From Bench to Big Data: What's new with MultiQC and Nextflow

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Background

PhD in the lab, epigenetics

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Postdoc, core bioinformatics

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Software development

INDUSTRY

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NATIONAL GENOMICS INFRASTRUCTURE

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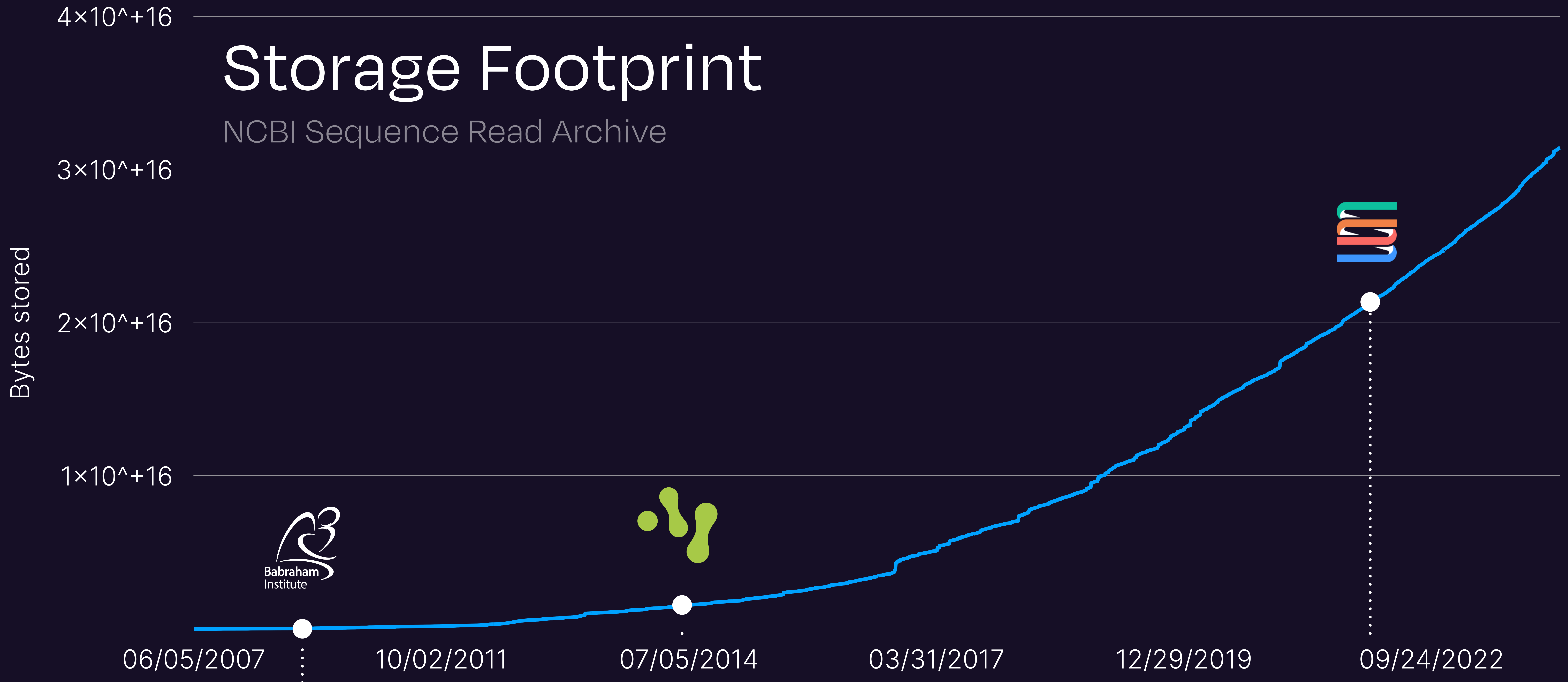
Storage Footprint

NCBI Sequence Read Archive



LAB

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seqera

Advancing Science For Everyone Through Software

Open Source Software

</> BUILD

Open Science Resources

DISCOVER

Science Infrastructure

SCALE

Product Manager for
Open Source Software

nextflow

multiqc

wave

fusion

Steering committee,
Core team

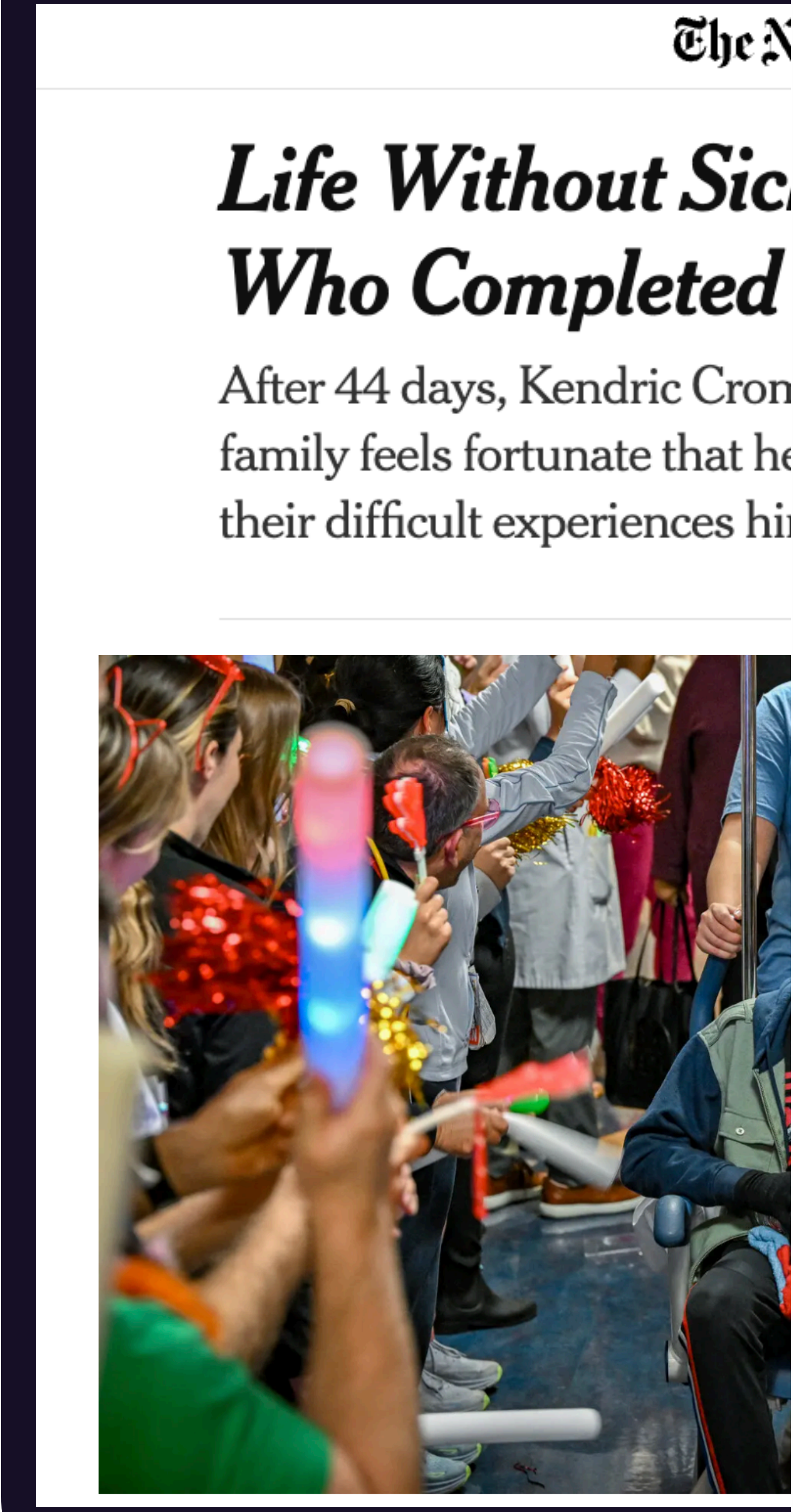
nf-core

Trustee

ossf

VERTEX

OUR WHY



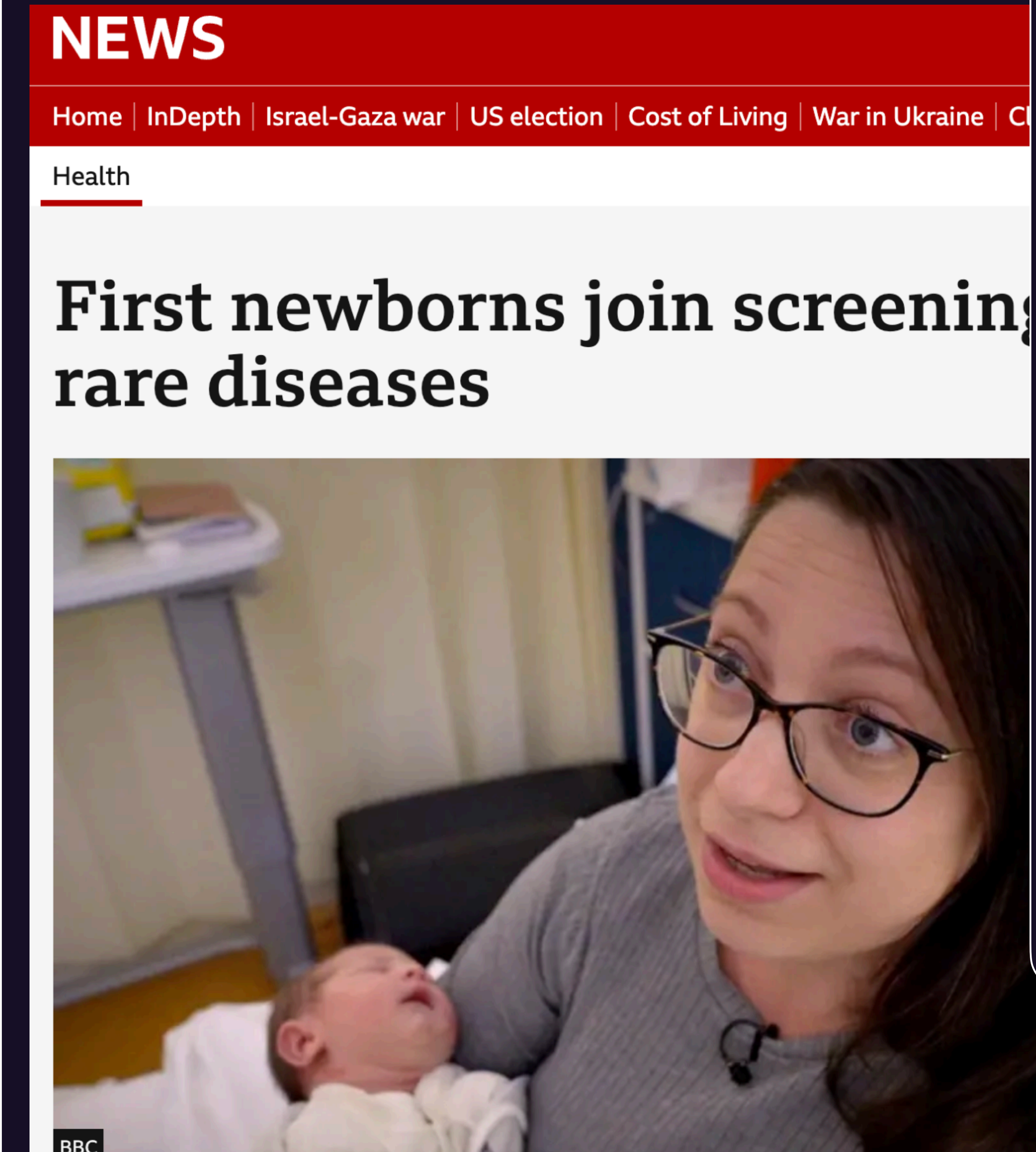
The N

Life Without Sic
Who Completed

After 44 days, Kendric Cron
family feels fortunate that he
their difficult experiences hi

Genomics England

OU



NEWS

Home | InDepth | Israel-Gaza war | US election | Cost of Living | War in Ukraine | Cl

Health

First newborns join screening
rare diseases

BBC

moderna

OUR WHY

‘Real hope’ for cancer cure as personal mRNA vaccine for melanoma trialled

Excitement among patients and researchers as custom-built jabs enter phase 3 trial

A nurse prepares to give Steve Young, one of the first patients in the trial, his first jab at UCLH in London. Photograph: Jordan Pettitt/PA

multiqc

Open-source reporting and analytics

x

multiqc

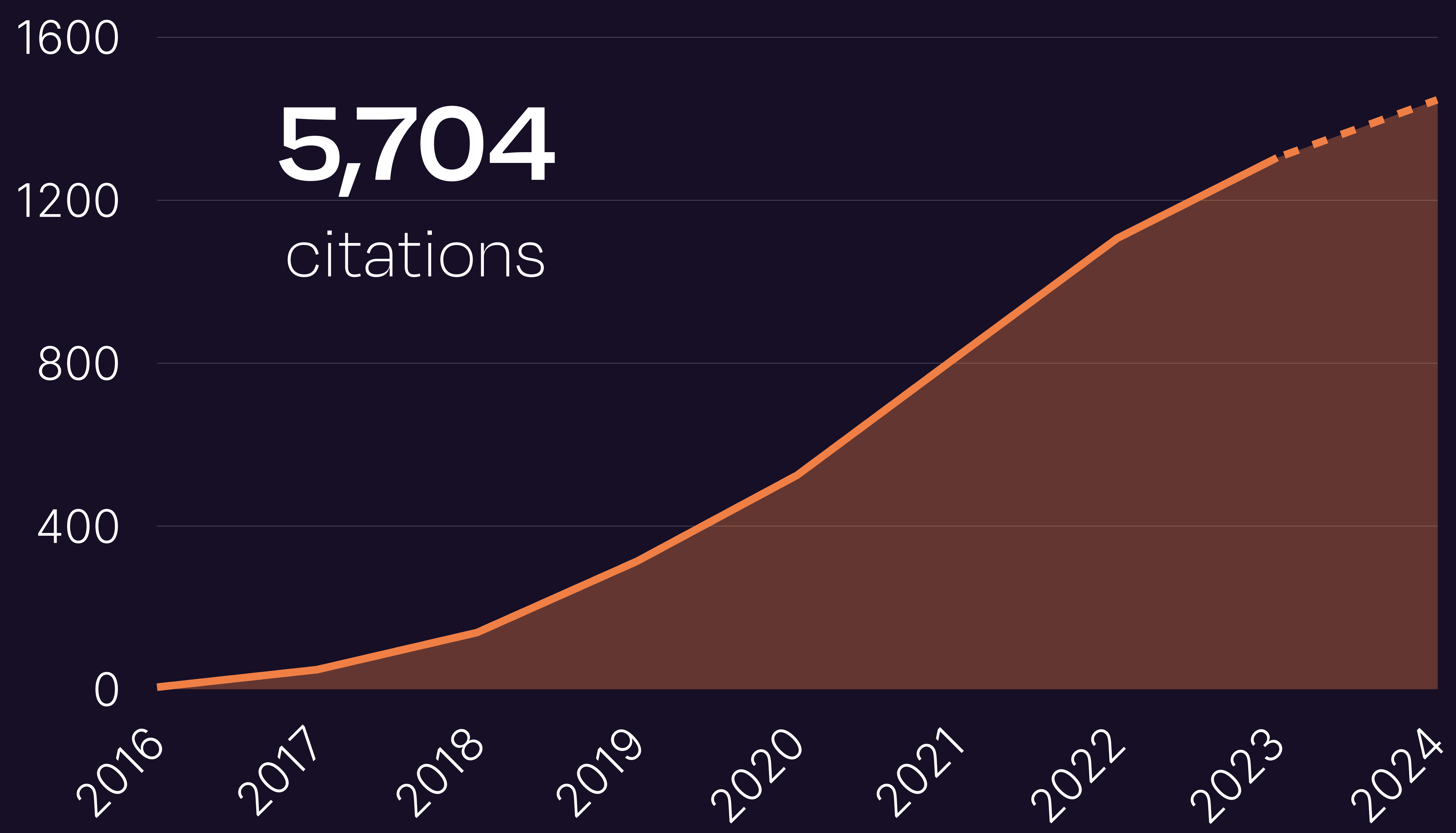
1,216
GitHub Stars

+25K
Runs per day

+1.5M
Downloads

x

Citations by year



Command Line Interface

Web interface

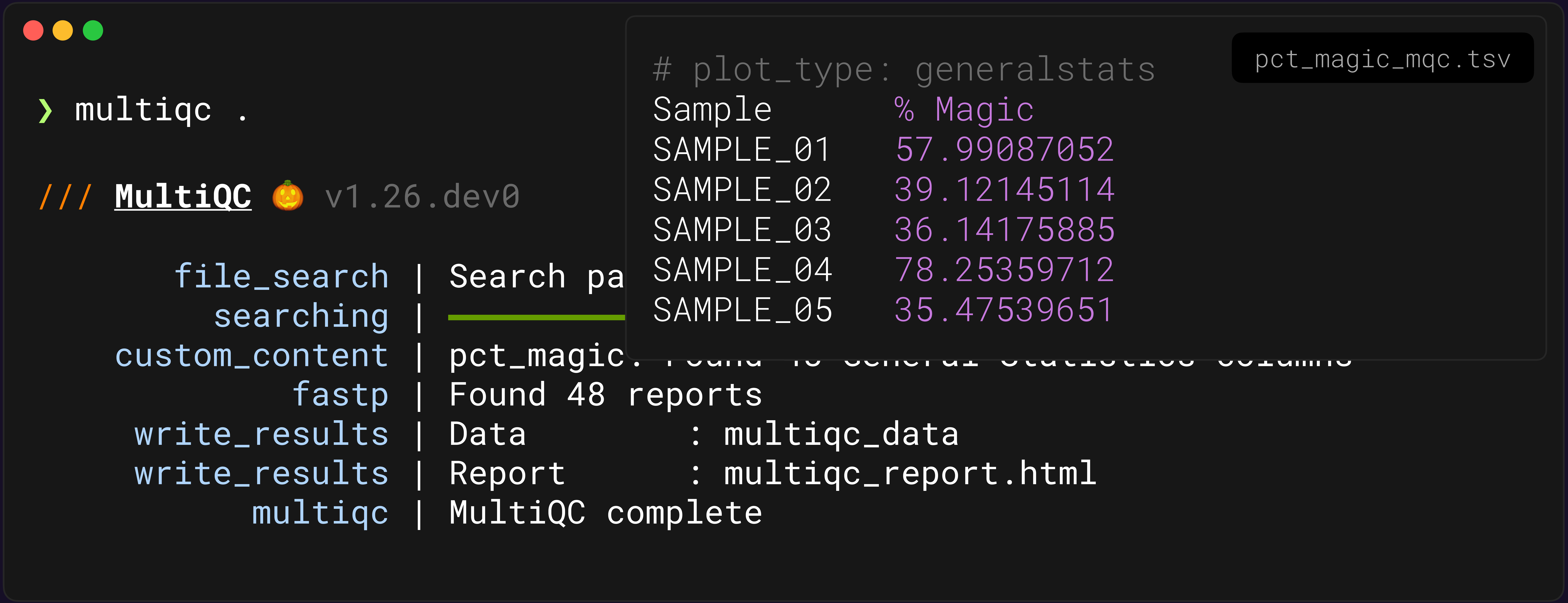
MultiQC Plugins

Custom Content

Notebooks and Scripts

Demo

https://seqera.io/multiqc/

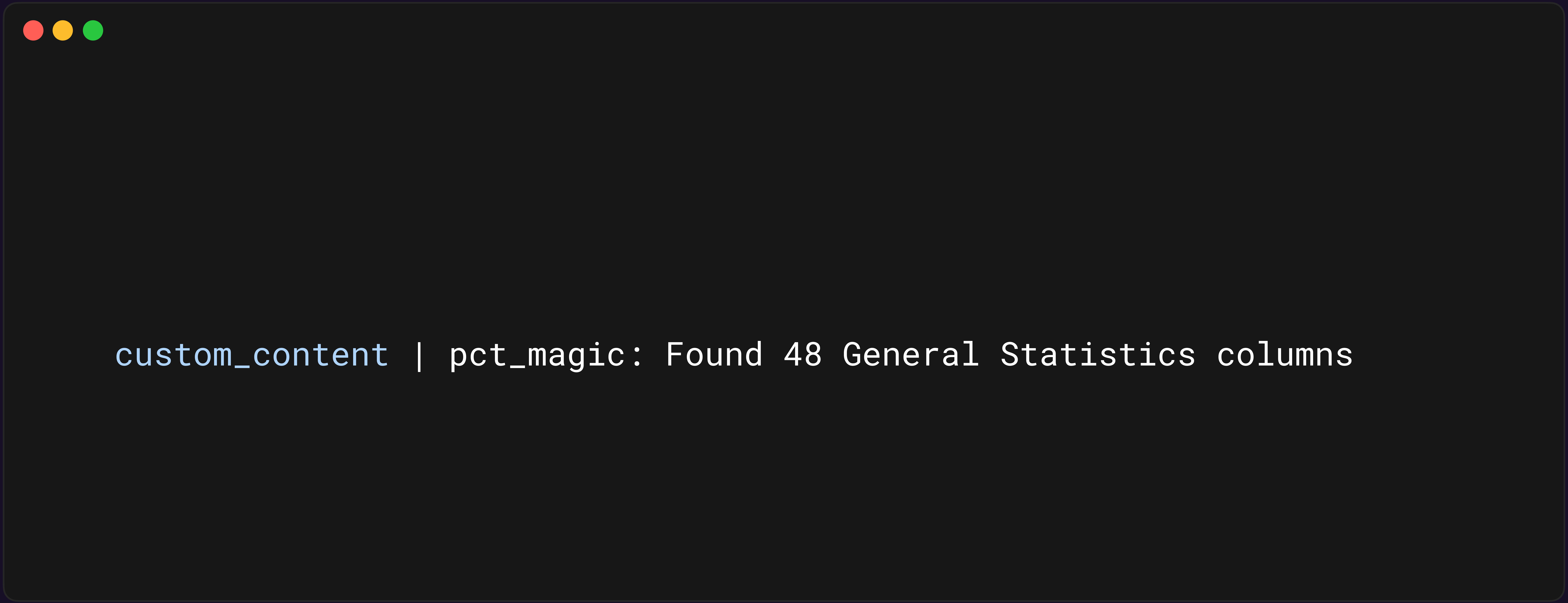


```
❯ multiqc .

/// MultiQC 🎃 v1.26.dev0

       file_search | Search pa
         searching | ━━━━━━━━━
    custom_content | pct_magic: Found 10 General Statistics columns
             fastp | Found 48 reports
     write_results | Data         : multiqc_data
     write_results | Report       : multiqc_report.html
           multiqc | MultiQC complete
```

pct_magic_mqc.tsv

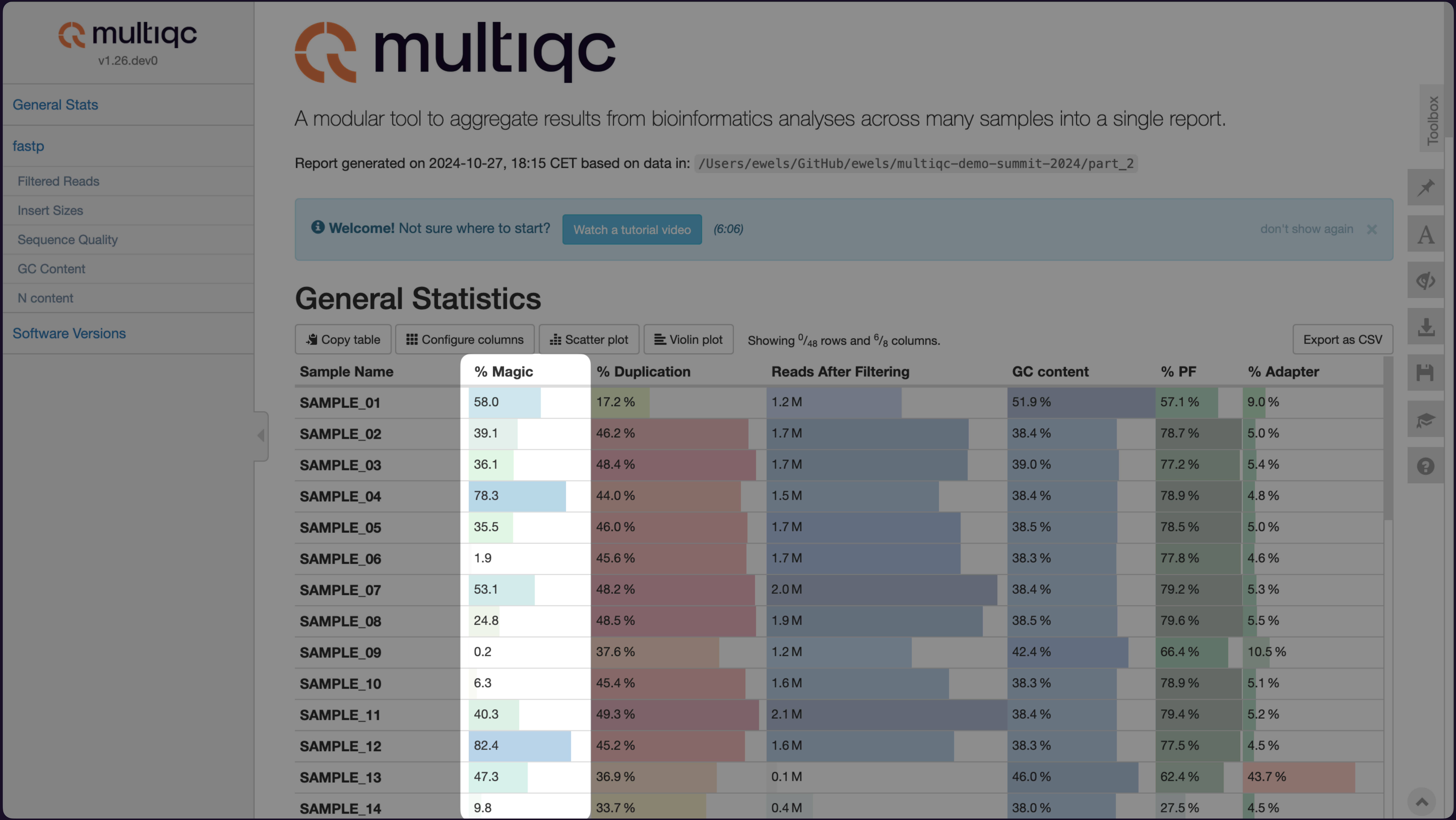
```
# plot_type: generalstats
Sample       % Magic
SAMPLE_01    57.99087052
SAMPLE_02    39.12145114
SAMPLE_03    36.14175885
SAMPLE_04    78.25359712
SAMPLE_05    35.47539651
```

```
fastp
fastqc
pct_magic_mqc.tsv
```



```
custom_content | pct_magic: Found 48 General Statistics columns
```

pct_magic_mqc.tsv



General Stats

fastp

- Filtered Reads
- Insert Sizes
- Sequence Quality
- GC Content
- N content

Software Versions

multiqc

A modular tool to aggregate results from bioinformatics analyses across many samples into a single report.

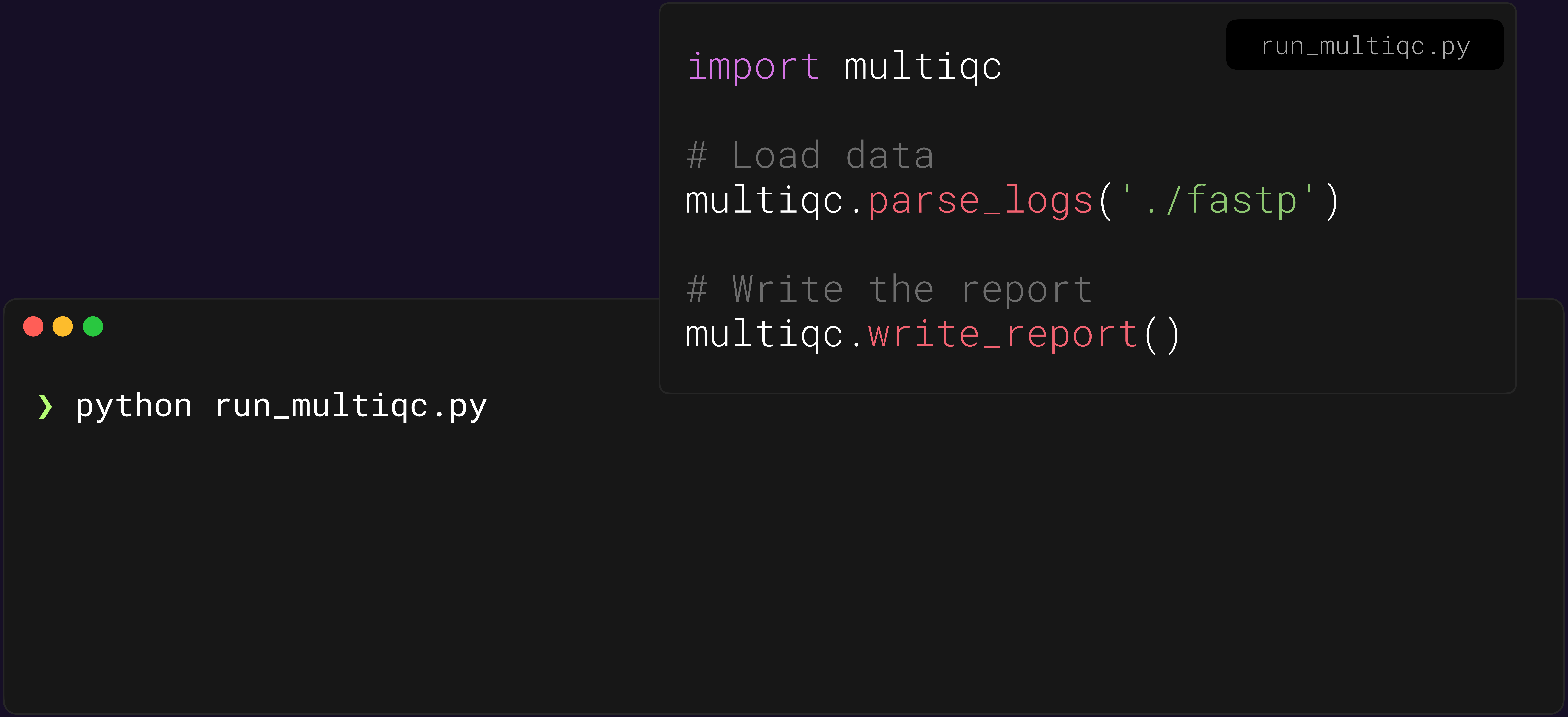
Report generated on 2024-10-27, 18:15 CET based on data in: `/Users/ewels/GitHub/ewels/multiqc-demo-summit-2024/part_2`

Welcome! Not sure where to start? Watch a tutorial video *(6:06)* don't show again ✕

General Statistics

Copy table | Configure columns | Scatter plot | Violin plot | Showing $^0/_{48}$ rows and $^6/_8$ columns. | Export as CSV

Sample Name	% Magic	% Duplication	Reads After Filtering	GC content	% PF	% Adapter
SAMPLE_01	58.0	17.2 %	1.2 M	51.9 %	57.1 %	9.0 %
SAMPLE_02	39.1	46.2 %	1.7 M	38.4 %	78.7 %	5.0 %
SAMPLE_03	36.1	48.4 %	1.7 M	39.0 %	77.2 %	5.4 %
SAMPLE_04	78.3	44.0 %	1.5 M	38.4 %	78.9 %	4.8 %
SAMPLE_05	35.5	46.0 %	1.7 M	38.5 %	78.5 %	5.0 %
SAMPLE_06	1.9	45.6 %	1.7 M	38.3 %	77.8 %	4.6 %
SAMPLE_07	53.1	48.2 %	2.0 M	38.4 %	79.2 %	5.3 %
SAMPLE_08	24.8	48.5 %	1.9 M	38.5 %	79.6 %	5.5 %
SAMPLE_09	0.2	37.6 %	1.2 M	42.4 %	66.4 %	10.5 %
SAMPLE_10	6.3	45.4 %	1.6 M	38.3 %	78.9 %	5.1 %
SAMPLE_11	40.3	49.3 %	2.1 M	38.4 %	79.4 %	5.2 %
SAMPLE_12	82.4	45.2 %	1.6 M	38.3 %	77.5 %	4.5 %
SAMPLE_13	47.3	36.9 %	0.1 M	46.0 %	62.4 %	43.7 %
SAMPLE_14	9.8	33.7 %	0.4 M	38.0 %	27.5 %	4.5 %



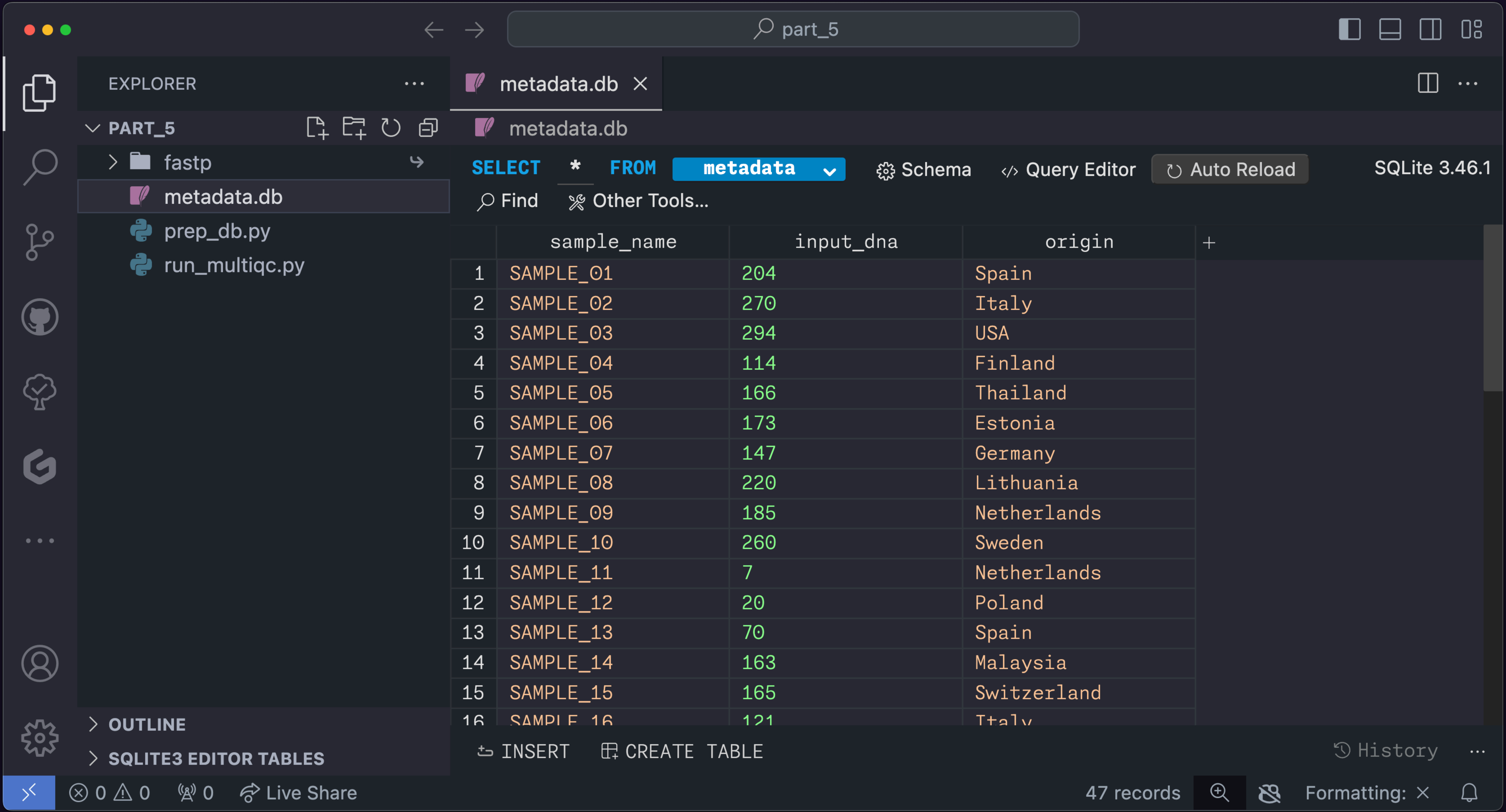
run_multiqc.py

```python
import multiqc

# Load data
multiqc.parse_logs('./fastp')

# Write the report
multiqc.write_report()
```

```
❯ python run_multiqc.py
```

run_multiqc.py

```python
# Fetch the custom data
reads = {}
for samp, data in multiqc.get_module_data(module='fastp').items():
    reads[samp] = {
      'Reads Before Filtering': data['summary']['before_filtering']['total_reads']
    }

# Add new column to the General Stats table
fastp_module = multiqc.report.modules[0]
fastp_module.general_stats_addcols(data_by_sample=reads)
```



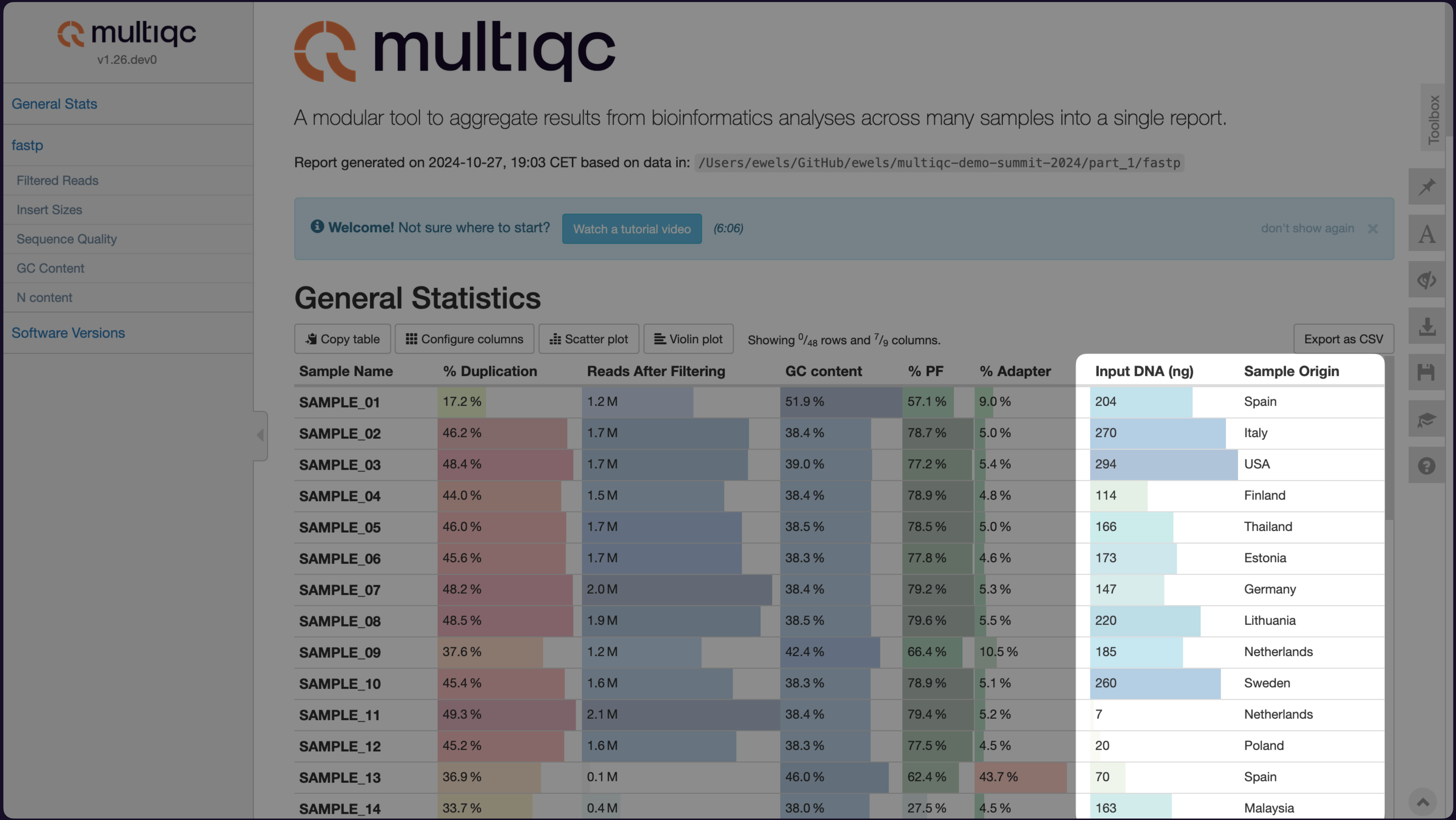
	sample_name	input_dna	origin
1	SAMPLE_01	204	Spain
2	SAMPLE_02	270	Italy
3	SAMPLE_03	294	USA
4	SAMPLE_04	114	Finland
5	SAMPLE_05	166	Thailand
6	SAMPLE_06	173	Estonia
7	SAMPLE_07	147	Germany
8	SAMPLE_08	220	Lithuania
9	SAMPLE_09	185	Netherlands
10	SAMPLE_10	260	Sweden
11	SAMPLE_11	7	Netherlands
12	SAMPLE_12	20	Poland
13	SAMPLE_13	70	Spain
14	SAMPLE_14	163	Malaysia
15	SAMPLE_15	165	Switzerland
16	SAMPLE_16	121	Italy

run_multiqc.py

```python
# Fetch from database
metadata = {}
cx = sqlite3.connect('metadata.db')
for row in cx.cursor().execute('SELECT * FROM metadata'):
    metadata[row[0]] = {
        'Input DNA (ng)': row[1],
        'Sample Origin': row[2]
    }

# Add data to report
metadata_module = multiqc.BaseMultiqcModule()
metadata_module.general_stats_addcols(data_by_sample=metadata)
multiqc.report.modules.append(metadata_module)
```

Fetch data

Add to report



multiqc

A modular tool to aggregate results from bioinformatics analyses across many samples into a single report.

Report generated on 2024-10-27, 19:03 CET based on data in: `/Users/ewels/GitHub/ewels/multiqc-demo-summit-2024/part_1/fastp`

Welcome! Not sure where to start? (6:06)

General Statistics

Showing $^{0}/_{48}$ rows and $^{7}/_{9}$ columns.

Sample Name	% Duplication	Reads After Filtering	GC content	% PF	% Adapter	Input DNA (ng)	Sample Origin
SAMPLE_01	17.2 %	1.2 M	51.9 %	57.1 %	9.0 %	204	Spain
SAMPLE_02	46.2 %	1.7 M	38.4 %	78.7 %	5.0 %	270	Italy
SAMPLE_03	48.4 %	1.7 M	39.0 %	77.2 %	5.4 %	294	USA
SAMPLE_04	44.0 %	1.5 M	38.4 %	78.9 %	4.8 %	114	Finland
SAMPLE_05	46.0 %	1.7 M	38.5 %	78.5 %	5.0 %	166	Thailand
SAMPLE_06	45.6 %	1.7 M	38.3 %	77.8 %	4.6 %	173	Estonia
SAMPLE_07	48.2 %	2.0 M	38.4 %	79.2 %	5.3 %	147	Germany
SAMPLE_08	48.5 %	1.9 M	38.5 %	79.6 %	5.5 %	220	Lithuania
SAMPLE_09	37.6 %	1.2 M	42.4 %	66.4 %	10.5 %	185	Netherlands
SAMPLE_10	45.4 %	1.6 M	38.3 %	78.9 %	5.1 %	260	Sweden
SAMPLE_11	49.3 %	2.1 M	38.4 %	79.4 %	5.2 %	7	Netherlands
SAMPLE_12	45.2 %	1.6 M	38.3 %	77.5 %	4.5 %	20	Poland
SAMPLE_13	36.9 %	0.1 M	46.0 %	62.4 %	43.7 %	70	Spain
SAMPLE_14	33.7 %	0.4 M	38.0 %	27.5 %	4.5 %	163	Malaysia

nextflow

Open-source orchestrator for deploying workflows

Nextflow DSL limitations

Nextflow was created as an extension of the Groovy programming language.

Missing a formal grammar and syntax parser.

Too fragile. Poor syntax error detection and reporting. Lack of tooling.

X

Introducing: Language server & VS Code integration for Nextflow

Roadmap

Bring new parsers into Nextflow CLI

- Better error messages
- Improve the `nextflow inspect` command
- New commands for linting, formatting

Move beyond Groovy syntax

- Type annotations
- Static type checking
- Simpler dataflow syntax

X

The future of code development is AI-driven

How can we generate code that works in bioinformatics?

Seqera AI

Seqera AI

Available today at

seqera.io/ask-ai

Convert any bash / language script to Nextflow

AI error debugging and code-testing

Rooted in Nextflow and best practices

Discover

Nextflow Summit 2024

(You missed it, sorry)

https://summit.nextflow.io

https://youtube.com/@Nextflow

Thank you

Phil Ewels

phil.ewels@seqera.io

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https://summit.nextflow.io

https://seqera.io