

Bactopia & it's usage of nf-core components

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## Lots of bacterial genomes and bioinformatic growth in the last decade



Can we make use of all these publicly available bacterial genomes?

# Yes, we can!





Bactopia is a scalable, reproducible, and portable all-in-one pipeline.

# A few Bactopia highlights

- Supports Illumina and Nanopore reads
   Local or from public databases
- Includes more than <u>140 bioinformatic tools</u>
- <u>45+ Bactopia Tools</u> provide more workflows for more science
- Extensively tested with 100+ tests for 10,000+ output files
- Available on Bioconda, Docker, and Singularity
- Well documented at <u>bactopia.github.io</u>



# Bactopia design principles



Bactopia requires tools be available from Bioconda



All modules in Bactopia Tools must be on nf-core/modules



Bactopia should be easy to install and adaptable to user needs

## Three Sides of Bactopia



Bactopia Helpers





Bactopia

### Bactopia Tools

# Bactopia Helpers, help get started using Bactopia



bactopia citations

- Print citations for all datasets, tools and Bactopia
- bactopia datasets
  - Download and setup useful datasets for Bactopia
- bactopia download
  - Build Conda, Docker or Singularity environments for all steps in bactopia
- bactopia prepare
  - Create a file of filenames for analysis
- bactopia search
  - Generate a list of SRA accessions for analysis





Blast

Align genes, proteins, or primers to assembled contigs

Sequence Type
Determine sequence type base on PubMLST profiles

## Bactopia Tools More workflows for more science

- Allow easy comparative analysis of Bactopia outputs
- Two Types:
  - Single tool (Kleborate, TB Profiler)
  - Multiple tools connected together
    - pangenome: Prokka -> PIRATE -> IQ-Tree
  - 45+ Bactopia Tools are available
    - Frame-worked for easy addition
    - Example: pangenome Bactopia Tool



#### BACTOPIA





More workflows for more science

#### ANTIMICROBIAL RESISTANCE

#### Abricate

Mass screening of contigs for antimicrobial and virulence genes

AMRFinder+ Identify antimicrobial resistance in genes or proteins

Resistance Gene Identifier

Predict antibiotic resistance from assemblies

#### ANNOTATION

#### Bakta

Rapid annotation of bacterial genomes and plasmids eggNOG-Mapper

Functional annotation of proteins using orthologous groups and phylogenies

#### DISTANCE

#### FastANI

Fast alignment-free computation of Average Nucleotide Identity (ANI)

mash dist Calculate Mash distances between sequences

mashtree distances

Quickly create a tree using Mash

#### **SEOUENCE** SURVEY

#### CheckM

Assess the assembly quality of your samples

mlst Automatic MLST calling from assembled contigs

Listeria



#### PANGENOME

Create a pan-genome and core-genome phylogeny of vour samples. Additionally, supplement your samples by including publicly available assemblies.

#### **TAXONOMIC CLASSIFICATION**

GTDB Identify marker genes and assign taxonomic classifications

Kraken2 Taxonomic classifications of sequence reads

#### **MOBILE GENETIC** ELEMENTS

ISMapper Identify insertion site positions in bacterial genomes

MOB-suite Reconstruct and annotate plasmids in bacterial assemblies

#### MERLIN

Use Merlin to automatically run species-specific tools for the following organisms Escherichia Mycobacterium

schenchia	mycobacterium
Haemophilus	Neisseria
(lebsiella	Salmonella
egionella	Staphylococcus
isteria	Streptococcus

#### SPECIES SPECIFIC

AgrVATE Rapid identification of Staphylococcus aureus agr locus type

ECTyper In-silico prediction of Escherichia coli serotype

emmtyper emm-typing of Streptococcus pyogenes assemblies

hicap cap locus serotype and structure in Haemophilus influenzae assemblies

HpsuisSero Serotype prediction of Haemophilus parasuis assemblies

Kleborate Screen Klebsiella assemblies for MLST, sub-species, and genes of interest

legsta Typing of Legionella pneumophila assemblies

LisSero Seroaroup typing prediction for Listeria monocytogenes

meningotype Serotyping of Neisseria meningitidis assemblies

ngmaster Multi-antigen sequence typing for Neisseria gonorrhoeae

SeqSero2 Salmonella serotype prediction from reads or assemblies

SISTR Serovar prediction of Salmonella assemblies

spaTyper Computational method for finding spa types in Staphylococcus aureus

SsuisSero Serotype prediction of Streptococcus suis assemblies

staphopia-sccmec Primer based SCCmec typing of Staphylococcus aureus genomes

TBProfiler Detect resistance and lineages of Mycobacterium tuberculosis

# In a few steps, go from raw data to investigating results



Adopting nf-core components has made much of this more achievable in Bactopia, and you should consider the same for you non-nf-core pipeline

A group of volunteers always ready to share their vast amount of experience



# A few ways Bactopia is making use of nf-core components

# nf-core library in Bactopia



- Bactopia has 45+ workflows in from a singleentry point (<u>main.nf</u>)
- <u>Dynamic imports</u> of JSON schemes based on workflow config
  - Each module gets its own <u>params.config</u> and <u>params.json</u>
- Required script to aggregate into a "nextflow\_schema.json" (Nextflow Tower)

# nf-core/modules in Bactopia

- Every Bactopia Tool is available from nf-core modules
  - Slight modifications on the Bactopia-side
  - Ex. AgrVATE: <u>nf-core/modules</u> vs <u>Bactopia</u>

- Similar pytest framework as nf-core/modules
  - Tests every step in <u>Bactopia</u> and <u>Bactopia Tools</u>
  - Uses self-hosted GitHub Action runner





# nf-core meta.yaml template for documentation



- Bactopia adds <u>additional metadata</u>
  - o <u>Citations, markdown tables, output tree</u>

- Yamls are used in <u>Bactopia docs</u>
  - Built with Jinja2, Mkdocs and GitHub Actions

• Writing docs while building

# What's next for Bactopia?

MultiQC Modules

*More nf-core/modules* 

Eyes on future of configs

rich-click everything



Report generation

More Bactopia Tools

*Custom workflows for surveillance* 

Enhanced CLI

Don't hesitate to reach out if you think I can help!

# Need help?

Repository: bactopia/bactopia

Documentation: bactopia.github.io

Always looking for feedback!



Taylor Fearing Jim Mildenberger Chayse Rowley Follow nf-core on



Chan Zuckerberg <sup>+</sup> Initiative <sup>(9)</sup>

https://nf-co.re

lcons: <u>openmoji.org</u>



Department of Medicine Timothy D. Read, PhD