Library Resources for Teaching and Research in the Health Sciences

Renae Barger, Associate Vice Chancellor, HSLS

Ansuman Chattopadhyay, Program Director for Molecular Biology Information Service







University Libraries





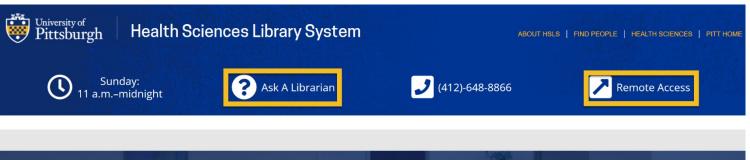


Falk Library – Level M, Alan Magee Scaife Hall (School of Medicine West Wing)





Virtual Front Door: www.hsls.pitt.edu











HSLS Liaison Librarians























Resources for Teaching





Customized Instruction for Your Class or Department https://www.hsls.pitt.edu/instruction/class-catalog

Topics:

- Evidence-based searching
- Research data management
- Data visualization
- Research Impact
- Instructional and visual design
- Next generation sequencing

Class Examples:

- Health Equity Research
- Preparing for the NIH Data Management and Sharing Plan
- Visualizing Research Impact
- Scientific Drawing with Illustrator
- Data Analysis using CLC Genomics Workbench
- Citizen Health Science: A Tool for Teaching
- Identifying & Combatting Health Misinformation
- Wikipedia for Health Sciences Students



Citation Management at HSLS

A citation manager can help you store, organize, and cite references.

HSLS offers support for citation management in a variety of ways:

- Classes
- Written guides
- Interactive tutorials
- Our citation management librarians are also happy to answer your questions or teach a customized class for your class, lab, or other group

HSLS provides support for three citation managers:



EndNote

- Web and desktop versions
- Free to Pitt students and faculty;
 \$50 for staff



Sciwheel

- Web-based
- Free for all Pitt affiliates



Zotero

- Web, desktop, and iOS versions
- Free and open source

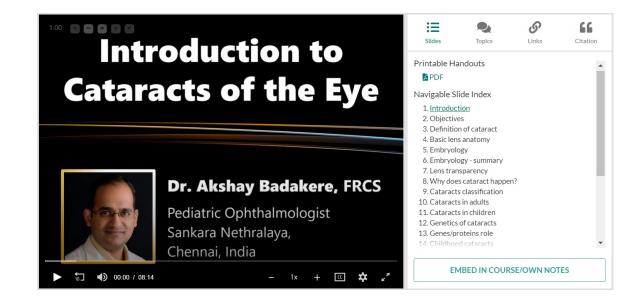




Multimedia Content

https://www.hsls.pitt.edu/streaming-media

- Visual guides
- Video protocols
- Documentaries
- Recorded Lectures
- Procedures



Sample video from HSTalks with slides and index. Content from HSTalks can be embedded directly into a course LMS.

HSLS VR LEARNSPACE

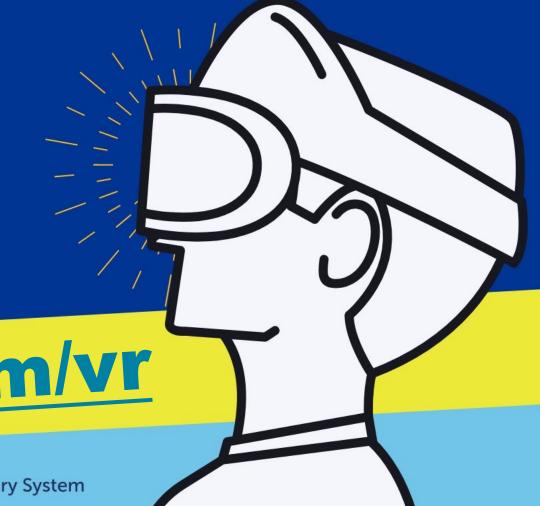
AVAILABLE APPS INCLUDE:

ANATOMY & PHYSIOLOGY ATLASES

CLINICAL SIMULATIONS

3D MEDICAL IMAGING

AND MORE!







ENHANCE YOUR TEACHING WITH HSLS VR LEARNSPACE'S

ANATOMYX

5,000 DETAILED ANATOMICAL MODELS

INCLUDES
ANATOMY
FUNCTIONS,
ETYMOLOGY,
AND MORE

CUSTOMIZABLE LEARNING EXPERIENCES



Resources for Research



Data Services



 Write a data management or sharing plan



Comply with data sharing policies



 Organize & describe your research data and code



Identify appropriate data repositories



 Create effective data visualizations



 Locate existing datasets for reuse



 Preserve your data and code for long-term access



Measuring Research Impact

- Discovering the impact of your work
- Tools for publication reporting
- Identifying impactful journals in your field
- Increasing your research visibility
- Using research metrics responsibly



Image from The University of Sheffield Library



Scholarly Publishing and Communication



Selecting and evaluating journals



Promoting your research



Open access publishing



 Author rights: copyright, fair use, licensing



Interpreting funder and journal policies



Communicating your research impact

Institutional Animal Care and Use Committee (IACUC) Support

Literature searches for the "3R's" are required for some IACUC protocols



• **Reduction**—Minimize the number of animals used, without jeopardizing statistical validity



• Refinement—Employ techniques that reduce pain & distress



• **Replacement**—Substitute animals with non-animal methods (i.e., computer simulation) or lower animal species



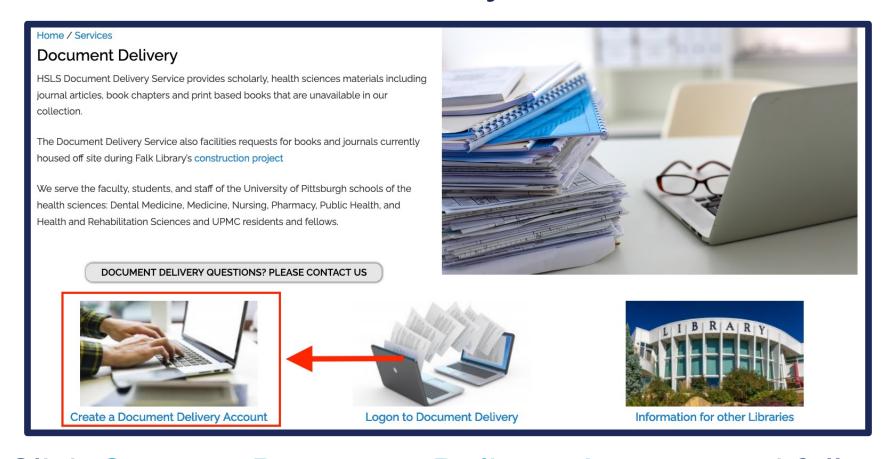


HSLS Systematic Review Program

- Who's eligible?
 - Faculty with primary appointments in schools of the health sciences
 - Residents/fellows affiliated with UPMC Office of GME
- What is required?
 - Submission of a detailed protocol
 - Protocol undergoes scientific review by HSLS librarians
- Be aware a protocol may be declined due to:
 - Concerns about project feasibility or timeline
 - Limited librarian availability



Create a Document Delivery Account



Click <u>Create a Document Delivery Account</u> and follow directions on that page.

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PowerPoint Slides: t.ly/PPNo1







Software Licensing



Bioinformatics Training Workshops



Web Tools



Consultations



Sri Chaparala, MS Bioinformatics Specialist srichaparala@pitt.edu



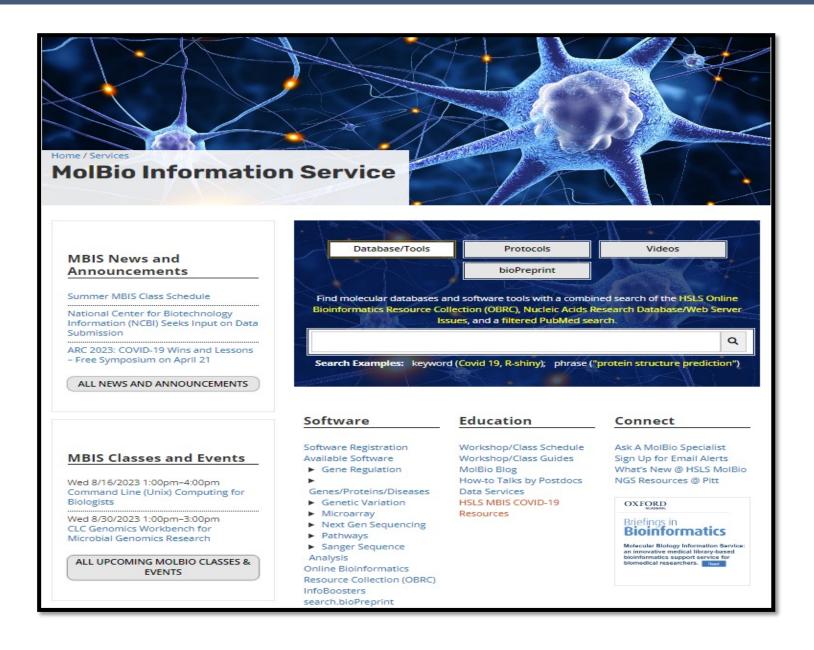
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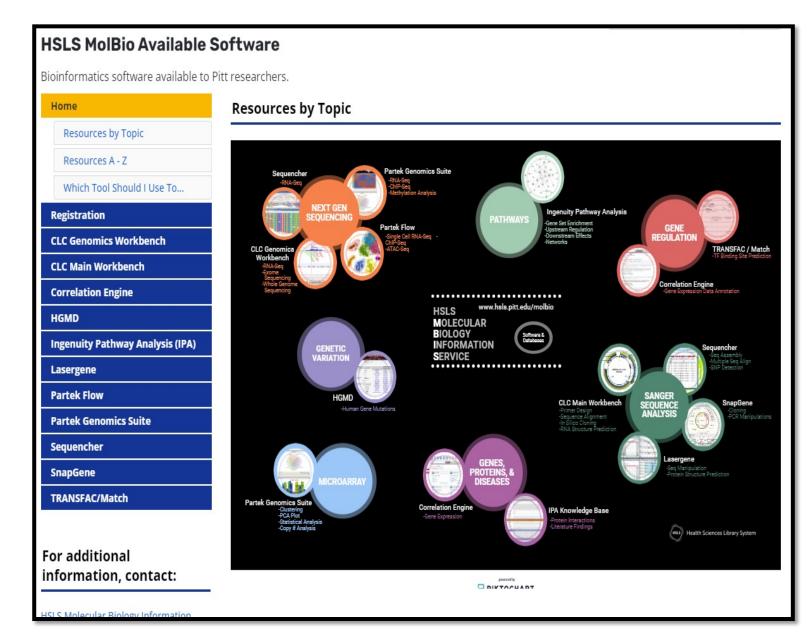








Licensed Software





BioinformaticsWorkshops

scRNA-Seq Data Analysis using PartekFlow

Wed 5/31/2023, 1:00pm to 3:00pm

IPA and Correlation Engine - A Comprehensive Approach to Pathway Enrichment Analysis

Wed 6/7/2023, 1:00pm to 3:00pm

Data Wrangling in R

Tue 6/13/2023, 12:00pm to 1:00pm

All of Us Researcher Workbench - Terminology and Data Models Training

Tue 6/13/2023, 1:00pm to 3:00pm

Data Visualization in R using ggplot2

Tue 7/11/2023, 12:00pm to 1:00pm

All of Us Researcher Workbench - EHR and Survey Data Analysis

Tue 7/11/2023, 1:00pm to 2:00pm

Single cell Multiomics Analysis with Partek Flow

Wed 7/12/2023, 1:00pm to 3:00pm

Transcriptome Analysis - From GEO Data Mining to Submission

Wed 7/26/2023, 1:00pm to 3:00pm

Command Line (Unix) Computing for Biologists

Wed 8/16/2023, 1:00pm to 4:00pm

CLC Genomics Workbench for Microbial Genomics Research

Wed 8/30/2023, 1:00pm to 3:00pm



Wed 5/31/2023, 1:00pm to 3:00pm

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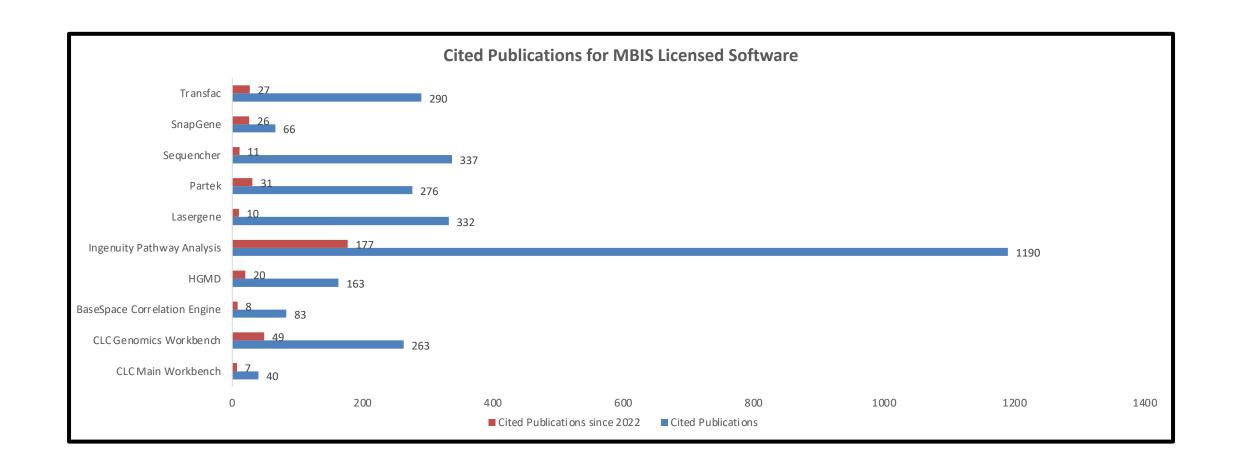
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Bioinformatics Workshops Guide Pages

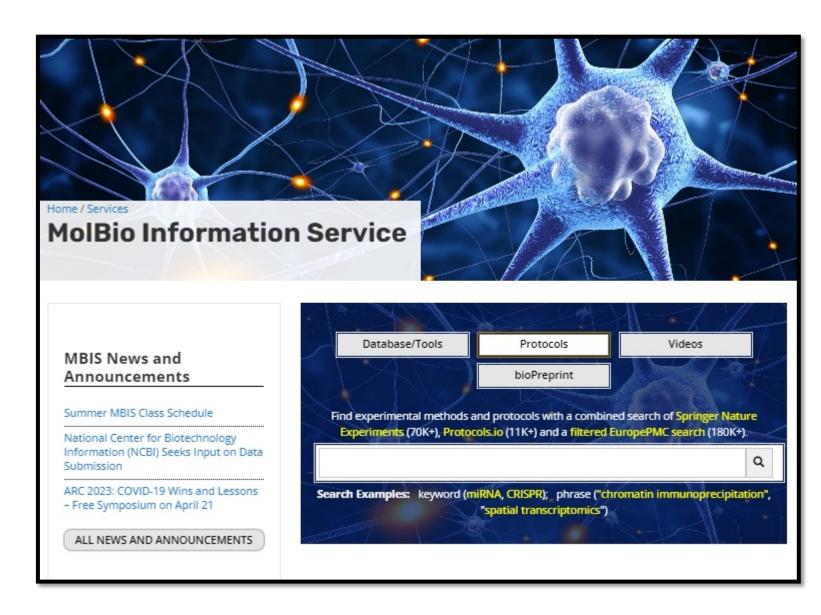
Since 2022, University of Pittsburgh researchers have referenced HSLS-licensed commercial software in

313 papers, as tracked by Google Scholar.





Life Sciences Search Engine







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Searc	n.Bi	orre	prini

Refine your preprints search via Topic Clusters to discover cutting edge, yet-to-be published or peer-reviewe
biomedical research articles retrieved from Europe PMC.

"protein structure prediction"

Search Examples: keyword (COVID-19); phrase ("Coronavirus disease")

Use quotation marks for searches with 2 words or more.

Results are sorted by date of publication (most recent on top; maximum of 1000; 25 per page). Resources include: AAS Open Res, bioRxiv, ChemRxiv, F1000Res, Gates Open Res, HRB Open Res, medRxiv, MNI Open Res, Peerl Preprints, Preprints.org, Research Square, Wellcome Open Res.

Results 1-2 of 2 in Enabled Large Language Models

Topic Clusters

Top 400 Results

- + SARS-CoV-2 (125)
- + Protein complexes (28)
- + Protein design (25)
- Language Model (18)
- + Single (8)
- · Enabled Large Language Models (2)
- · Existing Sequence-Based Methods Have Limited (2)
- · Esmfold, Omegafold (2)
- SARS-CoV-2 (2)
- · Other Topics (2)
- + Human proteins (17)
- + Model quality assessment (19)
- + Distance prediction (22)
- + Annotation (11)
- + Graph neural networks (11)
- + Cryo, Electron microscopy (11)
- + Homology search (7)
- + RNA structure (6)
- + Mutations On Protein (8)
- + Contact Map (11)
- + Protein-ligand complexes (6)
- + NMR data (9)
- + Cancer (8)
- + Residue-residue contact prediction (10)
- + Accurate contact predictions (9)

1. ProstT5: Bilingual Language Model for Protein Sequence and Structure new window

Advanced Artificial Intelligence (AI) enabled large language models (LLMs) to revolutionize Natural Language Processing (NLP). Their adaptation to protein sequences spawned the development of powerful protein language models (pLMs). Concurrently, AlphaFold2 broke through in protein structure prediction. For the first time, we can now systematically and comprehensively explore the dual nature of proteins that act and exist as three-dimensional (3D) machines and evolve in linear strings of one-dimensional (1D) sequences. Here, we leverage pLMs to simultaneously model both modalities by combining 1D sequences with 3D structure in one generic model. For this, we encode protein structures as token sequences using the 3Di-alphabet introduced by Foldseek. The resulting "structure-sequence" representation is processed by a pLM to extract features and patterns. Toward this end, we constructed a non-redundant dataset from AlphaFoldDB and fine-tuned an existing pLM (ProtT5) to translate between 3Di and amino acid sequences. As a proof-of-concept for our novel approach, dubbed Protein structure-sequence T5 (ProstT5), we showed improved performance for subsequent prediction tasks, and for "inverse folding", namely the generation of novel protein sequences adopting a given structural scaffold ("fold"). Our work showcased the potential of pLMs to tap into the information-rich protein structure revolution fueled by AlphaFold2. It paves the way for the development of tools optimizing the integration of this vast 3D structure data resource, opening new research avenues in the post AlphaFold2 era. We released our model at https://github.com/mheinzinger/ProstT5

Authors: Heinzinger M, Weissenow K, Sanchez JG, Henkel A, Steinegger M, Rost B.

https://doi.org/10.1101/2023.07.23.550085 - Europe PMC

2. Evolutionary-scale prediction of atomic level protein structure with a language model new window

Artificial intelligence has the potential to open insight into the structure of proteins at the scale of evolution. It has only recently been possible to extend protein structure prediction to two hundred million cataloged proteins. Characterizing the structures of the exponentially growing billions of protein sequences revealed by large scale gene sequencing experiments would necessitate a break-through in the speed of folding. Here we show that direct inference of structure from primary sequence using a large language model enables an order of magnitude speed-up in high resolution structure prediction. Leveraging the insight that language models learn evolutionary patterns across millions of sequences, we train models up to 15B parameters, the largest language model of proteins to date. As the language models are scaled they learn information that enables prediction of the three-dimensional structure of a protein at the resolution of individual atoms. This results in prediction that is up to 60x faster than state-of-the-art while maintaining resolution and accuracy. Building on this, we present the ESM Metage-nomic Atlas. This is the first large-scale structural characterization of metagenomic proteins, with more than 617 million structures. The atlas reveals more than 225 million high confidence predictions, including millions whose structures are novel in comparison with experimentally determined structures, giving an unprecedented view into the vast breadth and diversity of the structures of some of the least understood proteins on earth.







July 26: Transcriptome Analysis - From GEO Data Mining to Submission



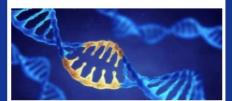
Wednesday, July 26, 2023, 1-3 p.m. Online

Register for Transcriptome Analysis – From GEO Data Mining to Submission

Learn to locate gene expression studies relevant to your topic in the Gene Expression Omnibus repository, and master the art of retrieving and analyzing gene expression count data using tools such as GEO2R, Correlation Engine, and iDEP.

Read more...

Just Released: HGMD Professional 2023.2



Four times a year, Cardiff University releases new updates to HGMD Pro, its market-leading database for finding disease-causing mutations. The summer update is now available, expanding the world's largest collection of human inherited disease mutations by an impressive 33,342 new entries.

Read more...

CMU and DNAnexus Seek Team Leads for October Hackathon



This fall, CMU Libraries is hosting a hackathon in partnership with DNAnexus on the topic of data management and graph extraction for large models in the biomedical space. The hackathon will be held in person at CMU, October 19-21, 2023.

Read more...



One-on-One Consultations hslsmolb@pitt.edu



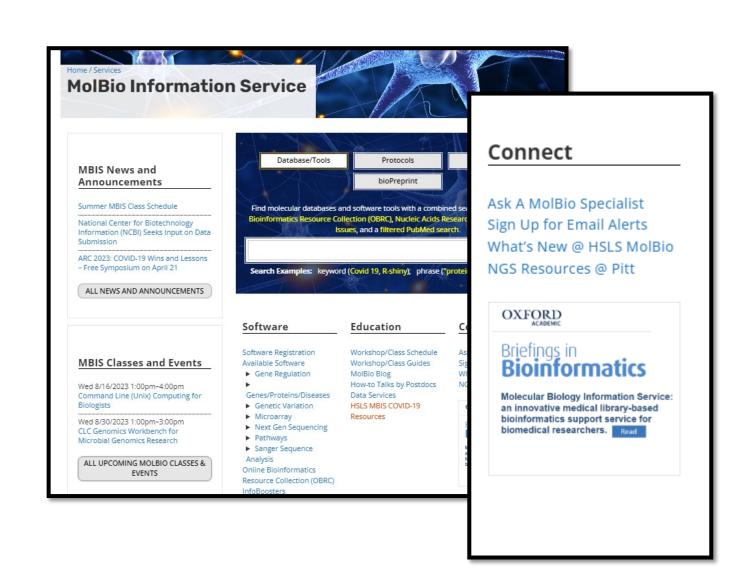
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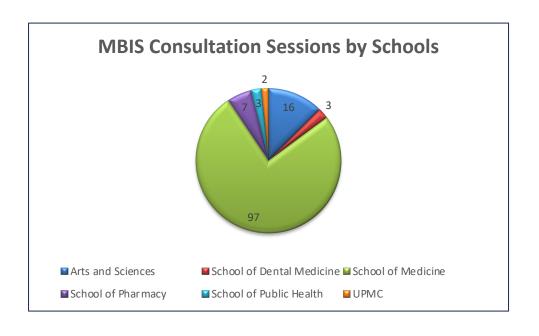
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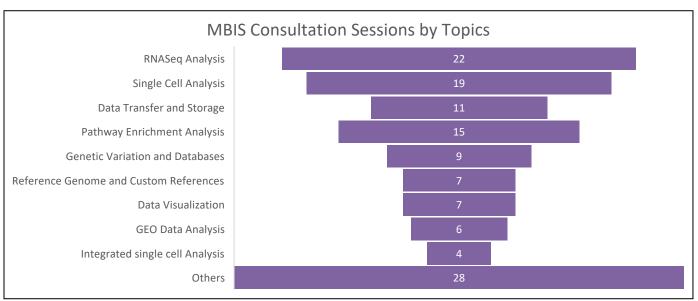


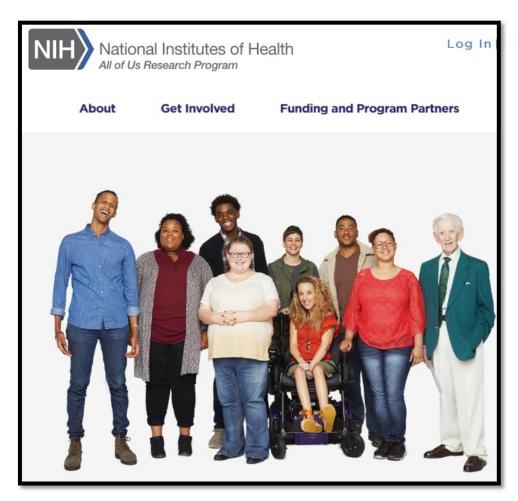
Ansuman Chattopadhyay Program Director ansuman@pitt.edu



In FY2023, MBIS conducted 128 individual consulting sessions for 144 researchers.







Training Initiatives for All of Us Researcher Workbench

Workshops

- Introduction to AoU Researcher Workbench
- Terminology and Data Models Training
- EHR and Survey Data Analysis

Summer Course for MD/Ph.D. students

- Translational Biomedical Analytics:
- Exploring, Analyzing, and Innovating with the All of Us (AoU) Research Program

Code templates
In-person Consultations
Friday Office Hours





Mission: Providing bioinformatics resources via software procurement, implementation, and training to assist biomedical scientists with solving their research questions.

Review

> Brief Bioinform. 2020 May 21;21(3):876-884. doi: 10.1093/bib/bbz035.

Molecular Biology Information Service: an innovative medical library-based bioinformatics support service for biomedical researchers



Ansuman Chattopadhyay ¹, Carrie L Iwema ¹, Barbara A Epstein ¹, Adrian V Lee ¹, Arthur S Levine ¹

Affiliations + expand

PMID: 30949666 DOI: 10.1093/bib/bbz035

FULL TEXT LINKS

OXFORD

ACTIONS



☐ Collections

Thank You!

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