

BioCompute Database and Transfer Mechanism Development Workshop

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Workshop Guidelines

- If you have questions during the talk, please type them into the chat.
- Q&A
 - Moderator: Charles Hadley King
 - Use “raise hand” feature during Q&A session to ask a question.
- This workshop will be recorded, and the recording will be sent to all attendees shortly after.

Thank you!

Goals of this Workshop

1. Introduce BioCompute Objects (BCO) for computational analysis
2. Provide BioCompute resources for future reference
3. Demonstrate tools available via BioCompute Portal and BCODB

Agenda

- Introduction: Use cases and BioCompute
- BioCompute Portal Walkthrough
- Demo of user account and DB access
- Description of DB and schema
- Transfer from Galaxy, HIVE, & local machine
- Q&A



Use-Case Examples

Test
Submission

Tuberculosis
Detection

Vaccine Safety

Provenance Domain

Name R Safety Assessment Algorithm for Aluminum in Infant Vaccines.

Version 1.0

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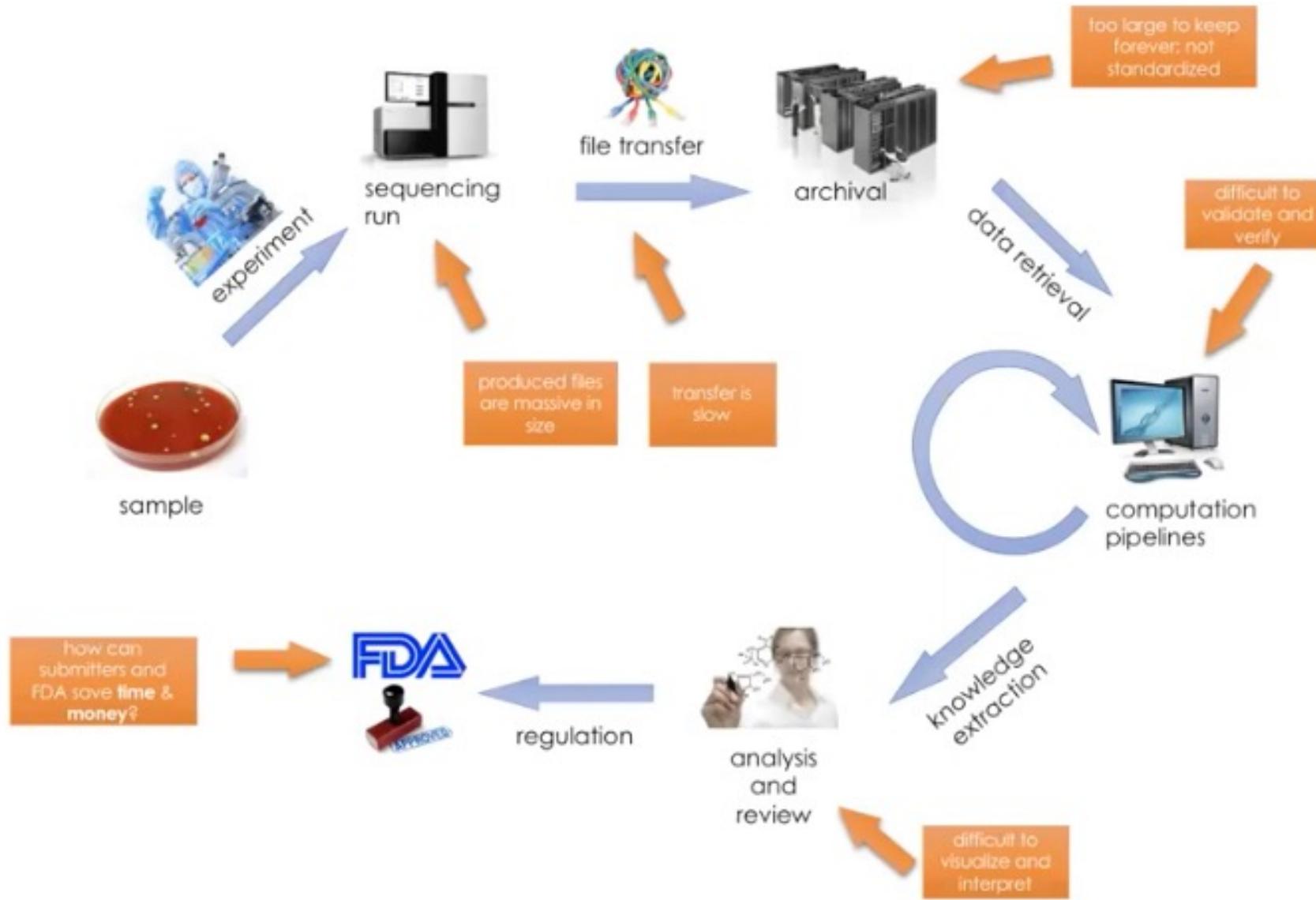
Created 2020-04-30T18:03:25.679Z

Modified 2021-12-03T19:23:45.074Z

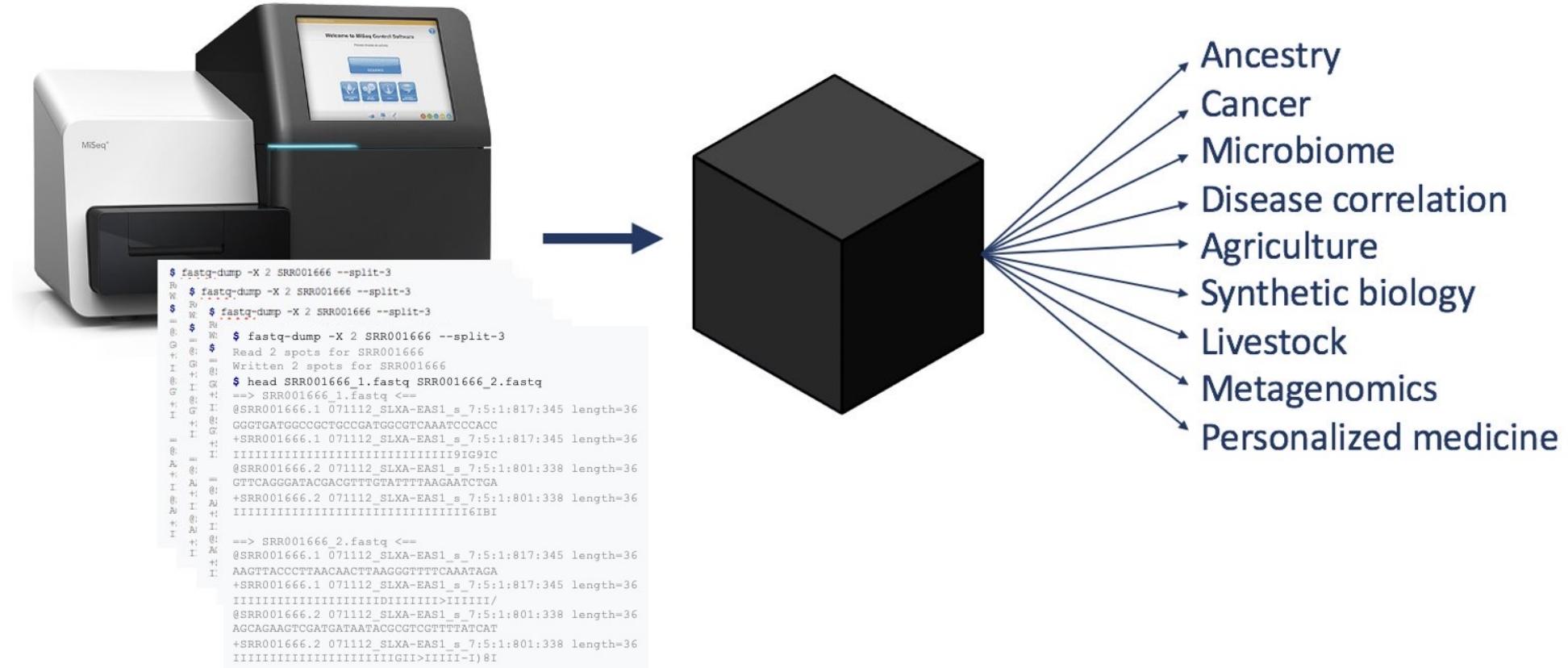
Contributors

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NGS life cycle



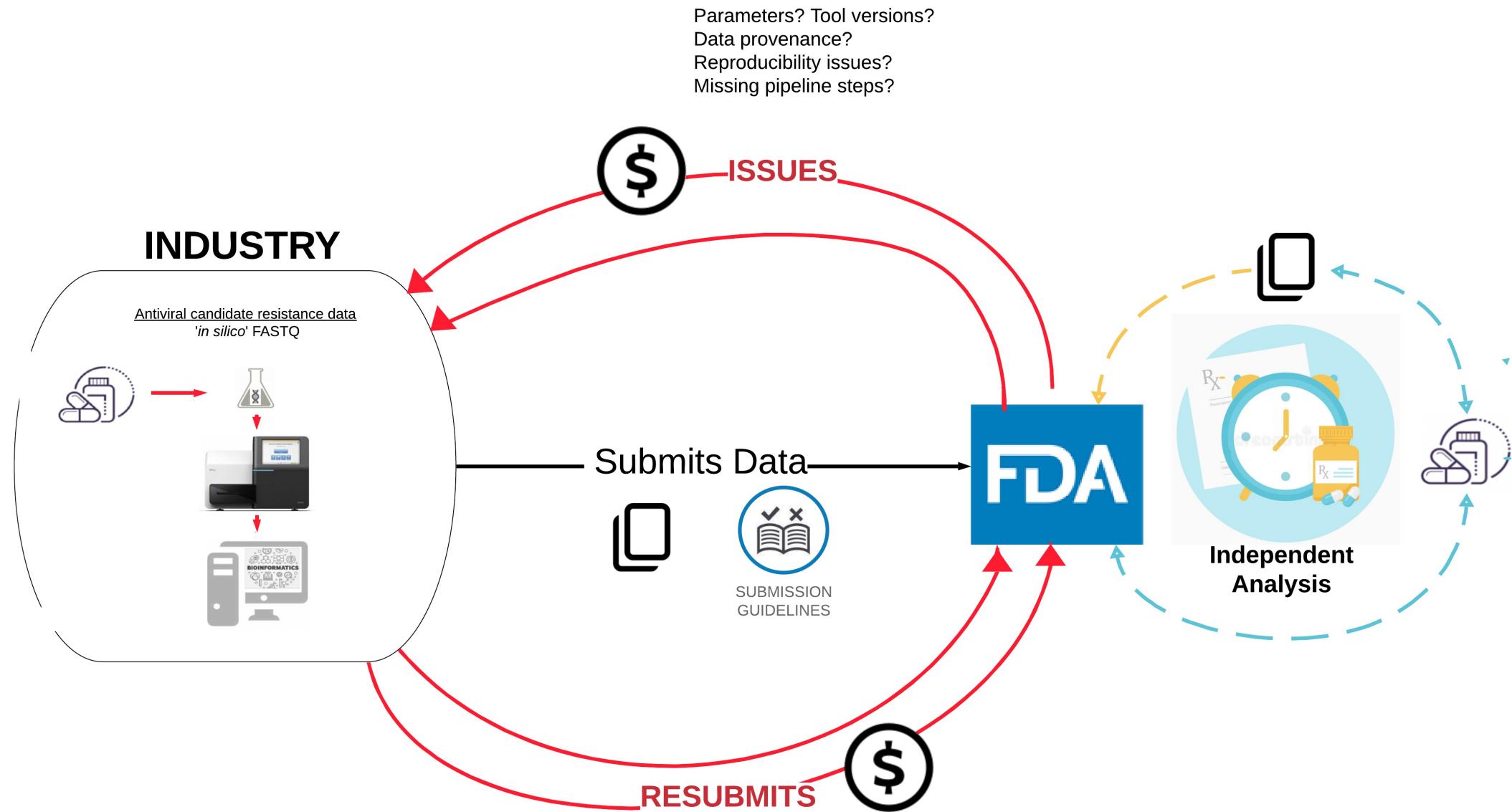
NGS Data Flows



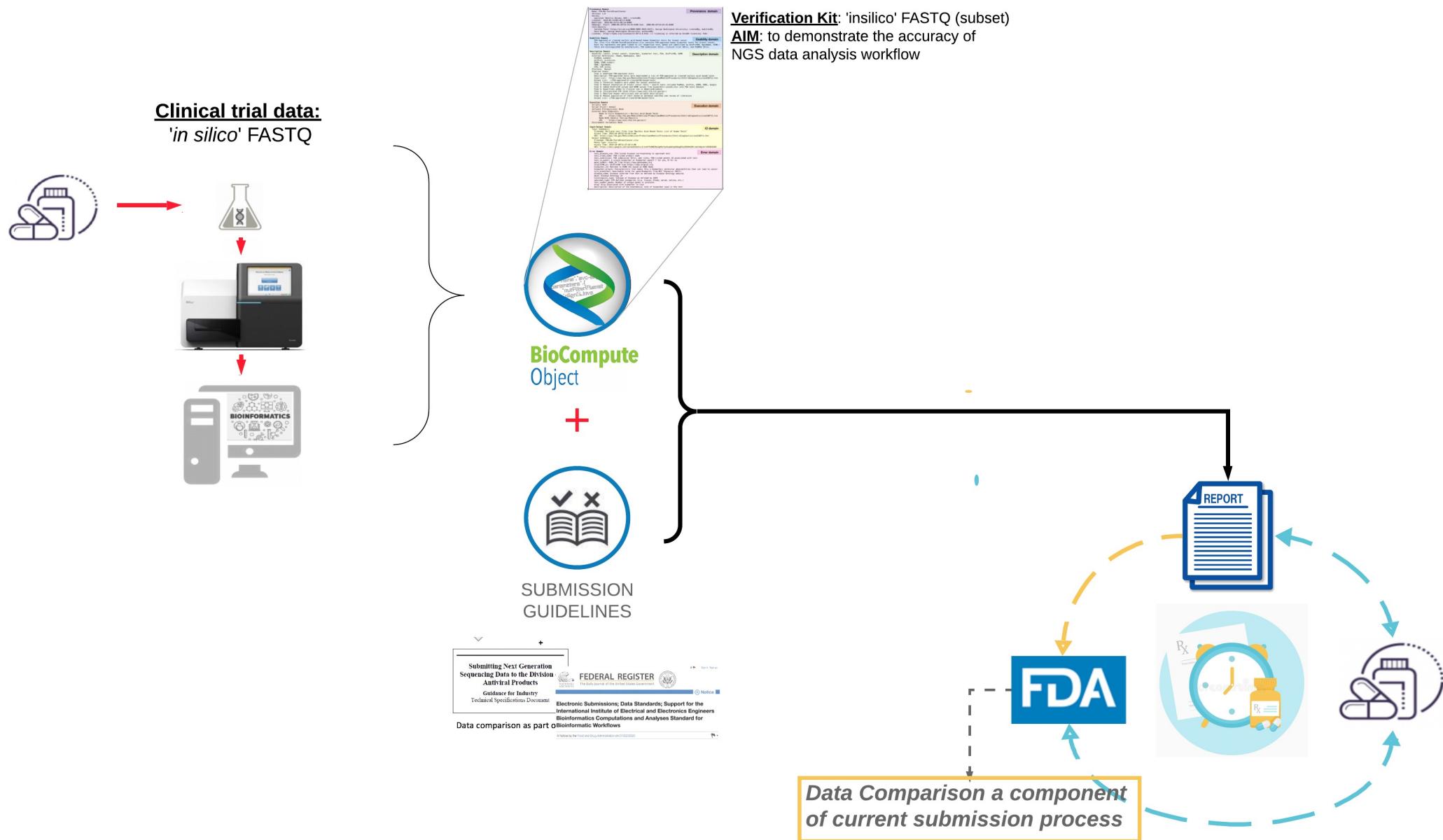
Introduction to BioCompute



BCO Value in Regulatory Submission



BCO Value in Regulatory Submission



A solution should...

In 2014, the Genomics Working Group convened a special session to discuss the problem, and came up with four key focus areas

1. Be **human readable**: like a GenBank sequence record
2. Be **machine readable**: structured information with predefined fields and associated meanings of values
3. Contain enough information to understand the computational pipelines, interpret information, maintain records, and reproduce experiments
4. Be **immutable**: ensure information has not been altered

Written in JSON

Categorized by domains

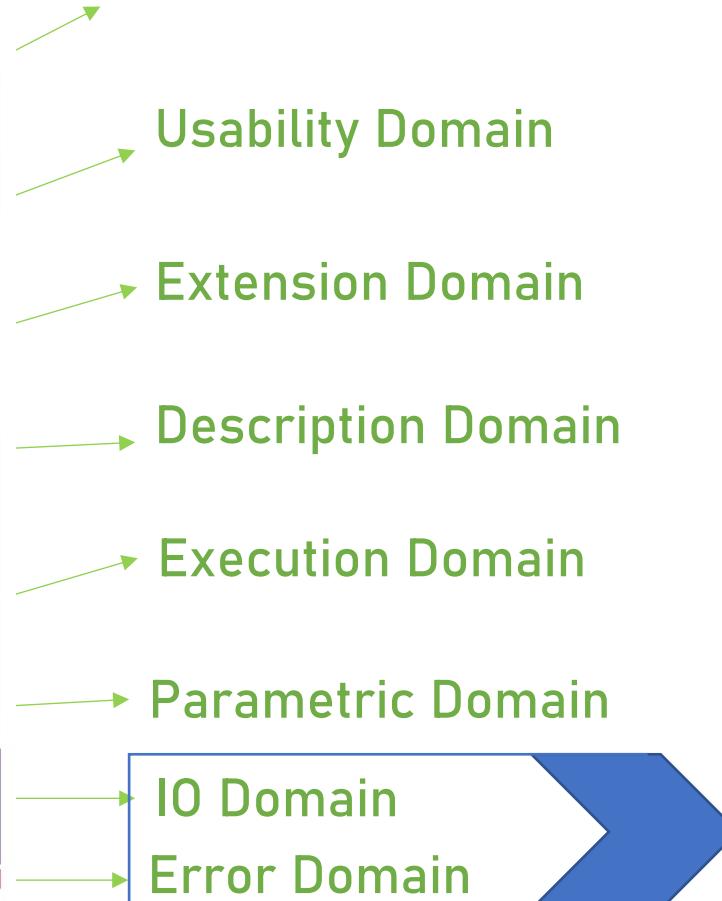
- Adaptable to other schemas

Adheres to and encourages F.A.I.R. principles

- Fully open source
- Preserves data provenance (unique IDs for versioning)

Top Level	BCO ID: https://w3id.org/biocompute/1.3.0/examples/FDA-NA-TestsBreastCancer
	Checksum: 86CACCE7067935B87A3D06FFEE04ED244AF58C2571204C37E5F1B3ADE4A31
	Specification: https://w3id.org/biocompute/1.3.0/
Provenance Domain	
Name:	FDA-NA-TestsBreastCancer
Version:	1.0
Review:	
approved:	Natalie Abrams, NIH : createdBy
Created:	2018-05-24T09:40:17-04:00
Modified:	2018-06-21T14:06:14-04:00
Last modified:	2000-09-26T14:43:04-04:00 End: 2000-09-26T14:43:45-04:00
Contributors:	
Janisha Patel (https://orcid.org/0000-0002-0824-4637), George Washington University; createdBy, modifiedBy	
Dara Baker, George Washington University; authoredBy	
License:	https://spdx.org/licenses/CC-BY-4.0.html --- licensing is inferred on OncoXylo licensing. Pub
Usability Domain	
FDA-approved or cleared nucleic acid-based human biomarker tests for breast cancer.	The .xlsx file FDA-NA-TestsBreastCancer.xlsx contains FDA-approved human biomarker tests for breast cancer. Each row represents one gene linked to its respective test. Genes are identified by UniProtKB, HGNCname, EDRN number. Tests are distinguished by manufacturer, FDA submission ID(s), clinical trial ID(s) and PubMed ID(s).
Extension Domain	
Dataset Extension:	Comment: Unique column headers for the dataset. Test_disease_use: FDA-listed disease corresponding to approved test test_trade_name: FDA-listed product name test_manufacturer: FDA-listed company for the approved test test_submission: FDA submission ID(s), web links: FDA-listed patent ID associated with test test_is_panel: A single biomarker or biomarker panel? Y for yes, N for no gene_symbol: HGNC ID from https://www.genenames.org uniprotKB_ac: UniProtKB accession: https://www.uniprot.org biomarker_id: linked to EDRN ID(s) linked to HGNC name biomarker_origin: Characteristic that makes this a biomarker; molecular abnormalities that can lead to cancer ncit_biomarker: Searchable terms for gene/Biomarker from NCI Thesaurus (NCIT)
Description Domain	
Keywords:	Cancer, breast cancer, biomarker, biomarker test, FDA, UniProtKB, EDRN
External References:	(Name, Namespace, IRI) PubMed; pubmed; UniProt accession; EDRN ID(s); biomarker; HGNC; HGNCname; GTR; GTR terms; Platform; Manual; PubMed; SRS;
Execution Domain	
Script: none	
Setup: never; manual	
Software Prerequisites: None	
External Data Endpoints:	
Name In Vitro Diagnostics - Nucleic Acid Based Tests	
URL: https://www.fda.gov/MedicalDevices/ProductsandMedicalProcedures/InVitroDiagnostics/ucm330711.htm	
Name NCDI Genetic Testing Registry	
URL: https://www.ncbi.nlm.nih.gov/gtr/	
Environment Variables: None	
Parametric Domain	N/A
Input/Output Domains	
Input Subdomain:	
Filename: Multiple test files from "Nucleic Acid Based Tests: List of Human Tests"	
Access Time: 2018-10-10T11:34:02-05:00	
URI: https://www.fda.gov/MedicalDevices/ProductsandMedicalProcedures/InVitroDiagnostics/ucm330711.htm	
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FDA-NA-TestsBreastCancer.xlsx	
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URI: https://docs.google.com/spreadsheets/d/1xI0Y7uJNE7HgCgH5SypxEuqAb:gVIIwgR2nC0tWh2BY/edit#gid=149206303	
Error Domain	

Provenance Domain



IEEE Standard



Institute of Electrical and Electronics
Engineers Standard

IEEE 2791-2020 approved January 2020

<https://standards.ieee.org/content/ieee-standards/en/standard/2791-2020.html>



FEDERAL REGISTER

The Daily Journal of the United States Government



N Notice

Electronic Submissions; Data Standards; Support for the International Institute of Electrical and Electronics Engineers Bioinformatics Computations and Analyses Standard for Bioinformatic Workflows

A Notice by the Food and Drug Administration on 07/22/2020

PUBLISHED DOCUMENT

AGENCY:
Food and Drug Administration, Health and Human Services (HHS).

ACTION:

DOCUMENT
Printed ve
PDF
Publicatio
07/22/20;
Agencies:

PUBLISHED DOCUMENT

AGENCY:

Food and Drug Administration, Health and Human Services (HHS).

ACTION:

Notice.

SUMMARY:

The Food and Drug Administration (FDA or Agency) is announcing support for use in regulatory submissions the current version of the International Institute of Electrical and Electronics Engineers (IEEE) bioinformatics computations and analyses standard for bioinformatic workflows (BioCompute) and an update to include this standard in the FDA Data Standards Catalog for the submission of high-throughput sequencing (HTS) data in new drug applications (NDAs), abbreviated new drug applications (ANDAs), biologics license applications (BLAs), and investigational new drug applications (INDs) to the Center for Biologics Evaluation and Research (CBER), Center for Drug Evaluation and Research (CDER), and Center for Food Safety and Applied Nutrition (CFSAN).

DATES:

Submit either electronic or written comments on the notice by August 21, 2020.

DOCUMENT DETAILS

Printed version:

[PDF](#)

Publication Date:

07/22/2020

Agencies:

[Food and Drug Administration](#)

Dates:

Submit either electronic or written comments on the notice by August 21, 2020.

Comments Close:

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Agency/Docket Number:

Docket No. FDA-2020-N-1450

Document Number:

2020-15771

DOCUMENT DETAILS

ACCESS NAME ORG ADDED BY ID

Private test-workflow dnanexus.science sam.westreich workflow-FQ7P7Vj05922F6k6J3b87yQ6

CREATED 2018-12-10 23:16:23

[Edit tags](#)

Revision: 1 Latest Edit Fork Export

Run Workflow rev1

SPEC WORKFLOW DIAGRAM

INPUTS

- file Input 1 REQUIRED workflow-app-1
- file Input 2 REQUIRED workflow-app-2

OUTPUTS

- file Output 1 REQUIRED workflow-app-1
- file Output 2 REQUIRED workflow-app-2



Galaxy Administration

Galaxy Analyze Data Workflow Shared Data Admin Help User Using 35.7

Administration

- Security
- Data
- Server
- Tool sheds
- Form Definitions
- Sample Tracking

Repository Actions Tool Shed Actions

Genome/Exome paired analysis (SNVMix1)

Boxes are red when tools are not available in this repository (this page displays SVG graphics)

Workflow diagram:

```

graph LR
    A[Input 1] --> B[Input 2]
    B --> C[Input 3]
    C --> D[Input 4]
    D --> E[Input 5]
    E --> F[Input 6]
    F --> G[Input 7]
    G --> H[Input 8]
    H --> I[Input 9]
    I --> J[Input 10]
    J --> K[Input 11]
    K --> L[Input 12]
    L --> M[Input 13]
    M --> N[Input 14]
    N --> O[Input 15]
    O --> P[Input 16]
    P --> Q[Input 17]
    Q --> R[Input 18]
    R --> S[Input 19]
    S --> T[Input 20]
    T --> U[Input 21]
    U --> V[Input 22]
    V --> W[Input 23]
    W --> X[Input 24]
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    Y --> Z[Input 26]
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    EE15 --> FF15[Input 422]
    FF15 --> GG15[Input 423]
    GG15 --> HH15[Input 424]
    HH15 --> II15[Input 425]
    II15 --> JJ15[Input 426]
    JJ15 --> KK15[Input 427]
    KK15 --> LL15[Input 428]
    LL15 --> MM15[Input 429]
    MM15 --> NN15[Input 430]
    NN15 --> OO15[Input 431]
    OO15 --> PP15[Input 432]
    PP15 --> QQ15[Input 433]
    QQ15 --> RR15[Input 434]
    RR15 --> SS15[Input 435]
    SS15 --> TT15[Input 436]
    TT15 --> UU15[Input 437]
    UU15 --> VV15[Input 438]
    VV15 --> WW15[Input 439]
    WW15 --> XX15[Input 440]
    XX15 --> YY15[Input 441]
    YY15 --> ZZ15[Input 442]
    ZZ15 --> AA16[Input 443]
    AA16 --> BB16[Input 444]
    BB16 --> CC16[Input 445]
    CC16 --> DD16[Input 446]
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    KK16 --> LL16[Input 454]
    LL16 --> MM16[Input 455]
    MM16 --> NN16[Input 456]
    NN16 --> OO16[Input 457]
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    PP16 --> QQ16[Input 459]
    QQ16 --> RR16[Input 460]
    RR16 --> SS16[Input 461]
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    VV16 --> WW16[Input 465]
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    YY16 --> ZZ16[Input 468]
    ZZ16 --> AA17[Input 469]
    AA17 --> BB17[Input 470]
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    HH17 --> II17[Input 477]
    II17 --> JJ17[Input 478]
    JJ17 --> KK17[Input 479]
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    LL17 --> MM17[Input 481]
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    OO17 --> PP17[Input 484]
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    RR17 --> SS17[Input 487]
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    TT17 --> UU17[Input 489]
    UU17 --> VV17[Input 490]
    VV17 --> WW17[Input 491]
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    DD18 --> EE18[Input 499]
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    VV19 --> WW19[Input 543]
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    BB20 --> CC20[Input 549]
    CC20 --> DD20[Input 550]
    DD20 --> EE20[Input 551]
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    FF20 --> GG20[Input 553]
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    JJ20 --> KK20[Input 557]
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    MM20 --> NN20[Input 560]
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    UU20 --> VV20[Input 568]
    VV20 --> WW20[Input 569]
    WW20 --> XX20[Input 570]
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    YY20 --> ZZ20[Input 572]
    ZZ20 --> AA21[Input 573]
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    BB21 --> CC21[Input 575]
    CC21 --> DD21[Input 576]
    DD21 --> EE21[Input 577]
    EE21 --> FF21[Input 578]
    FF21 --> GG21[Input 579]
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    II21 --> JJ21[Input 582]
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    LL21 --> MM21[Input 585]
    MM21 --> NN21[Input 586]
    NN21 --> OO21[Input 587]
    OO21 --> PP21[Input 588]
    PP21 --> QQ21[Input 589]
    QQ21 --> RR21[Input 590]
    RR21 --> SS21[Input 591]
    SS21 --> TT21[Input 592]
    TT21 --> UU21[Input 593]
    UU21 --> VV21[Input 594]
    VV21 --> WW21[Input 595]
    WW21 --> XX21[Input 596]
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    ZZ21 --> AA22[Input 599]
    AA22 --> BB22[Input 600]
    BB22 --> CC22[Input 601]
    CC22 --> DD22[Input 602]
    DD22 --> EE22[Input 603]
    EE22 --> FF22[Input 604]
    FF22 --> GG22[Input 605]
    GG22 --> HH22[Input 606]
    HH22 --> II22[Input 607]
    II22 --> JJ22[Input 608]
    JJ22 --> KK22[Input 609]
    KK22 --> LL22[Input 610]
    LL22 --> MM22[Input 611]
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    NN22 --> OO22[Input 613]
    OO22 --> PP22[Input 614]
    PP22 --> QQ22[Input 615]
    QQ22 --> RR22[Input 616]
    RR22 --> SS22[Input 617]
    SS22 --> TT22[Input 618]
    TT22 --> UU22[Input 619]
    UU22 --> VV22[Input 620]
    VV22 --> WW22[Input 621]
    WW22 --> XX22[Input 622]
    XX22 --> YY22[Input 623]
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    AA23 --> BB23[Input 626]
    BB23 --> CC23[Input 627]
    CC23 --> DD23[Input 628]
    DD23 --> EE2
```

BioCompute participants



EPINOMICS

Google



GENOME NEXT



CUROVERSE



EMBL-EBI



DNAexus



NIST



FLATIRON

Galaxy
PROJECT



MANCHESTER
1824
The University of Manchester



CU
NY

Agenda

- Introduction to BioCompute
- **BioCompute Portal Walkthrough**
- Demo of user account and DB access
- Description of DB and schema
- Transfer from Galaxy, HIVE, & local machine
- Q&A



BioCompute Portal Walkthrough



Demo

How to navigate the Portal?
How to create a BioCompute Object?
How do you edit a BioCompute Object?





Resources

Builder

BioCompute Objects

Log In/Register

BioCompute Documentation

External site

User Guide
Best Practices
SOP
Tutorials

IEEE 2791-2020

IEEE Standard for Bioinformatics Analyses Generated by High-Throughput Sequencing (HTS) to Facilitate Communication



BCO TSC

The Technical Steering Committee of the BioCompute Partnership (TSC) is a body of experienced professionals with BioCompute standard subject matter expertise. See here for the Meeting notes and agenda for all past and the upcomming meetings.

News and Events

FDA Notice on BioCompute

Electronic Submissions; Data Standards; Support for the International Institute of Electrical and Electronics Engineers Bioinformatics Computations and Analyses Standard for Bioinformatic Workflows.

Tweets by @BioComputeObj

BioCompute Retweeted



GW SMHS
@GWSMHS

A consortium led by @GW_HIVE_Lab, @rmazumde, and @Embleema, with @TempleUniv, has received @FDA funding to advance the work against #infectiousdiseases. Read more: bit.ly/3FaDCvY via @TheVDT

Cloud-based tools for BioCompute

See our resources page for additional tools and services.



Access AWS HIVE, the High-Performance Integrated Virtual Environment, on AWS. HIVE is a cloud-based environment optimized for the storage and analysis of extra-large data, such as biomedical data, clinical data, next-generation sequencing (NGS) data, mass spectrometry files, confocal microscopy images, post-market

BioCompute Builder



Use the BioCompute Builder or view objects in the database. The BioCompute Builder is a platform-free, form-based editor. The builder walks a user through building a BCO through text boxes, indicating which entries are required to adhere to the IEEE standard.



Use Galaxy on AWS, the open source, web-based platform for data intensive biomedical research.

Assemble your [pipeline](/about) in the workspace, designate the outputs in the module boxes, and record the entire pipeline as a BCO.



Embleema and George Washington University-led Co...

METUCHEN, N.J.--(BUSINESS WIRE)--Oct 28, 2021--

validdatedailytins.com



Nov 15, 2021

BioCompute Retweeted

Demo



User account and DB access





Demo

Register a new account
Build an Object
Create a draft
Edit a draft
Save edits
Validate Object
Publish



Description of DB and Schema



BioCompute Schema Files

IEEE.org | IEEE Xplore Digital Library | IEEE Standards | IEEE Spectrum | More Sites

IEEE SA OPEN

☰ Menu

2791 object > ieee-2791-schema

ieee-2791-schema

Project ID: 116

24 Commits 2 Branches 3 Tags 276 KB Files 276 KB Storage 1 Release

master

ieee-2791-schema

History

Find file

Clone



Update README.md

Joshua Gay authored 1 year ago

45683af9



README

Other

Auto DevOps enabled

Name	Last commit	Last update
.gitignore	Creates initial release of BioCompute Obj...	2 years ago
2791object.json	replaces https://w3id.org/2791/ with https:...	1 year ago
AUTHORS	Update AUTHORS	1 year ago
CONTRIBUTORS	Update CONTRIBUTORS	1 year ago
LICENSE	Update LICENSE	1 year ago
README.md	Update README.md	1 year ago
description_domain.json	replaces https://w3id.org/2791/ with https:...	1 year ago
error_domain.json	replaces https://w3id.org/2791/ with https:...	1 year ago

<https://opensource.ieee.org/2791-object/ieee-2791-schema/>

Demo

Repositories



Transfer from external sources using Swagger site for API access



BioCompute Object Data Base API (BCODB API) 1.3.0

[Base URL: biocomputeobject.org/]
<https://biocomputeobject.org/api/docs/?format=openapi>

A web application that can be used to create, store and edit BioCompute objects based on BioCompute schema described in the BCO specification document.

[Terms of service](#)

[Contact the developer](#)

[MIT License](#)

Schemes

HTTPS ▾

Django Login

Authorize

Filter by tag

Account Management

GET /api/accounts/activate/{username}/{temp_identifier} Activate an account

api_accounts_activate_read

POST /api/accounts/describe/ Account details

api_accounts_describe_create

POST /api/accounts/new/ Account creation request

api_accounts_new_create

Swagger site for API access

Group Management

POST /api/groups/create/ Create group

api_groups_create_create

Demo



Transfer from Galaxy



Thank you!

Your time and feedback are greatly appreciated.



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John Didion



Vahan Simonyan
Jeremy Goecks
Gil Alterovitz
Carole Goble
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Michael Crusoe
Stian Soiland-Reyes
Konstantinos Krampus
Elaine Thompson
Nicola Soranzo
Jason Travis
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Acknowledgements and Contact

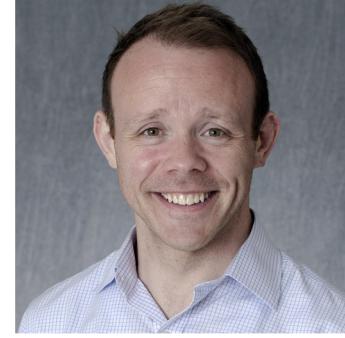


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Recording on workshop: <youtube link>

- Introduction: Use cases and BioCompute
- BioCompute Portal Walkthrough
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Q&A

