BIOINFORMATICS RESOURCE CENTERS

A knowledgebase of Integrated Data, Metadata, & Analysis Tools to Support Data-enabled Infectious Disease Research

Ishwar Chandramouliswaran Office of Data Science & Emerging Technologies NIAID, NIH, DHHS



KEY CAPABILITIES



THE CENTERS ORGANIZED BY PATHOGEN GROUPS

| Institute name | PI name | BRC | Pathogen |
|-------------------------------|------------------------|------------------|---|
| University of Notre Dame | Mary Ann McDowell | VectorBase | Invertebrate vectors of human pathogens |
| University of Pennsylvania | David Roos | EuPathDB/FungiDB | Eukaryotic/fungal pathogens |
| Northrop Grumman | Richard Scheuermann | Vipr/IRD | Viruses/Influenza |
| University of Chicago | Rick Stevens | PATRIC | Bacteria |
| Round FY04 | Rour FY | | |

COLLABORATE TO INTEGRATE DATA ACROSS NIAID PROGRAMS





VECTORBASE BRC FOR INVERTEBRATE VECTORS OF HUMAN PATHOGENS

- An unique and integrated bioinformatics resource for vector community
 - Genome of 35 organisms with annotated gene features, genome variation, transcript and protein expression
 - Population genetics data integrated with variation and insecticide-resistance phenotypes, field-associated samples from surveillance studies, and pathogen transmission data
 - Transcriptomes (RNA-seq) and gene expression data
 - Pathways
- Data access, analysis and visualization tools
 - Data-centric search system
 - Computational tools made accessible through a Galaxy instance implemented in VB
 - Expression map
 - Ontology browser

Welcome to VectorBase!

VectorBase is a NIAID Bioinformatics Resource Center providing genomic, phenotypic and population-centric data to the scientific community for invertebrate vectors of human pathogens.



TOOLS & RESOURCES

Pause

Improved RNAseq tracking and analysis

Improved RNAseq tracking and analysis



A beta release of the VectorBase RNAseq tracking and analysis system is now available for use. RNAseq experiments are being aligned to the reference genome in a standardised fashion across all VectorBase species, and the results are exposed in the Web Apollo gene annotation and the genome browser systems. You can now query for RNAseq experiments of interest via the VectorBase site search, or via the track hub system within the genome browser for each species. A **tutorial** explaining how to use the new system is available, and we look forward to receiving suggestions for how to further improve the new system.

SUBMIT YOUR DATA TO VECTORBASE VectorBase is not just for accessing data and using tools - we

Tweets by @VectorBase



EUPATHDB BRC FOR INVERTEBRATE VECTORS OF HUMAN PATHOGENS

An unique resource for protozoan & fungal pathogens



- A comprehensive collection genomic and functional genomic data, isolate data and phylogenomics
 - genome sequences and annotation, strand-specific RNA-seq data, splice junction predictions, phosphoproteomic data, high-throughput phenotyping data, single nucleotide polymorphism, and expression quantitative trait loci data.
- Sophisticated search strategies using metadata
- Computational analysis on Galaxy

EuPathDB provides a unified entry point for the Eukaryotic Pathogen Bioinformatics Resource Center where you can ask questions that leverage data across organisms using orthlogy: http://EuPathDB.org

OrthoMCL allows you to identify phylogenetically conserved or unique proteins among genomes from all branches of life:

http://OrthoMCL.org Organism specific websites allow you search diverse data types from multiple species:

AmoebaDB Amoebozoa specific resource including Entamoeba - Acanthamoeba coming soon:

http://AmoebaDB.org CryptoDB Cryptosporidium specific resource: http://CryptoDB.org GlardiaDB Giardia specific resource includes assemblages A, B and E: http://GiardiaDB.org MicrosporidiaDB Includes multiple microsporidia species: http://MicrosporidiaDB.org

PiroplasmaDB Babesia and Theileria specific resource:

http://PiroplasmaDB.org PlasmoDB Resource for Plasmodium species. http://PlasmoDB.org

ToxoDB Toxoplasma, Neospora and Eimeria resource:

http://ToxoDB.org TrichDB Resource for Trichomonas vaginalis:

http://TrichDB.org TriTrypDB Resource for kinetoplastida including Trypanosoma spp. and Leishmania spp.

http://TriTrypDB.org



VIRUS PATHOGEN RESOURCE (VIPR) INFLUENZA RESEARCH DATABASE (FLUDB)

- A comprehensive collection of influenza and multiple virus family related data.
 - sequences and annotations, immune epitopes, 3D protein structures, HTP omics data, clinical phenotype, surveillance, serology, host factor data, and curated antiviral drug data.
- A suite of analytical and visualization tools
 - phylogenetic tree, sequence variation determination, metadata-driven Comparative Analysis Tool for Sequences (meta-CATS), short peptide identification, PCR primer design, Sequence Feature and Phenotypic Variant Type (PVT) annotation, HA clade classification, HA subtype numbering conversion, surveillance data visualization, protein structure visualization, and host factor data enrichment analysis
- Personal workbench spaces for data storage, sharing and analysis
- An infrastructure for antiviral drug data management and analysis.
 - Drug interaction site curation
 - Integration of host factor data with drug target
 - Anti-viral drug resistance risk assessment tool



Surveillance



Tutorial

Human, avian and non-human mammalian surveillance data can be searched based upon location and various host characteristics for download and display on a map with bird flyway overlay. Create a report showing counts of surveillance records grouped by user-driven criteria.

Key Highlights:

- Human, avian and non-human mammalian surveillance data
- User-driven serotype comparison
- Display data on Google Map with flu prevalence color coded and bird flyways overlayed
- color co
 - · View results by metadata matrix report



PATHOGEN RESOURCE INTEGRATION CENTER (PATRIC) BRC FOR BACTERIAL SPECIES

Integrated Data Collections

Genomes, Transcriptomes (uArray and RNAseq), Proteomics, Metabolomics, Curated gene collections, Protein-Protein Interactions, Tn-Seq

AMR panel data, Disease & isolation phenotype metadata,, Virulence, Drug Targets, Biochemical Pathways

Computational Analysis Services



| DATA WORKSPA | CES SERVICES HEL | P. |
|---|--|----|
| Antibiotic Resistance Genomes Genomic Features Pathways Protein Families Specialty Genes Transcriptomics Download Data FTP Server | Specialty Data Collections PATRIC Collaborations PATRIC DBPs NIAID Clinical Proteomics NIAID Genome Sequencing NIAID Structural Genomics NIAID Systems Biology NIAID Functional Genomics | 1 |

Personal Workspace for analysis of User data and "Virtual Integration" of user data in the context of all the public datasets



View all AMR on

RESPOND TO NEEDS OF ID RESEARCHERS







- Clinical & Epidemiological Data
- PopBio Data & Tools





- AMR data collection
- AMR prediction tools

HANDS-ON TRAINING WORKSHOPS GLOBALLY



TO INCREASE USAGE & IMPACT



SCIENCE ENABLED BY THE BIOINFORMATICS RESOURCE CENTERS



EVOLUTION OF THE RESOURCES



THE NIAID DATA CHALLENGE



Image Courtesy: Dr. Emily Erbelding (modified)

NEW MODELS OF DATA-DRIVEN HYPOTHESIS GENERATION

Expanding the Immunology Toolbox: Embracing Public-Data Reuse and Crowdsourcing

Rachel Sparks,¹ William W. Lau,² and John S. Tsang^{1,*}

¹Systems Genomics and Bioinformatics Unit, Laboratory of Systems Biology, National Institutes of Allergy and Infectious Diseases, National Institutes of Health

²Office of Intramural Research, Center for Information Technology, National Institutes of Health

*Correspondence: john.tsang@nih.gov

http://dx.doi.org/10.1016/j.immuni.2016.12.008

New technologies have been propelling dramatic increases in the volume and diversity of large-scale public data, which can potentially be reused to answer questions beyond those originally envisioned. However, this often requires computational and statistical skills beyond the reach of most bench scientists. The development of educational and accessible computational tools is thus critical, as are crowdsourcing efforts that utilize the community's expertise to curate public data for hypothesis generation and testing. Here we review the history of public-data reuse and argue for greater incorporation of computational and statistical sciences into the biomedical education curriculum and the development of biologist-friendly crowdsourcing tools. Finally, we provide a resource list for the reuse of public data and highlight an illustrative crowdsourcing mouse models. Through education, tool development, and community engagement, immunologists will be poised to transform public data into biological insights.



FAIR GUIDELINES

Findable Accessible Interoperable Reusable



Comment OPEN Published: 15 March 2016

The FAIR Guiding Principles for scientific data management and stewardship

Mark D. Wilkinson, Michel Dumontier [...] Barend Mons 🖾

Scientific Data 3, Article number: 160018 (2016) Download Citation 🛓

REVISIT DATA MANAGEMENT & SHARING PLANS

Resource Sharing Plan

compliance with current NH requirements, we herewith outline a plan to share materials and r management of infeliectual property. We will adhere to the NH Grant Policy on Sharing of lique Research Resources including the Sharing of Biomedical Research Resources pilott onth genybolicytic guide. Instalhent: We w melic and phenotypic data upon request. Material protective terms than in the Simple Latter A; agements: Material such as microbial stratms pository or other public repositories. The BEI supermetry work be followed in such cases. S; pailes for the search community in accords

Principles and Guidelines document. The following Table outlines the data types and to v along with timelines for deposition.

| Data and/or Reagent Type | Public Repository for Raw and Finished Data | |
|---|--|--|
| RNA sequencing (transcriptomics) | GEO / NCBI | |
| ONA Sequencing (clinical isolates) | NCBI SRA | |
| Genome Assemblies and associated metadata | NCBI Assembly and/or NIAID BRC or other repositories (e.g., PATRIC) | |
| Model Organisms / Strains | Stock center / BEI Resources Repository / or other approved repository | |
| Other data types (e.g., metabolomics) | NIAID BRCs or other repositories (e.g., PATRIC) | |

Data and Resource Sharing Plan U01 A1134255: PL YOURO, VMCENT (Contact) In the original proposal the Notwing table was included to is from the proposed wirk. This table is included how for refer

124 61

| - 1 | 6 m | Desir Aydan | Sola Type | |
|--|--|--|---|---|
| 18. | Moderna | of COL acquisition | CM | |
| 14. | i weiss of | angulation | CM. HEL.MET | |
| 14. | S Model for | of severe disease | CM | |
| 14. | want . | Invers disease | CH. HE MET. | |
| - | Ci anvea | Inene branch | CM. 188 | |
| - | Denatic a | contailians with CDI | CM, 182, W00 | |
| 18. | 1 Mendeer | InfCD Incuration | 165 | |
| 26. | | colorisation/#CU | CM | |
| 14 | 1CU total | matter angulation | CM | |
| | Mendant | ne long laim colorization | CM. BYGS. 185 | |
| | | te coloribellari etadollari | | |
| n ider De bro die typ speens die en station | Hy cases of CDI to statute in the hospita as: CM—climical m 8 alpha lypes: SL—m 8, network analysis | calecter of de cambled, sol and an peakles laboratory rec rate searchister. Hadate, 105-email recommi- pervised berring, USL-unit Types and recources the | ufs. "NA CDI casas d suburt game are geneted learning | |
| | Nucleic acid se | | at was the general | |
| | a. 155-end b. C. stiffici c. Metaper d. Metaplat | oding gene amplicon lib le genome sequence da nomic sequence dataset hisotiptomic sequence da | ta ('WGS') | |
| 23 | Metabolomics of a. Targete | d analysis | | 1 |
| | b. Urearge Clinical metada Fecal speciment a. Frozen 1 b. Fecal sp | la 15 Veces | | |

Data accessibility/therming The omics data in this proposal can be split into 4 categories. These data are all collected with IiLumina sequencing technology, which are shared with the targer scientific community through appropriate databases including the NCIB Sequence Read Archive for raw sequencing data, or the NCIB Gene Expression Commisso

FAIR principles and metrics for evaluation



Michel Dumontier, Ph.D.

Distinguished Professor of Data Science



| Staphylococcus aureus Strains (e.g. new mutants or revetants) | Years 3-6 | BEI Resources (NH) or true Pr per MTA | walidated replaces / reventents, are republy make available per faint polytom |
|--|---|--|---|
| One or more deposition also will be startifie Deposition will scour as publicly as a approx | | | |
| B. Resource or Data Use Polici | es & Practices | | |
| Per CMID general policies, u contribution of the data generators/pr unpublished data. Such guidelines ca A System of Tripartia Responsibility | roducers by followi in be found in Sha | ng normal standards of scie | entific eliquette and fair use of Biological Research Projects: |

Het Sharing Plan: RCM, University of Houston, Taxas AMA and UCLA are convertiled to public monthem of its souther results and evolvinging heads to provide that provide plant and entry to the most nevert NH publics on data baking and open ancients to research on select agents, series mundited by subsequently enclode laws, mpainters instand to research on select agents, res will comply using publics and the subsect of the most never the subsect agents, res will comply using publics for the subsect of the subsect on the subsect of the subsect

> publicly investor as soon as produce in 0. Deey will be quickly protected to facilitate 1 and in peer-reviewed scientific journals, webicitive seres than in a Dimple Letter intelectual property arise which requires a he research community in accordance with

sai has been performed with utilization of

ce of the investigators on this project anti-on-multiple censis. Data and specimen means having an experimented in Maharing at Baytar Callege of Maddices in the HMM Baytar Callege of Maddices in the HMM at an experiment of the Management at an experiment of the Management Industry and the commented on the appropriate frashing will be contexted on the appropriate frashing and will be transformed to the local

data and that is most compatible with any II at Housine). We will have a dedicated names of sur local data repository. This will try, wrated at BCM and legt in secure sitts component that sugged individual data shows that can be able to be shown at the support beam of the shows able to be able to be able to be shown at the beam of the source is the shows at the beam of the source is the shows at the beam of the source is the source is the shows at the beam of the source is the source is the shows at the beam of the source is the source is the shows at the beam of the source is the source is the shows at the source is the source is the source is the source is the shows at the source is the

 this proposal are committed to ion. Specifically, we propose to essench community by depositing following the NAMD Data Sharing re generated from focal samples fs, we will exercise the stricted a to the research community. As

> ers and oral presentations). all times, including dissemination dentified data formats. its (e.g. Data Use Agreements)

rchers interested in the project(s). licely available via <u>BEI Resources</u> ally (non-disclosure) Acreements.

community. any data in the case of vulnerable

r legal consequences. Associated t guidance from Program staff.

ad Archive (SRA) of NCBI

a per semplei sell be submitte

@ micheldumontier::#DANSLOD:2017-05-01 program and a statement of the stat

Whole metagenemic sequencing data (100 uangles / year) with be extended to time interval of every 6 member, people approximately 60 samples into ercularisation - baby. Whole metagenerrise sequencing data will be submitted rapidly as possible, and no later than 45 calendar days of being generated, as p the NAAD Division of Microbiology and Infectious Diseases (DMD) Data Bharina as

CO-LOCATE DATA & TOOLS ON CLOUD

Traditional Way: Bring data to the researchers



Problems Data sharing = data copying Limits Access Largely fixed compute Individual security implementations

<u>Cloud Way:</u> Bring researchers to the data



Solutions True data sharing Democratizes access Elastic compute and storage Centralized security implementation

MINT DIGITAL OBJECT IDENTIFIERS



DATA INDEXING



Google Dataset Search Beta

Search for Datasets

Q

Try boston education data or weather site:noaa.gov

Not an endorsement but an example

USE OF JUPYTER NOTEBOOKS



Not an endorsement but an example

CONTAINERIZATIONS OF TOOLS

NIH Data Science Learning and Testing Hackathon

February 23, 2018!

The NIH will host a Learning and Testing Data Science hackathon on February 23rd, 2018 on the main campus in Bethesda, MD. Learners will test alpha and beta code that have been generated in full, collaborative development hackathons for a wide range of scientific problems, including general bioinformatics and genomic analyses in addition to text, image, and sequence processing. This event is for researchers who are in the early stages of their data science journey, including students and postdocs. Other non-scientific developers, mathematicians, or librarians in a similar educational place are also welcome! Learning in this event will be primarily hands-on and self-driven, but will also include short workshops on topics such as Docker and GitHub. Mentors will also be available to assist with questions.





present in a metagenomic sample, which will allow for both smarter drug selection by clinicians and faster research in an academic environment.

USE OF APPLICATION PROGRAMMING INTERFACES



Not an endorsement but an example

USE OF SMART-IRB, AUTHN, AUTHZ SOLUTIONS



Supporting single IRB review Advancing collaborative research



DUOS



Not an endorsement but an example

REALIZE DATA SHARING

- Aligns with multiple federal and NIH Missions:
 - 2011: Precision Medicine Report
 - > 2012: Data and Informatics Working Group (DIWG) of the Advisory Committee to the NIH Director
 - > 2013: OSTP White House Memo Increasing Access to Federally Funded Scientific Research Results
 - > 2013: NIH Big Data to Knowledge (BD2K) Initiative
 - > 2014: National Strategy for Combating Antibiotic-Resistant Bacteria (CARB)
 - > 2018: NIH Strategic Plan for Data Science



| Γ | ۲ | |
|---|---|--|
| | National Institutes of Health | |
| | | |
| | Data and Informatics Working Group Draft Report to The Advisory Committee to the Director | |
| | | |
| | June 15, 2012 | |

| | EXECUTIVE OFFICE OF THE PRESERVED OPPED OF EXECUTIVE AND TELEWORKSHICK PRESERVED. |
|---|--|
| | Polyany 22, 2011 |
| MINRO | NOUT FOR THE BEADS OF EXECUTIVE DEPARTMENTS AND AGENCIES |
| TRONG | http://itenatur |
| NRICT | becoming to one to the Results of Federally Funded Scientific Research |
| L 14 | to Principles |
| hadrenty for | consistent is commuted for encourage that, in the prospect court and with the linearial providing and consistent and the and the adjustment set and before. The dense results related assessible are seenich are studied as adjusted to and another for the patient, industry, and a community, "back togethe industry part encourand publications and digital data. |
| drive out to | essarch suggested by the Eulerial Concentrate cardy are seen struct brackdoning to the sensity. The tracks of that tensorial become the grint for new singlets and are seen in more such as buildly, energy, the on-moreneous, agriculture, and takened ascerty. |
| data andre aparente da patriciales arrices el patriciales de reput | light dass en schlang, ben bischel, hogde naven if divers singeneis to ben direkter en stehendensette gehabet, auf ochsig geneten sogenens pallet, soldtet so sol her konstrukter gehabet, auf ochsig geneten sogenens pallet, soldtet her sol and stehendensette gehabet, auf och geneten solgenen solgen and all and and and and and beneten sol and and and and and and and a stehet be construction, auf och and and and and and all and and the sol and and and and and and and and and all and a stehet be and and and and and and and and and all and |
| adulate p atariate p | constraints disc complexes that publicless provide valuable are easy, architecting the $r \sim p_{\rm prot}$ reviews, that are transmits the interval (statistical physical straight) of the discussors. It is used that there we constraints the number valuable to its are set of builded patters are advected with the discussion of the number of builded to be the Tablet of Constraints its discussion are approximately as the number of builders to the Tablet of Constraint its discussion are provide as reads of their number of the number of the tablet of the number of the number of the number of the number of the number of the tablet of the number of the number of the number of the number of the number of the number of the number of the number of the number of the number of the number of the number of the |
| To ashare | He Administration's committeent in increase access in faderally. Social published d digital scientific data, Paleral supresso resting of resounds and development rea and conditional policies the restinancy last access. |







EXPAND USER BASE - INTERACTIONS OF USERS & CONTRIBUTORS





Computational Research Scientist Python, R, SQL



Algorithm Developer ssh, programmatic access

Image Courtesy: Dr. Sheila Reynolds, ISB

ANTICIPATED OUTCOMES – DEMOCRATIZE RESOURCES

Discover & access relevant generated data, tools, & standards

Identify/provide home for research data that needs a home

Enable new paradigm/model of data-driven hypothesis-driven science

Continuous assessment and optimization of data science research resources

Reduce informatics costs in the long run

FUNDING OPPORTUNITY ANNOUNCEMENTS (FOA)

Secondary Analysis of Existing Datasets for Advancing Infectious Disease Research (R21 Clinical Trial Not Allowed)

R21 Exploratory/Developmental Research Grant

New

None

PA-19-068

Informatics Methodology and Secondary Analyses To Explore Shared Immunology Study Data in ImmPort

Program Announcement With Special Receipt, Referral, and or Review Considerations-proposed FY 2020 initiative



Ishwar Chandramouliswaran Office of Data Science & Emerging Technologies NIAID, NIH, DHHS



@ishwartweets https://www.linkedin.com/in/ishwarc/

