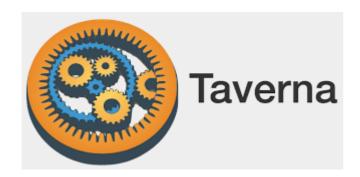
- 1. Data formats in bioinformatics,
- 2. Popular software libraries (BioPerl, BioPython)
- 3. Most important bioinformatics databases (UniProt, PDB, RefSeq, GenBank, ENA, InterPro, etc.)
- 4. Software licensing for scientific purposes. Free-software licensing. Patents.
- 5. Generic model Organism database (GMOD) project assumptions, history and usage
- 6. Genome browsers, problem description and state of the solutions
- 7. Version control systems (CVS, SVN, git), and online collaboration ad distribution platforms (github, sourceforge).
- 8. Software testing, automated testing frameworks.
- 9. Scientific workflow systems taverna and galaxy. MyExperiment platform. Reproducible research.
- 10. Literate programming idea and sweave, markdown, software documentation.
- 11. Interactive scripting platforms, Rstudio, Jupyter.

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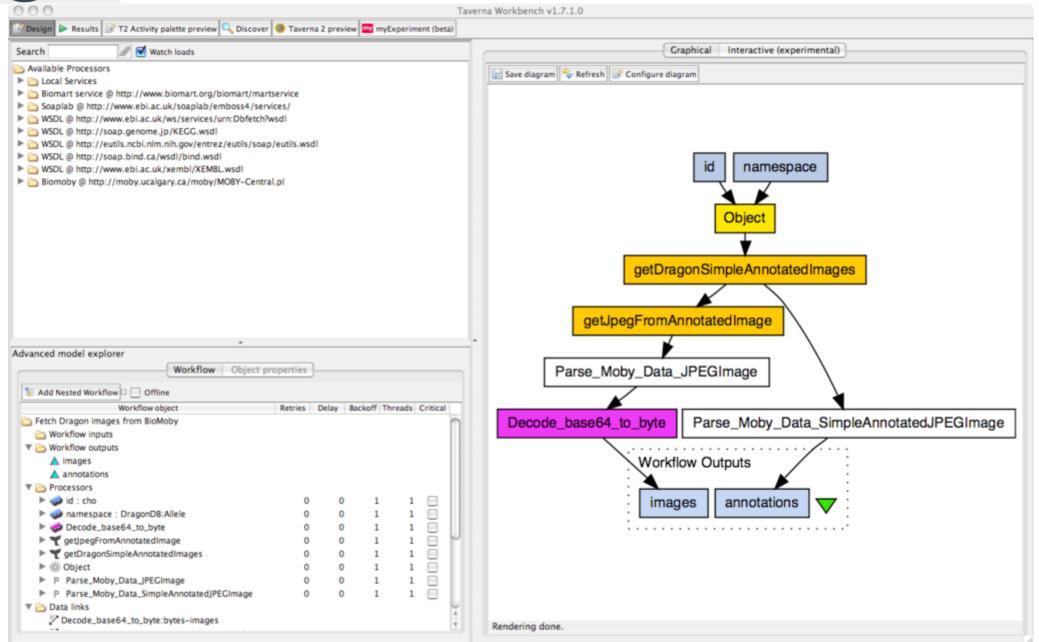
Scientific workflow systems

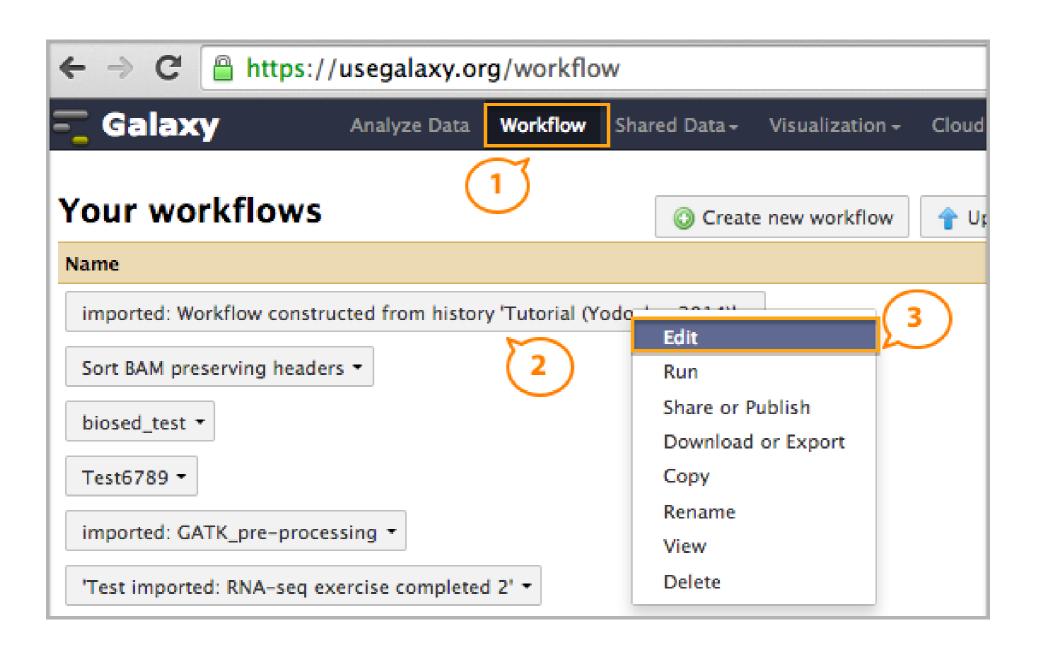
Scientific workflow systems

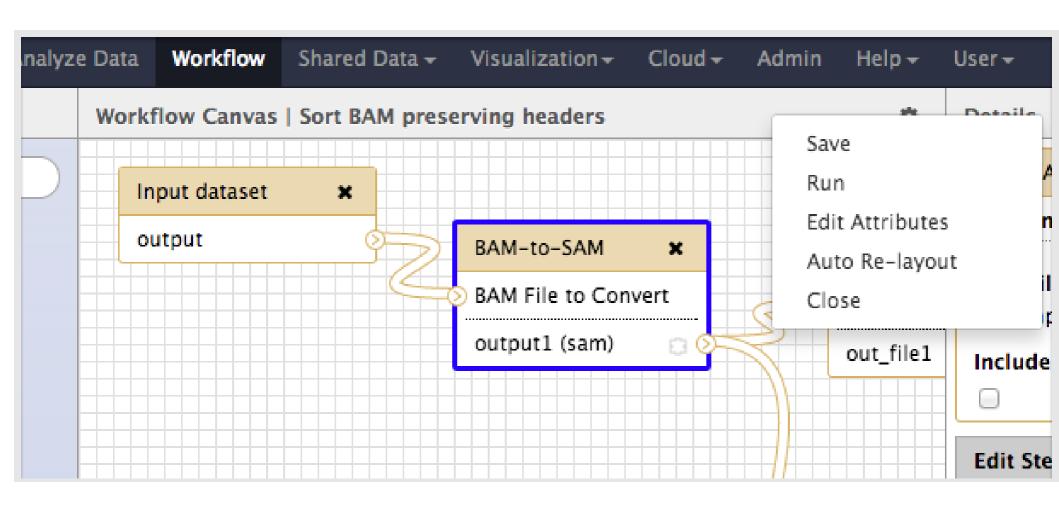




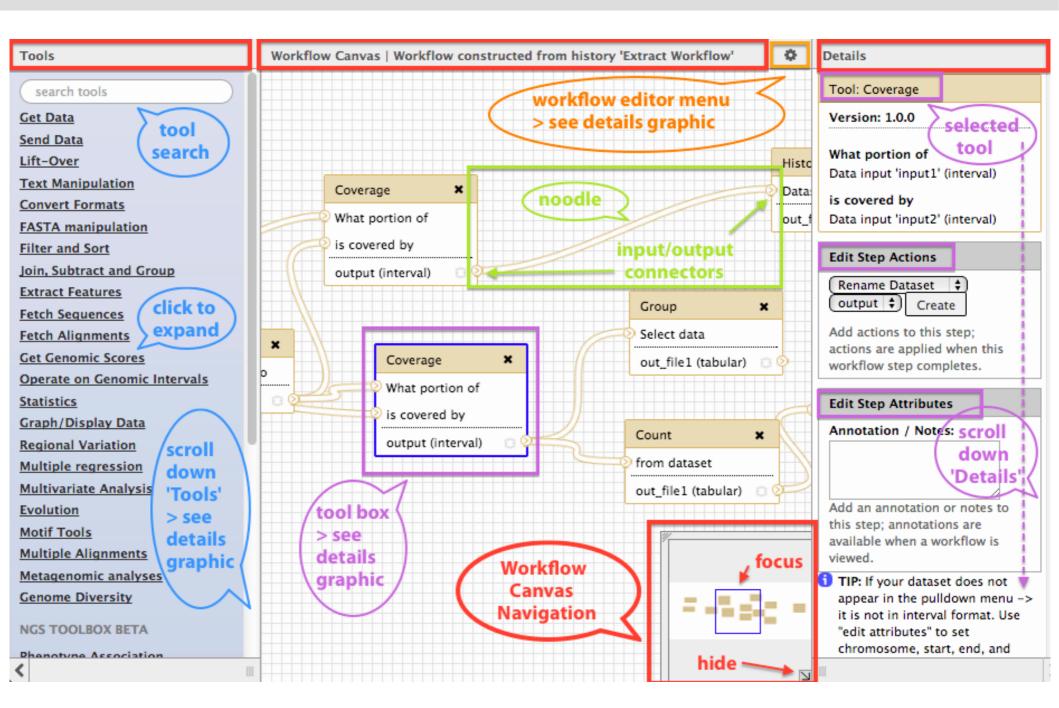




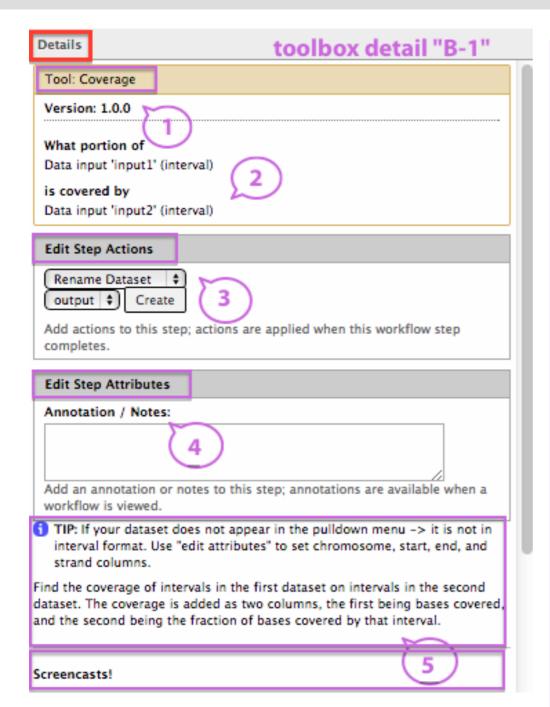




Galaxy ADP



Galaxy ADP



Screencasts!

toolbox detail "B-2"

See Galaxy Interval Operation <u>Screencasts</u> (right click to open this link in another window).

Example

if First dataset are genes



```
chr11 5203271 5204877 NM_000518 0 -
chr11 5210634 5212434 NM_000519 0 -
chr11 5226077 5227663 NM_000559 0 -
chr11 5226079 5232587 BC020719 0 -
chr11 5230996 5232587 NM_000184 0 -
```

and Second dataset are repeats:

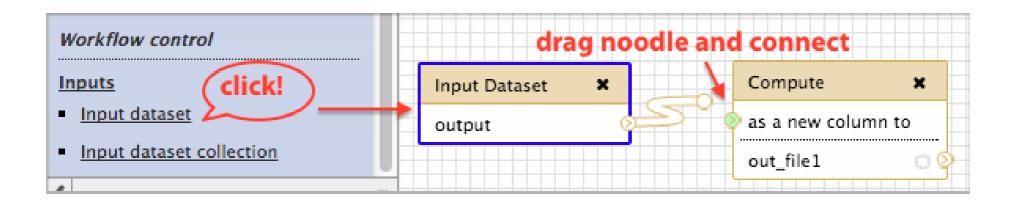
```
5203895 5203991 L1MA6
chr11
                                    500 +
          5204163 5204239 A-rich
chr11
                                    219 +
chr11
          5211034 5211167 (CATATA)n 245 +
chr11
          5211642 5211673 AT rich
chr11
          5226551 5226606 (CA)n
chr11
          5228782 5228825 (TTTTTG)n 208 +
          5229045 5229121 L1PA11
chr11
chr11
          5229133 5229319 MER41A 1106 +
chr11
          5229374 5229485 L2
                                    244 -
chr11
          5229751 5230083 MLT1A
                                    913 -
          5231469 5231526 (CA)n
                                    330 +
```

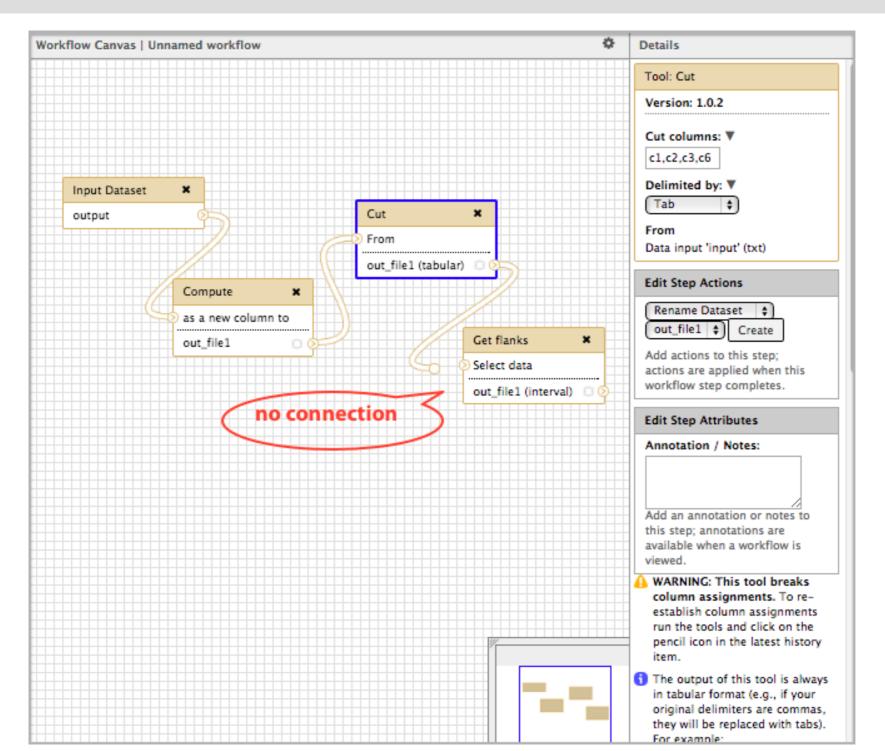
the Result is the coverage density of repeats in the genes:

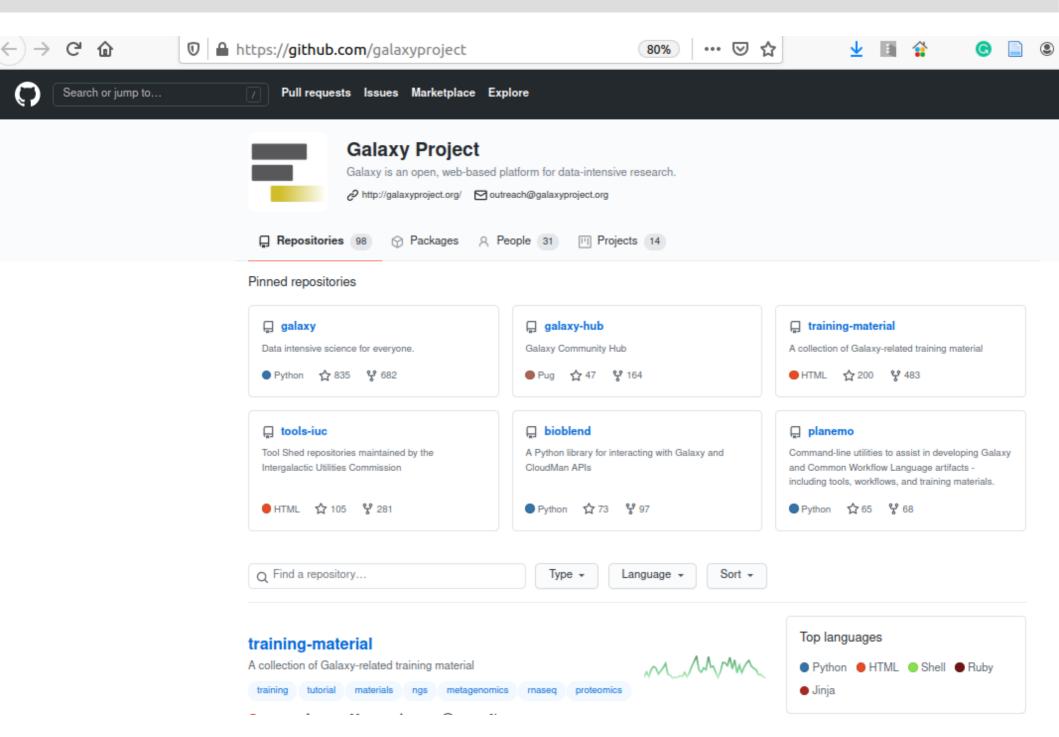
For example, the following line of output:

```
chr11 5203271 5204877 NM 000518 0 - 172 0.107098
```

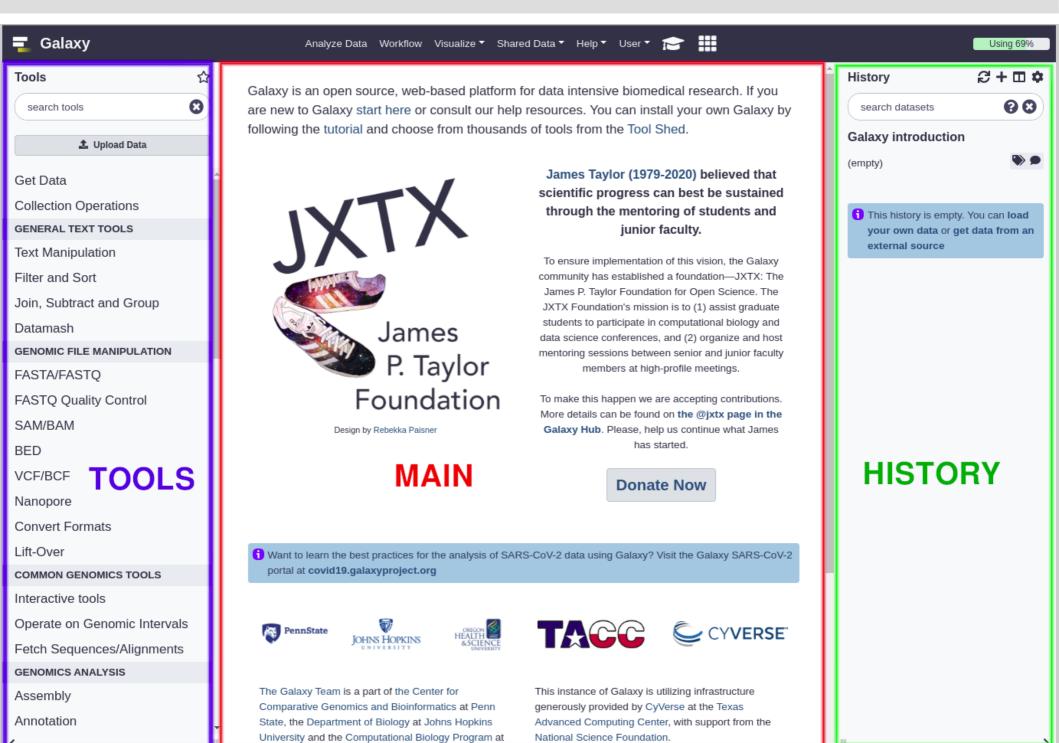
implies that 172 nucleotides accounting for 10.7% of the this interval (chr11:5203271-5204877) overlap with repetitive elements.

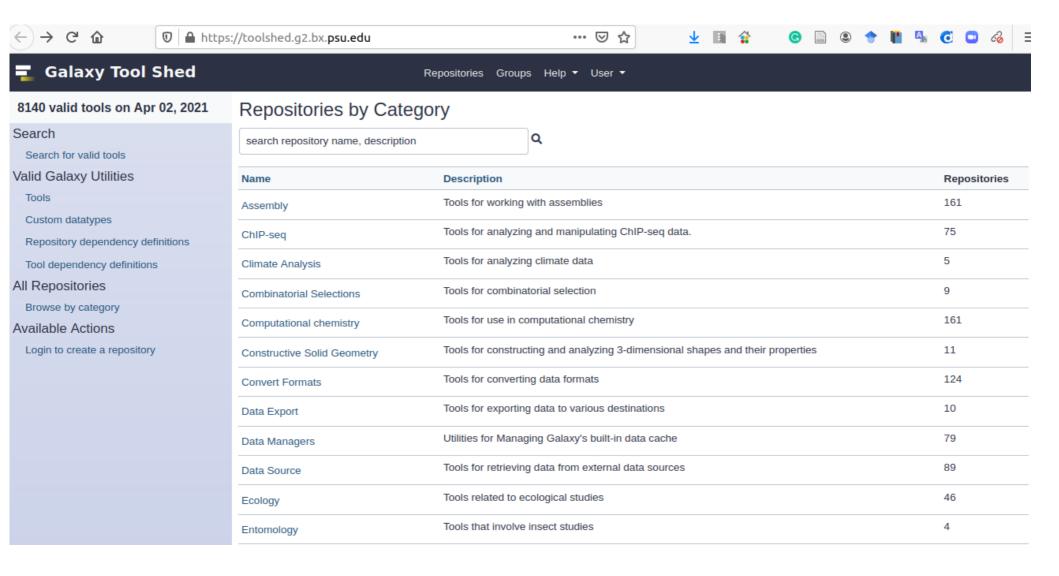


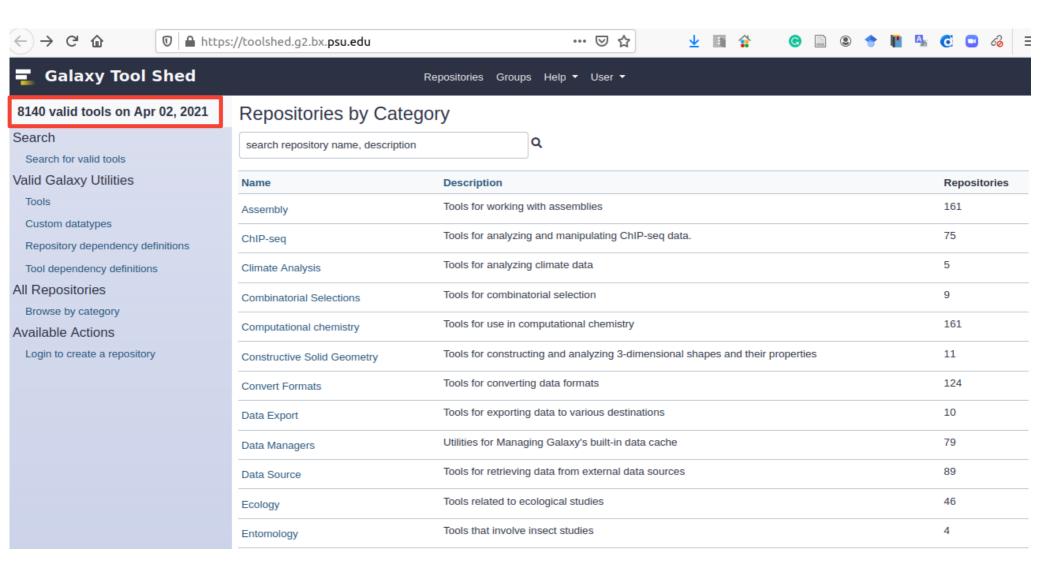


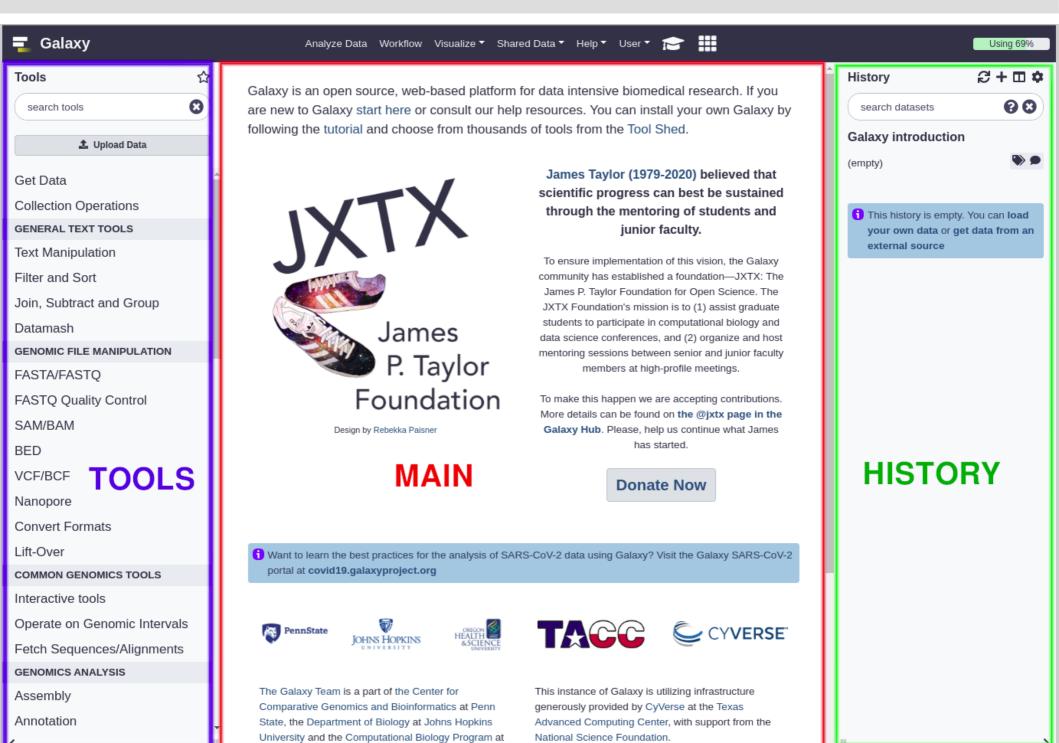


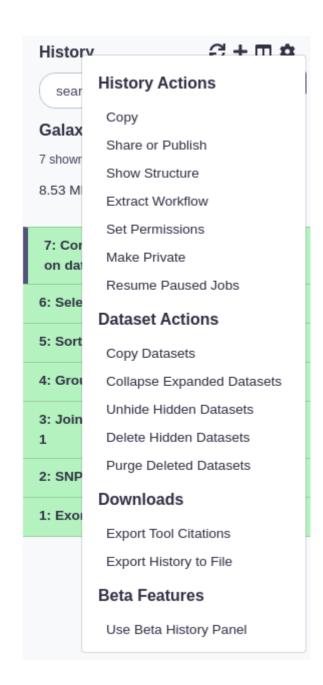




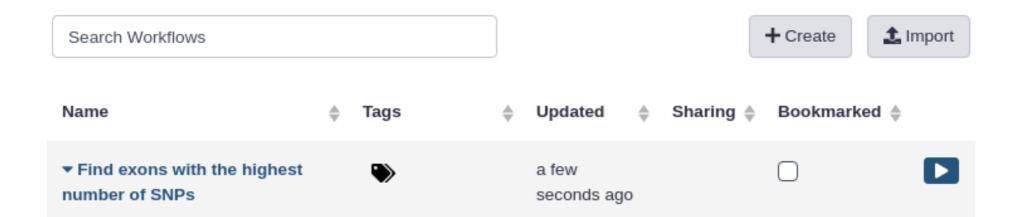


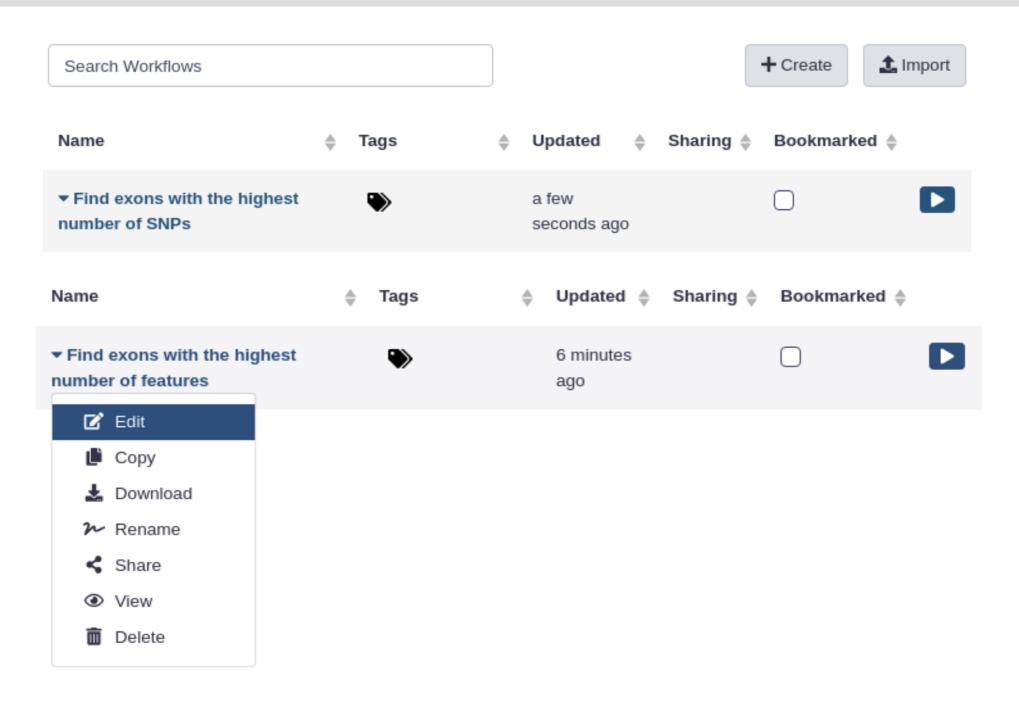


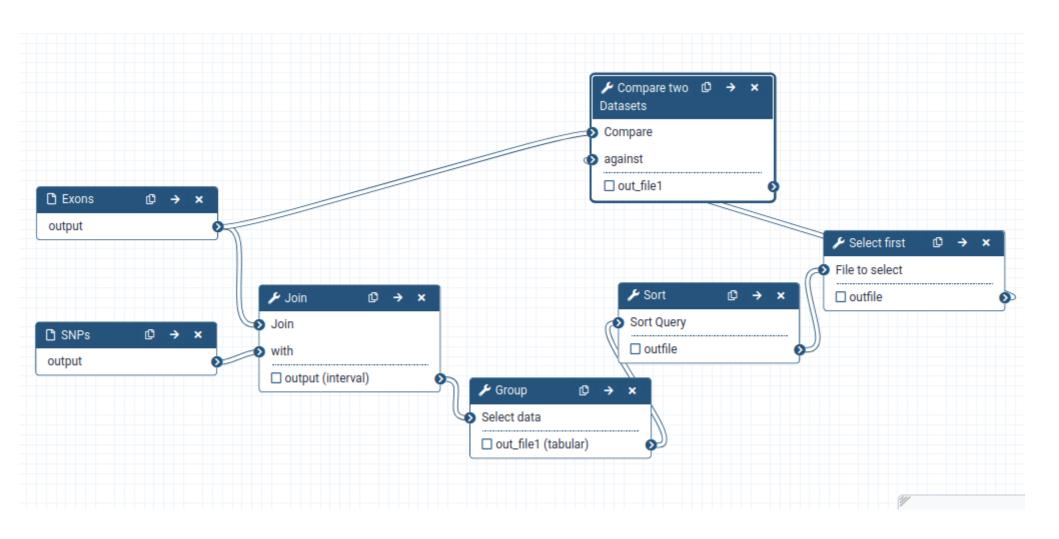


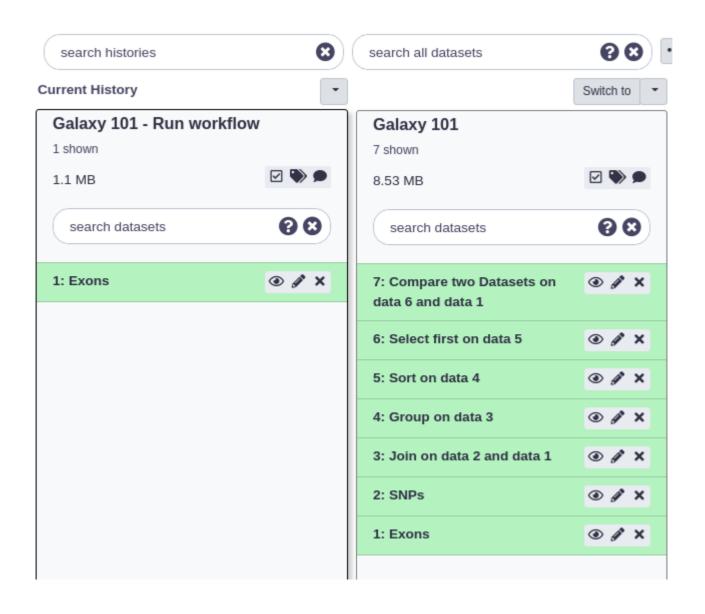


Workflow name	
Find exons with the highest number of SNPs	
Create Workflow Check all Uncheck all	
Tool	History items created
UCSC Main This tool cannot be used in workflows	1 Exons ✓ Treat as input dataset Exons
UCSC Main This tool cannot be used in workflows	2 SNPs ✓ Treat as input dataset SNPs
Join ✓ Include "Join" in workflow	▶ 3 Join on data 2 and data 1
Group ✓ Include "Group" in workflow	► 4 Group on data 3
Sort ✓ Include "Sort" in workflow	▶ 5 Sort on data 4
Select first ✓ Include "Select first" in workflow	► 6 Select first on data 5
Compare two Datasets ✓ Include "Compare two Datasets" in workflow	► 7 Compare two Datasets on data 6 and data 1









Share your work

To share a history, click on the galaxy- **gear icon** in the history panel and select **Share or Publish**. On this page you can do 3 things:

Make History Accessible via Link. This generates a link that you can give out to others. Anybody with this link will be able to view your history.

Make History Accessible and Publish. This will not only create a link, but will also publish your history. This means your history will be listed under Shared Data \rightarrow Histories in the top menu.

Share with a user. This will share the history only with specific users on the Galaxy instance.

Python PyPi ADP

Share your work





Python PyPi

Share your work



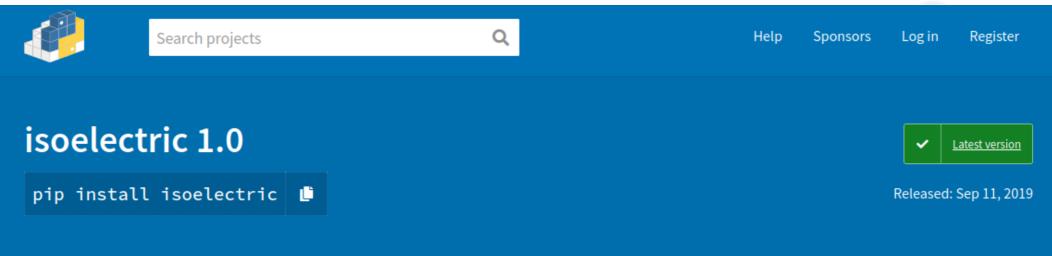






Python PyPi





IPC (Isoelectric Point Calculator) - prediction of isoelectric point of proteins and peptides





Project description

IPC is a program (available also as web service at isoelectric.org) for the accurate estimation of protein and peptide isoelectric point (pI) using Henderson-Hasselbach equation and pKa sets.





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isoelectric 1.0

pip install isoelectric 📙



Latest version

Released: Sep 11, 2019

Meta

License: Public Domain

Author: Lukasz Pawel Kozlowski

protein, peptide, isoelectric point, pl, biochemistry, proteomics

Requires: Python >= 3.0

Maintainers



lukaskoz

Classifiers

License

Public Domain

Operating System

OS Independent

INSTALLATION:

wget http://isoelectric.org/ipc.zip; unzip ipc.zip; # sudo apt-get install unzip (if not present) cd ipc; sudo python setup.py install

USAGE:

python ipc.py <fasta_file> <pKa set> <output_file> <plot_file>

ipc <fasta file> <pKa set> <output file> <plot file> (if installed into system using setup.py)

```
protein sequence(s) in fasta format, see ./examples
<fasta_file>
                one from pKa sets which will be used to calculate pI, default 'ALL' (report pI
<pKa set>
                valid options are:
                        'ALL', 'IPC_protein', 'IPC_peptide',
                        'Bjellqvist', 'Dawson', 'Grimsley',
                        'Toseland', 'EMBOSS', 'Kozlowski',
                        'DTASelect', 'Wikipedia', 'Rodwell',
                        'Patrickios', 'Sillero', 'Thurlkill',
                        'Solomon', 'Nozaki_Tanford',
```





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pip install isoelectric 🕒





Released: Sep 11, 2019

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License: Public Domain

Author: Lukasz Pawel Kozlowski ☑

protein, peptide, isoelectric point, pl, biochemistry, proteomics

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Maintainers



lukaskoz

Classifiers

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Operating System

o OS Independent

R Bioconductor ADP



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The mission of the *Bioconductor* project is to develop, support, and disseminate free open source software that facilitates rigorous and reproducible analysis of data from current and emerging biological assays. We are dedicated to building a diverse, collaborative, and welcoming community of developers and data scientists.

Bioconductor uses the R statistical programming language, and is open source and open development. It has two releases each year, and an active user community. Bioconductor is also available as Docker images.

News

- Bioconductor Bioc 3.17 Released.
- Bioconductor Community Blog
- Bioconductor browsable code base now available.
- See our google calendar for events, conferences, meetings, forums, etc.
- Bioconductor F1000 Research Channel is

Bioc2023 Conference»

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This changes affects maintainers of packages.

For more details see:

- 1. biocblog post
- 2. branch renaming FAO

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Using Bioconductor

The current release of *Bioconductor* is version 3.13; it works with *R* version 4.1.0. Users of older *R* and *Bioconductor* must update their installation to take advantage of new features and to access packages that have been added to *Bioconductor* since the last release.

The development version of *Bioconductor* is version 3.14; it works with *R* version 4.1.0. More recent 'devel' versions of *R* (if available) will be supported during the next *Bioconductor* release cycle.

Install the latest release of R, then get the latest version of Bioconductor by starting R and entering the commands

```
if (!requireNamespace("BiocManager", quietly = TRUE))
  install.packages("BiocManager")
BiocManager::install(version = "3.13")
```

It may be possible to change the *Bioconductor* version of an existing installation; see the 'Changing version' section of the BiocManager vignette.

The current release of *Bioconductor* is version 3.17; it works with *R* version 4.3.0. Users of older R and *Bioconductor* must update their installation to take advantage of new features and to access packages that have been added to *Bioconductor* since the last release.

The development version of *Bioconductor* is version 3.18; it works with *R* version 4.3.0. More recent 'devel' versions of *R* (if available) will be supported during the next *Bioconductor* release cycle.

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  install.packages("BiocManager")
BiocManager::install(version = "3.17")
```

It may be possible to change the *Bioconductor* version of an existing installation; see the 'Changing version' section of the BiocManager vignette.

Details, including instructions to <u>install additional packages</u> and to <u>update</u>, <u>find</u>, and <u>troubleshoot</u> are provided below. A <u>devel</u> version of *Bioconductor* is available. There are good <u>reasons for using BiocManager::install()</u> for managing *Bioconductor* resources.

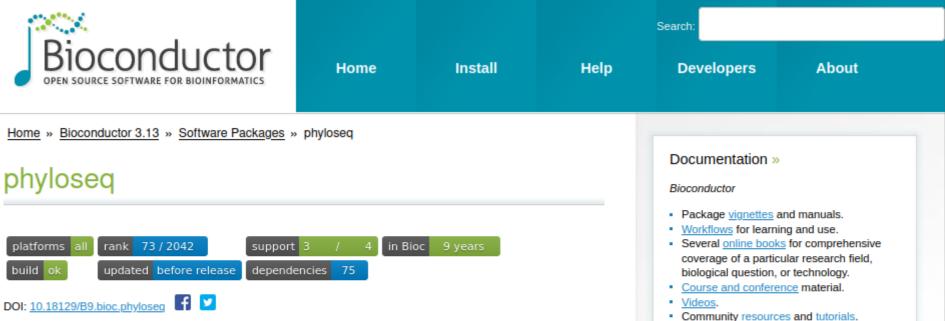
Install specific packages, e.g., "GenomicFeatures" and "AnnotationDbi", with

```
BiocManager::install(c("GenomicFeatures", "AnnotationDbi"))
```

The install() function (in the BiocManager package) has arguments that change its default behavior; type ?install for further help.

https://www.bioconductor.org/install/

R Bioconductor ADP



Handling and analysis of high-throughput microbiome census data

Bioconductor version: Release (3.13)

phyloseq provides a set of classes and tools to facilitate the import, storage, analysis, and graphical display of microbiome census data.

Author: Paul J. McMurdie <joey711 at gmail.com>, Susan Holmes <susan at stat.stanford.edu>, with contributions from Gregory Jordan and Scott Chamberlain

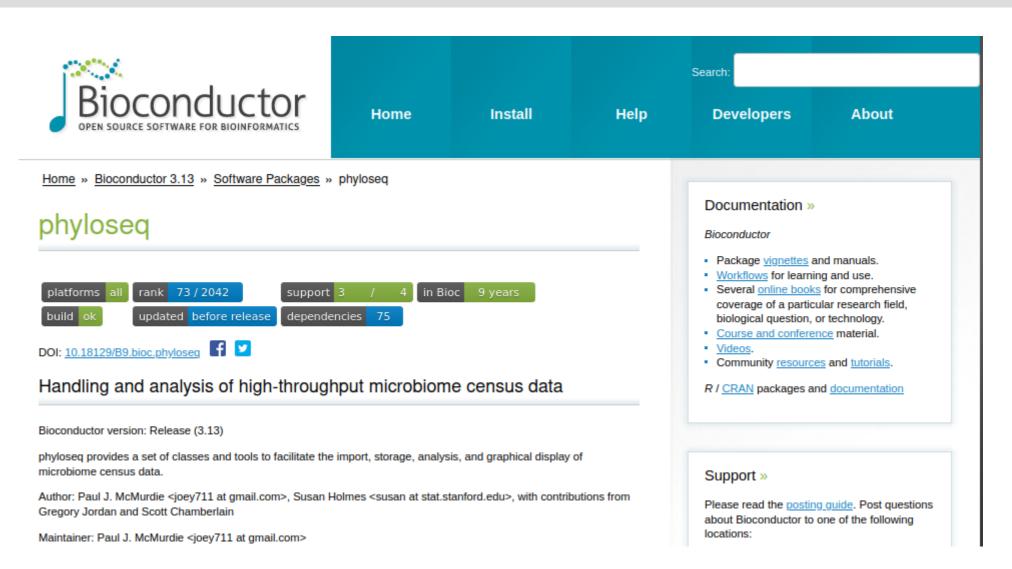
Maintainer: Paul J. McMurdie <joey711 at gmail.com>

R / CRAN packages and documentation

Support »

Please read the posting guide. Post questions about Bioconductor to one of the following locations:

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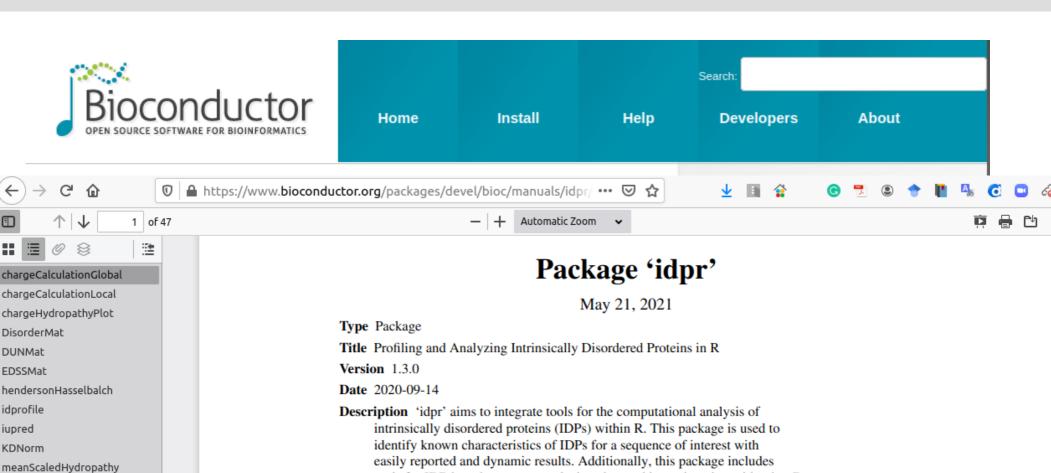


Documentation

To view documentation for the version of this package installed in your system, start R and enter:

browseVignettes("phyloseq")

R Bioconductor ADP



identify known characteristics of IDPs for a sequence of interest with easily reported and dynamic results. Additionally, this package includes tools for IDP-based sequence analysis to be used in conjunction with other R packages.

BugReports https://github.com/wmm27/idpr/issues

License LGPL-3
Encoding UTF-8
LazyData true

netCharge

scaledHydropathyGlobal

scaledHydropathyLocal

sequenceMapCoordinates

sequenceCheck sequenceMap

sequencePlot

structuralTendency

TP53Sequences

Index

structuralTendencyPlot

pKaData

biocViews StructuralPrediction, Proteomics, CellBiology

RoxygenNote 7.1.1

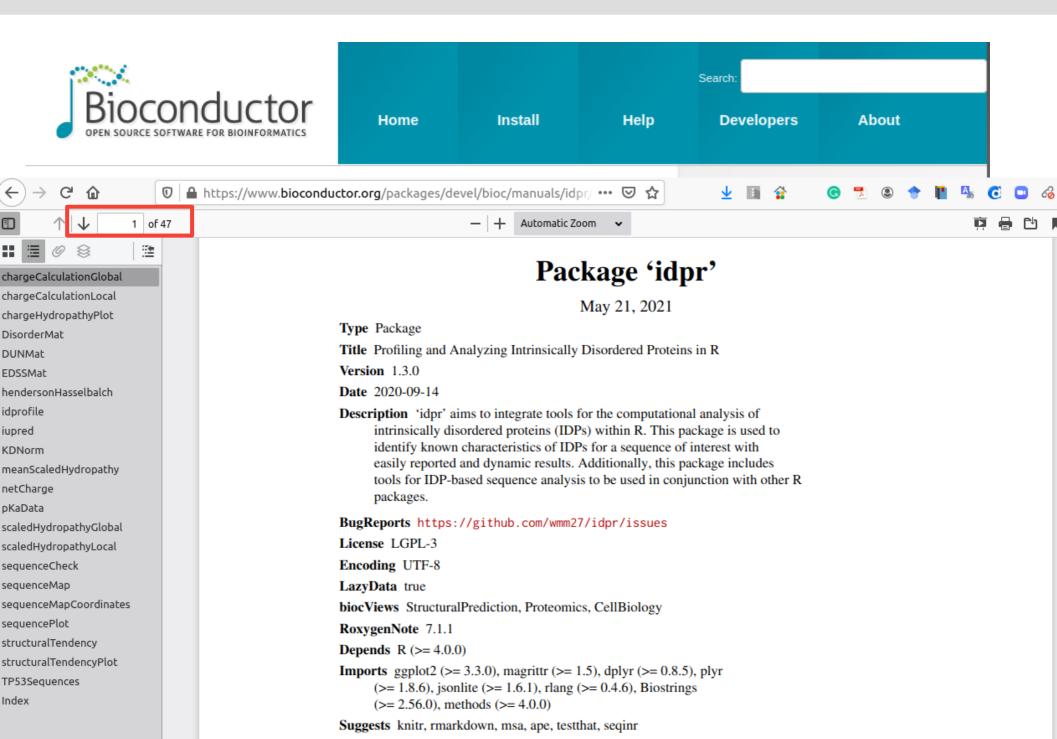
Depends R (>= 4.0.0)

Imports ggplot2 (>= 3.3.0), magrittr (>= 1.5), dplyr (>= 0.8.5), plyr (>= 1.8.6), jsonlite (>= 1.6.1), rlang (>= 0.4.6), Biostrings (>= 2.56.0), methods (>= 4.0.0)

Suggests knitr, rmarkdown, msa, ape, testthat, seqinr

VignetteBuilder knitr

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VignetteBuilder knitr

Scientific project timeline







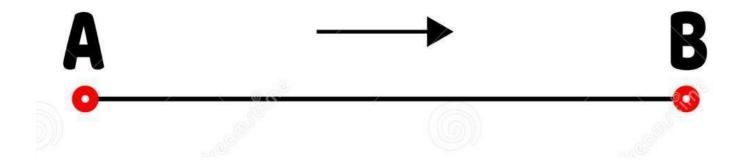
Problem to solve







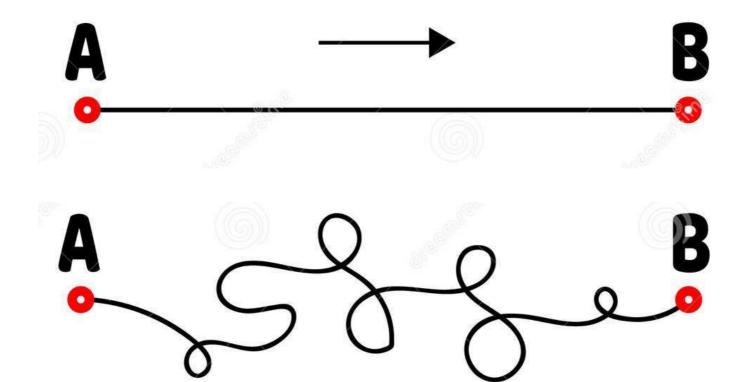
Problem to solve







Problem to solve





















































Grant assessment takes (at least) 6 months

(the bigger project, more parties involved, the longer)





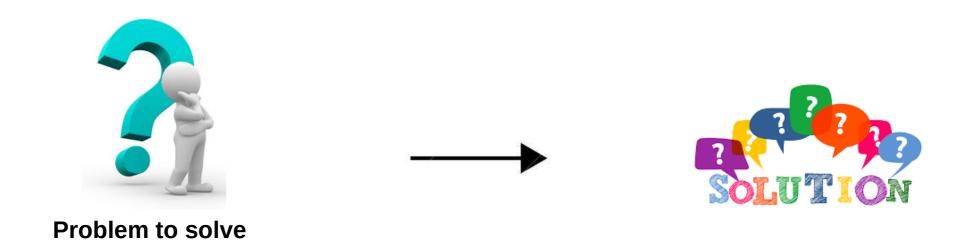


Grant assessment takes (at least) 6 months

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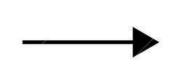
Success rate is ~20%

(even if you have very good track record)



The research (1-2 years, if you are lucky)







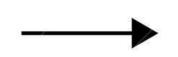
Problem to solve

The research (1-2 years, if you are lucky)







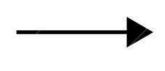


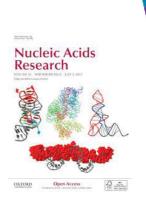


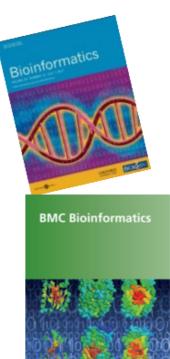
Problem to solve

Presenting results

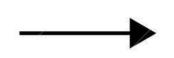












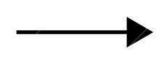


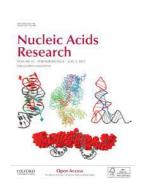
Problem to solve

Presenting results

(6-12 months, if you are lucky)



















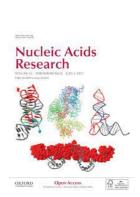


















8 Results for term "Lukasz Kozlowski"

Items/Page 10 → Order by Newest First →

IPC - Isoelectric Point Calculator

Lukasz P. Kozlowski

bioRxiv 049841; doi: https://doi.org/10.1101/049841

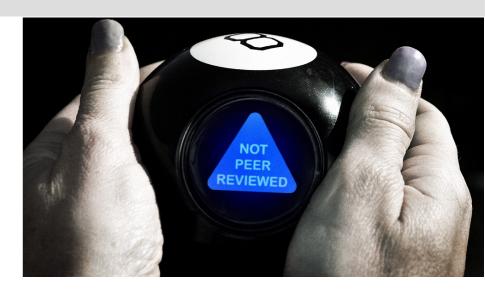
+ Add to Selected Citations

A high-throughput screen for transcription activation domains reveals their sequence characteristics and permits reliable prediction by deep learning

Ariel Erijman, Lukasz Kozlowski, Salma Sohrabi-Jahromi, James Fishburn, Linda Warfield, Jacob Schreiber, William S. Noble, Johannes Söding, Steven Hahn

bioRxiv 2019.12.11.872986; doi: https://doi.org/10.1101/2019.12.11.872986

+ Add to Selected Citations











bioRxiv posts many COVID19-related papers. A reminder: they have not been formally peer-reviewed and should not guide health-related behavior or be reported in the press as conclusive.

New Results

A high-throughput screen for transcription activation domains reveals their sequence characteristics and permits reliable prediction by deep learning

O Ariel Erijman, Lukasz Kozlowski, Salma Sohrabi-Jahromi, James Fishburn, Linda Warfield, Jacob Schreiber, William S. Noble, Johannes Söding, Steven Hahn

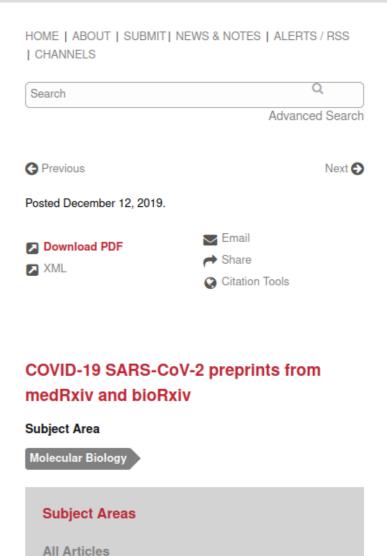
doi: https://doi.org/10.1101/2019.12.11.872986

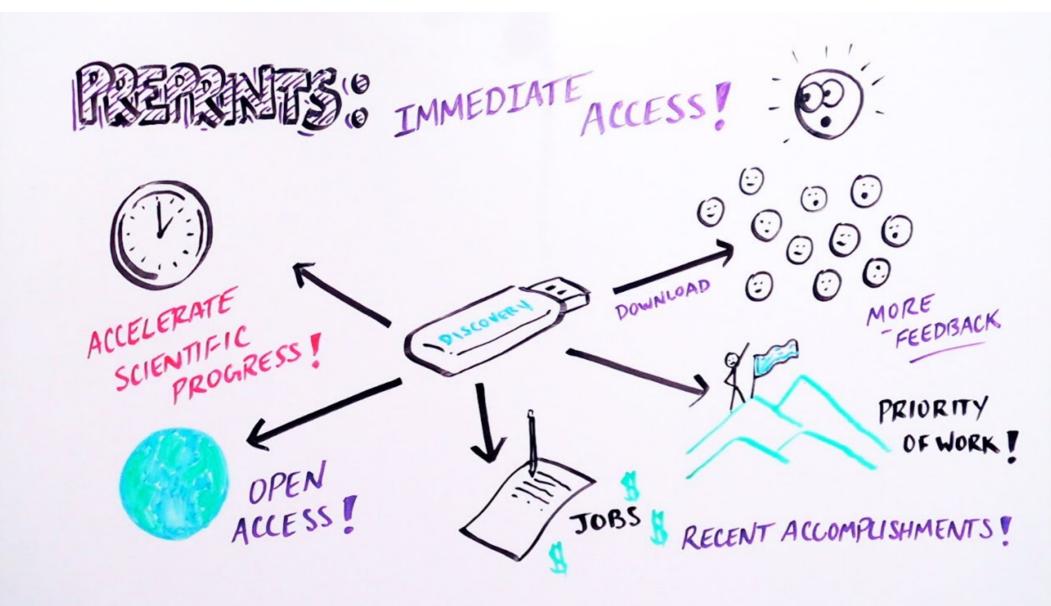
Now published in Molecular Cell doi: 10.1016/j.molcel.2020.04.020



Abstract

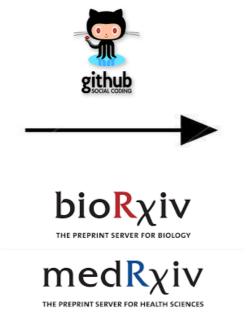
Transcription activation domains (ADs) are encoded by a wide range of seemingly unrelated

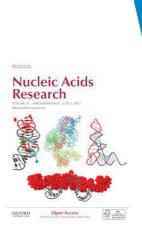








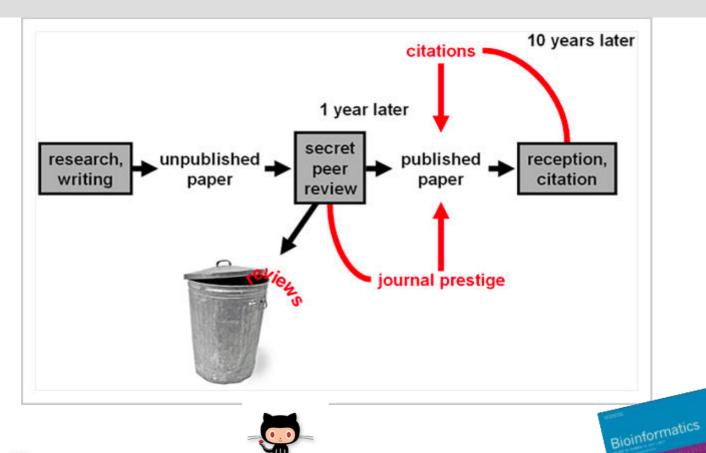




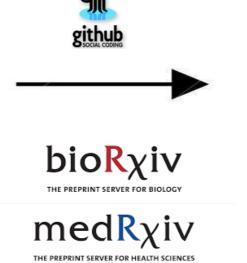


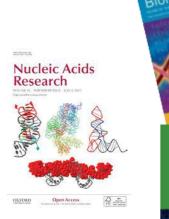
General workflow in science



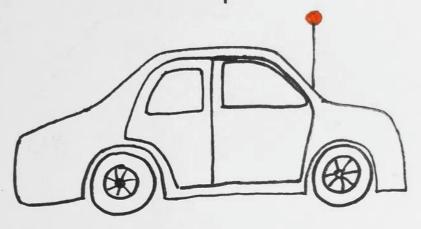




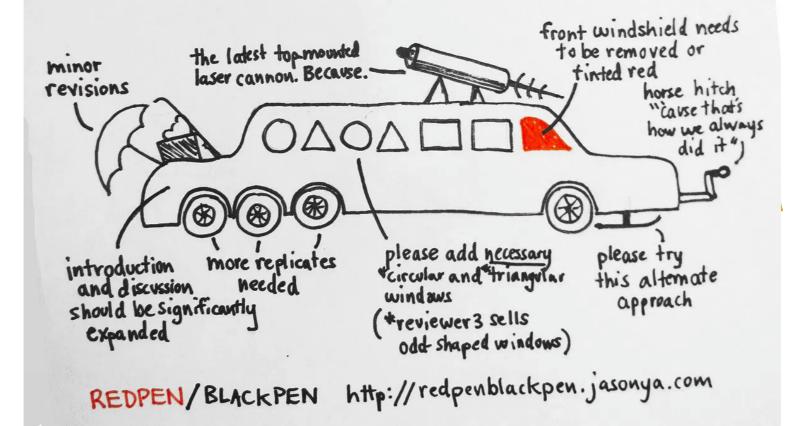


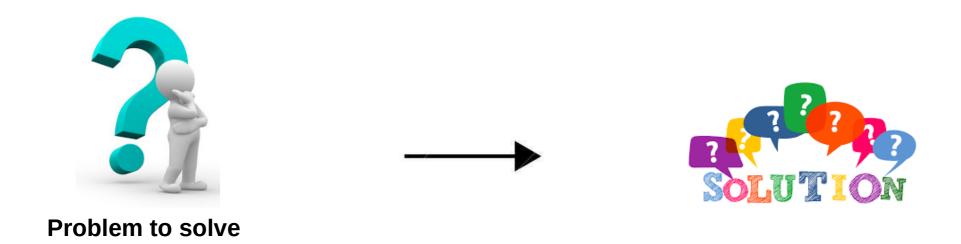






... and after peer review and revision

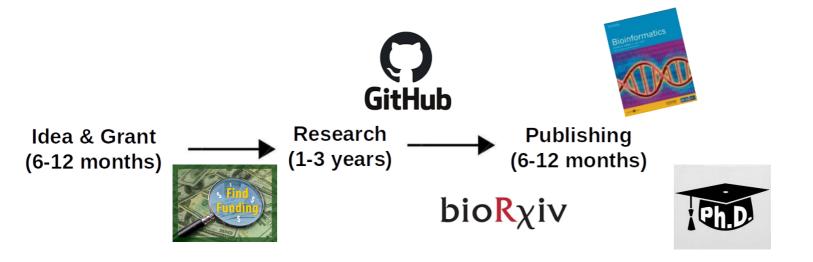




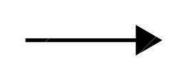






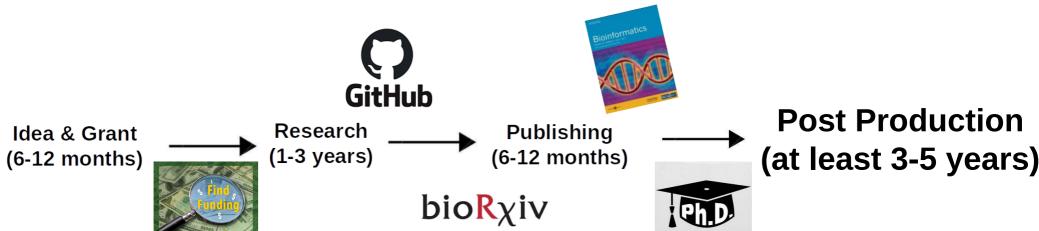




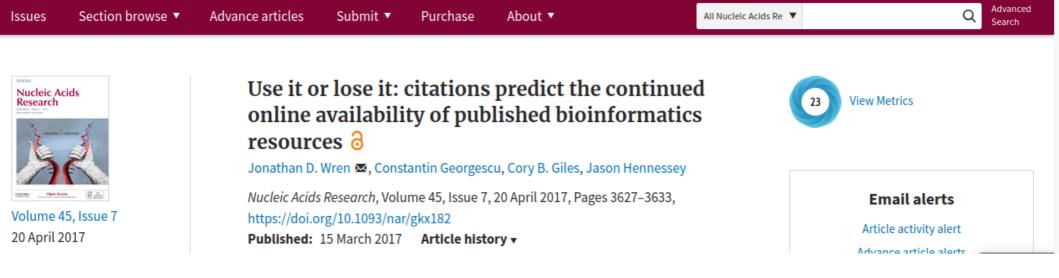


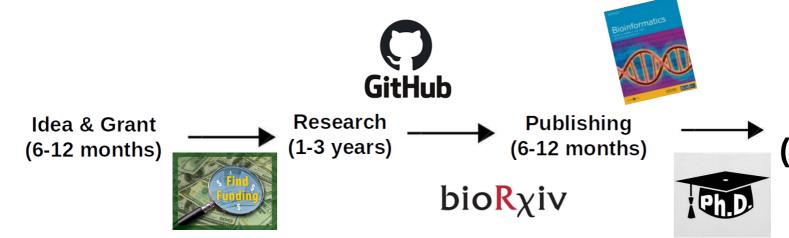






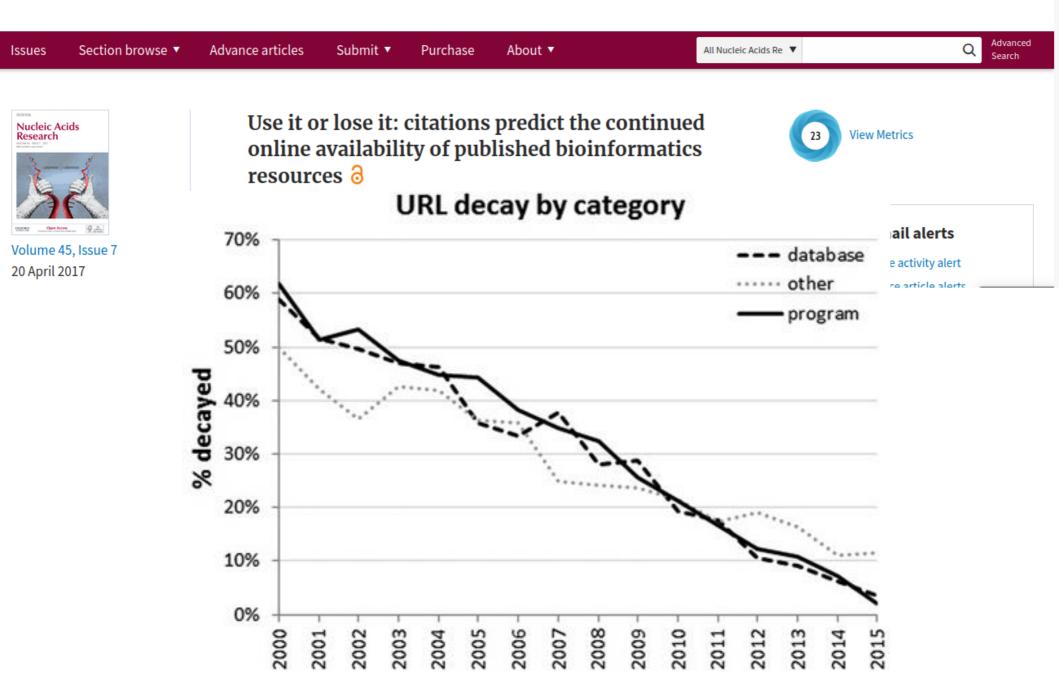
Nucleic Acids Research



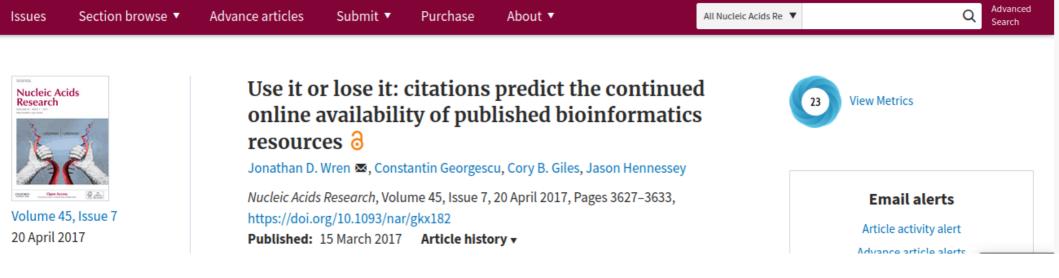


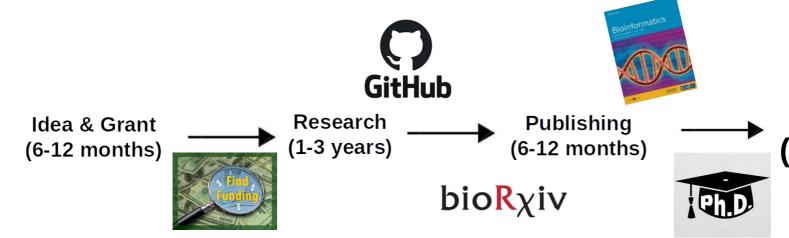
Post Production (at least 3-5 years)

Nucleic Acids Research



Nucleic Acids Research





Post Production (at least 3-5 years)

Projects

Projects presentation will be done during last week (11.06.24)

Formal requirements:

- the project has the github repository
- the project has the documentation
- license, data, scripts, test/examples are provided

Additionally, the project will be described by the leader of the Group (or few members) in short presentation (up to 20 min, plus 5-10 min for discussions).

The format: pdf/ppt and/or if possible interactive presentation of the project in the browser

Projects presentation will be done during last week (11.06.24)

Presentation should include:

- the introduction of the project (problem to be solved)
- the objectives (what you wanted to achieve)
- the results (what you achieved)
- the conclusions & possible directions for the future (what the software can do and what can be improved if more people would join)

Projects presentation will be done during last week (11.06.24)

Presentation should include:

- the introduction of the project (problem to be solved)
- the objectives (what you wanted to achieve)
- the results (what you achieved)
- the conclusions & possible directions for the future (what the software can do and what can be improved if more people would join)

The project and presentations should be finished up to 09.06. (please upload the presentation to the github of your repository up to 09.06)

Thank you for your time and See you at the next lecture

Any other questions & comments

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