

CoP Bioinformatics

Meeting 3 – June 2024



6 June 2024

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The Problem



Bioinformatics CoP

- Mailing list
 - Subscribe: bioinfo-list-join@seqshare.org
- Monthly meet-up
 - Informal, hands-on, brief, “BoF session”
 - 1. Stand-up: who’s doing what (10-15mn)
 - 2. Soapbox: talk, demo, discussion, ... (15-20mn)
 - 3. Open mic: questions, tips, ideas (10-15mn)
- More?
 - Face-to-face? “Walk-in” meeting? Topical meetings?

Stand-up Round

“Stand-up Meeting”

Original (SCRUM)

- What did you do yesterday?
- What will you do today?
- Is anything blocking you?



Idea: in 1-2mn max(!)

- What are you working on?
- What will you (or would you like to) be working on?
- Is anything blocking you / how can we help?

Soapbox Time

Some notes & links from Frontiers Webinar: Pathogen Genomic Surveillance

- Utility of Genomic Surveillance \propto **threat** \times **capacity** \times **response**
 - “A lack in any of these is a lack in overall utility of GS”
- Success factors: **density of sampling** & **rapidity of sharing**
 - “Surveillance is largely a documentation of past failures”
 - “Data sharing fosters trust, integrity and reciprocity”
- GPAS ‘Global Pathogen Surveillance Service’: <https://gpas.global/>
- (TERRA? <https://terra.bio>)
- Evaluation of ONT-only genomic surveillance (PMCID:9997738)

Nanopore-only assemblies for genomic surveillance of the global priority drug-resistant pathogen, *Klebsiella pneumoniae*

Ebenezer Foster-Nyarko ¹, Hugh Cottingham ², Ryan R Wick ², Louise M Judd ², Margaret M C Lam ², Kelly L Wyres ², Thomas D Stanton ¹, Kara K Tsang ¹, Sophia David ³, David M Aanensen ³, Sylvain Brisse ⁴, Kathryn E Holt ^{1 2}

The Final SPAdes (4.0)



- Open Source, moved to GitHub
 - Repo: <https://github.com/ablab/spades>
 - Docs: <https://ablab.github.io/spades/>
 - Protocols: <https://currentprotocols.onlinelibrary.wiley.com/doi/abs/10.1002/cpbi.102>
- 4.0 features
 - Assemble NCBI SRA files
 - BinSPreader: MAG refinement using GFA
 - Run HMMs over a GFA
 - Modes: meta, plasmid, rna, corona, etc

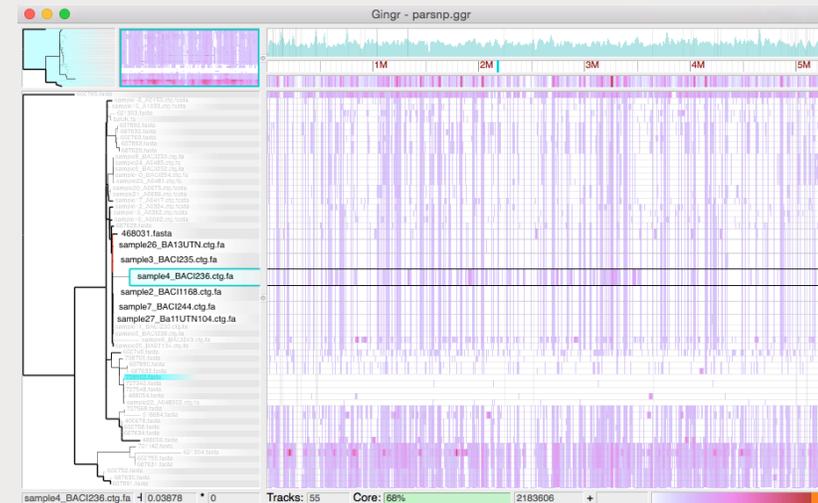
Parsnp 2.0

- First update since v1 (2014) (v1)
 - doi: [10.1093/bioinformatics/btae311](https://doi.org/10.1093/bioinformatics/btae311)
 - <https://github.com/marbl/parsnp>
- Multiple Sequence Alignment of 100s-1000s of genomes
 - Input: assemblies & finished genomes
 - Output: MSA, variant calls, core genome phylogeny
- Gingr for visualisation

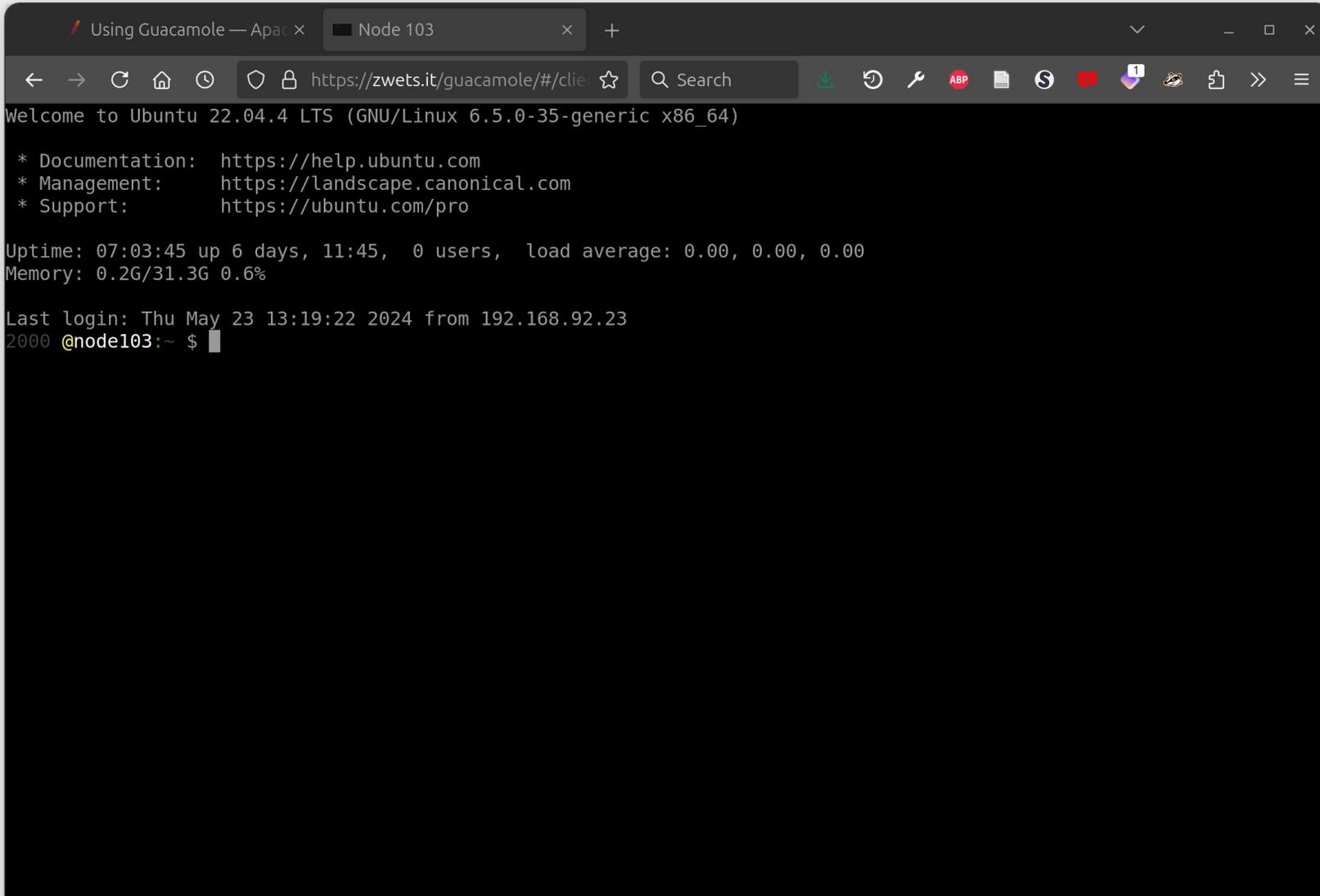
Genome analysis

Parsnp 2.0: scalable core-genome alignment for massive microbial datasets

Bryce Kille ^{1,*}, Michael G. Nute¹, Victor Huang¹, Eddie Kim¹, Adam M. Phillippy ²,
Todd J. Treangen ^{1,3,*}



Apache Guacamole (1)



```
Using Guacamole — Apac x Node 103
https://zwets.it/guacamole/#/cli
Welcome to Ubuntu 22.04.4 LTS (GNU/Linux 6.5.0-35-generic x86_64)

* Documentation:  https://help.ubuntu.com
* Management:    https://landscape.canonical.com
* Support:       https://ubuntu.com/pro

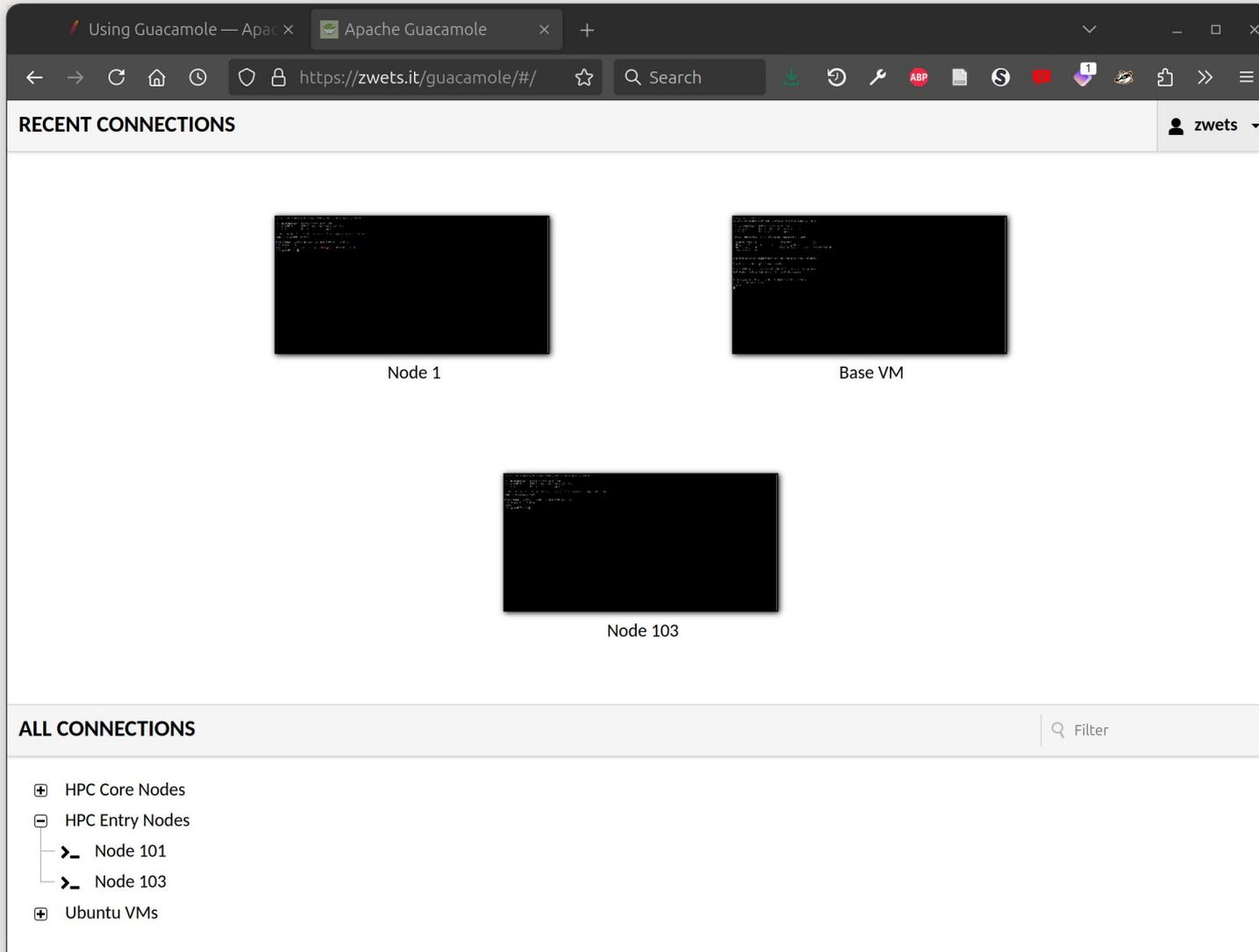
Uptime: 07:03:45 up 6 days, 11:45,  0 users,  load average: 0.00, 0.00, 0.00
Memory: 0.2G/31.3G  0.6%

Last login: Thu May 23 13:19:22 2024 from 192.168.92.23
2000 @node103:~ $
```

Client-less Remote Desktop

- In-browser
 - Terminal (SSH)
 - Console (VNC)
 - Desktop
 - Linux (VNC)
 - Windows (RDP)
 - Kubernetes VMs

Apache Guacamole (2)

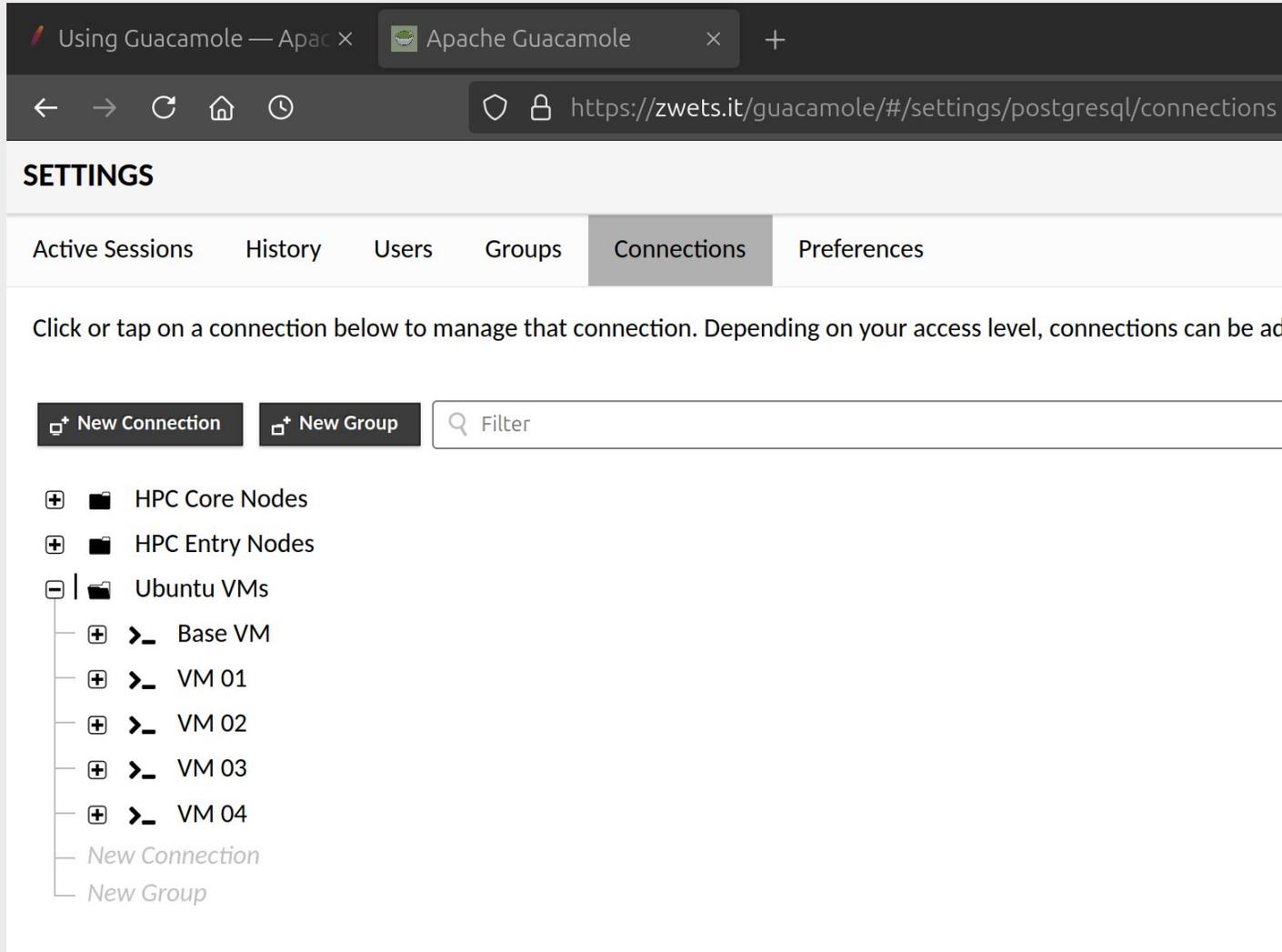


The screenshot shows the Apache Guacamole web interface in a browser. The address bar displays the URL `https://zwets.it/guacamole/#/`. The main content area is titled "RECENT CONNECTIONS" and shows three connection thumbnails: "Node 1", "Base VM", and "Node 103". Each thumbnail is a black rectangle with some white text visible, representing a terminal window. The user "zwets" is logged in. Below the "RECENT CONNECTIONS" section is the "ALL CONNECTIONS" section, which includes a search filter and a tree view of connection categories: "HPC Core Nodes", "HPC Entry Nodes" (with sub-items "Node 101" and "Node 103"), and "Ubuntu VMs".

Guacamole

- Tiers
 - Browser
 - Proxy
 - Web-Server
 - Guacamole Server
 - Backends through Plugins
 - SSH, VNC, RDP, K8S

Apache Guacamole (3)



Using Guacamole — Apac x Apache Guacamole x +

← → ↻ 🏠 🕒 <https://zwets.it/guacamole/#/settings/postgresql/connections>

SETTINGS

Active Sessions History Users Groups **Connections** Preferences

Click or tap on a connection below to manage that connection. Depending on your access level, connections can be added or removed.

+ New Connection + New Group 🔍 Filter

- + 📁 HPC Core Nodes
- + 📁 HPC Entry Nodes
- ☰ 📁 Ubuntu VMs
 - + ➤ Base VM
 - + ➤ VM 01
 - + ➤ VM 02
 - + ➤ VM 03
 - + ➤ VM 04
 - New Connection
 - New Group

Management

- Users
- Groups
- Connections
 - Authorization
 - Connection sharing
 - “On-demand” VMs

hAMRonization

- [doi:10.1101/2024.03.07.583950](https://doi.org/10.1101/2024.03.07.583950)
- PHA4GE = Public Health Alliance for Genomic Epidemiology
- Standardised output specification for bioinformatic AMR detection
- hAMRonization
 - <https://github.com/pha4ge/hAMRonization>
 - Python package: unifies output from (18) tools to the hAMRonize spec
 - Output: tabular, JSON, interactive HTML

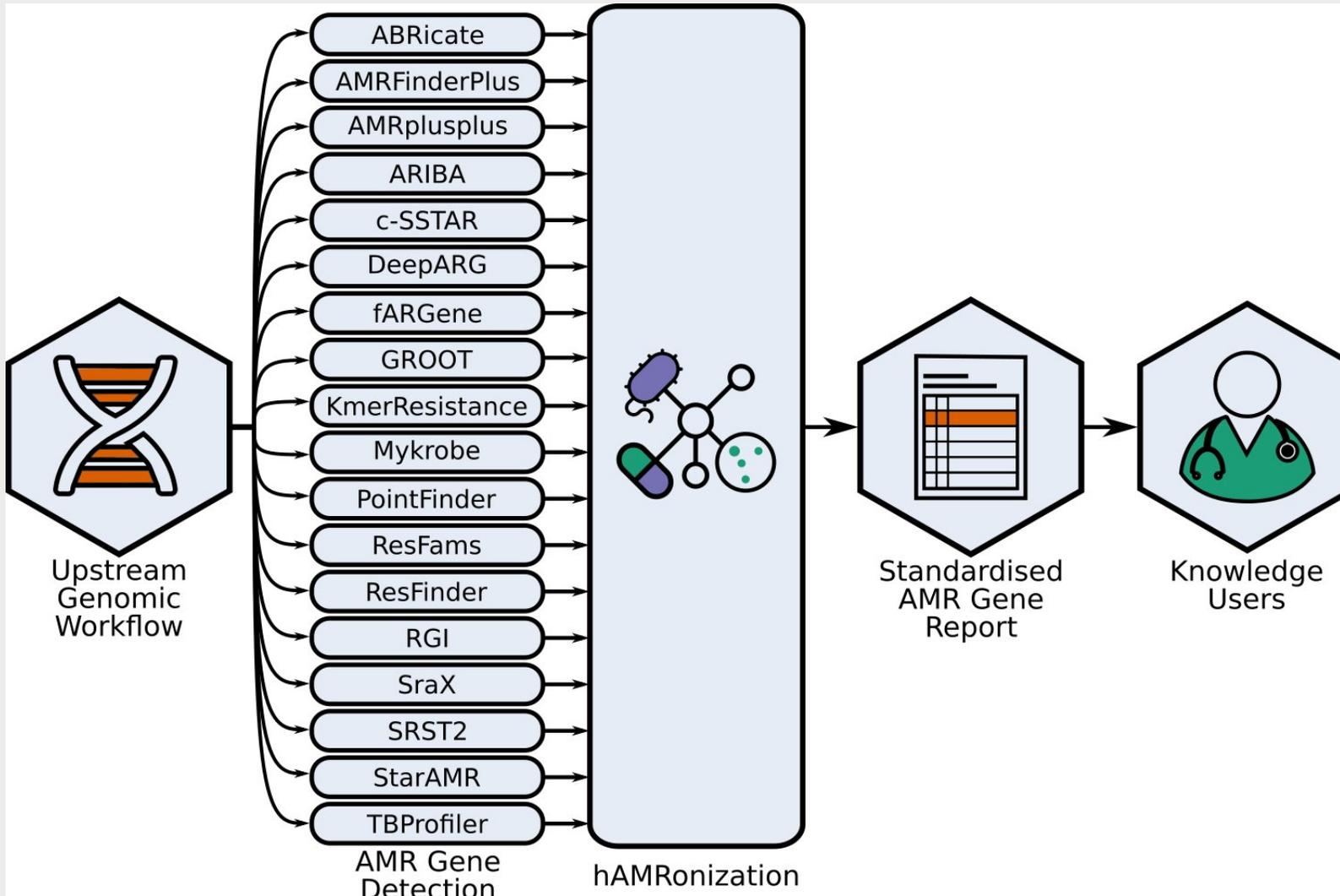


hAMRonization: Enhancing antimicrobial resistance prediction using the PHA4GE AMR detection specification and tooling

 Inês Mendes,  Emma Griffiths,  Alex Manuele,  Dan Fornika,  Simon H Tausch,  Thanh Le-Viet,  Jody Phelan,  Conor J. Meehan,  Amogelang R. Raphenya,  Brian Alcock,  Elizabeth Culp,  Federico Lorenzo,  Maria Sol Haim,  Adam Witney,  Allison Black,  Lee Katz,  Paul Oluniyi,  Idowu Olawoye,  Ruth Timme,  Hui-min Neoh,  Su Datt Lam,  Tengku Zetty Maztura Tengku Jamaluddin,  Sheila Nathan,  Mia Yang Ang,  Sabrina Di Gregorio,  Koen Vandellannoote,  Rutaiwan Dusadeepong,  Leonid Chindelevitch,  Muhammad Ibtisam Nasar,  David Aanensen,  Ayorinde Oluwatobiloba Afolayan,  Erkison Ewomazino Odih,  Andrew Grant McArthur,  Michael Feldgarden,  Marcelo M Galas,  Josefina Campos,  Iruka N. Okeke,  Anthony Underwood,  Andrew J. Page,  Duncan MacCannell,  Finlay Maguire

doi: <https://doi.org/10.1101/2024.03.07.583950>

hAMRonization (2)



hAMRonization

- Piloted in 17 PH Labs
- Standardised vocabulary, e.g.
 - “Gene Name”
 - “% Coverage (breadth)”
 - “Drug Class”
 - Provenance (tool, database, versions)
- Harmonised with ontologies
- Conversion from 18 tools that are:
 - In active use
 - Maintained
 - Species-agnostic
 - Open Source
- PoC Workflow (12 tools)

Public Health Alliance for Genomic Epidemiology

Search: blaOXA Show Only Genomes With Hits

	abricate: config 0	amrfinderplus: config 0	csstar: config 0	resfinder.py: config 0	staramr: config 0
ERR873305	11 hits	10 hits	10 hits	6 hits	9 hits
	aac(6')-29a	aac(6')-29a	aac(6')	aac(6')-29a	aac(6')-29a
	aph(3')-IIb	aph(3')-IIb	aph(3')	blaVIM-2	aph(3')-IIb
	blaOXA-395	blaOXA-395	bcr1	catB7	blaOXA-50
	blaPDC-158	blaPDC-3	blaOXA	crpP	blaPAO
	blaPDC-55	blaVIM-2	blaPAO	fosA	blaVIM-2
	blaVIM-2	catB7	blaVIM	sul1	catB7
	catB7	crpP	catB7		crpP
	cmlB1	fosA	crpP		fosA
	crpP	qacEdelta1	fosATR		sul1
	fosA-354827590	sul1	sul1		
	sul1				
ERR873306	11 hits	10 hits	10 hits	6 hits	9 hits

Search Results

Total hits: 347

Genomes with hits: 85

Tools with hits: 5

? Differential results: 84

Selected

Compare Clear

hAMRonization (3)

- Interactive HTML report
- Samples × tools × genes
- Genes only (tabular report has all)

Open Mic

- Feedback?
- Future themes?
- **Next month: Niamh**

Thank you



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The views expressed do not necessarily reflect the UK Government's official policies.