### **Breakout Session 2: Track B**

# Migration of Core Applications from the NIDDK information Network (dkNET)

Dr. Jeffrey Grethe PI, NIDDK Information Network (dkNET), University of California at San Diego



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# Breakout Session 2 – Track B

Jeffrey S. Grethe, Ph.D. FAIR Data Informatics Laboratory University of California San Diego, School of Medicine January 17, 2024





# What is dkNET?

- dkNET provides a single point of access to information about diverse research resources, including data, information, materials, tools, funding opportunities, literature, services, events, news, and projects that advance the mission of the NIDDK.
- dkNET provides tools and services in support of rigor and reproducibility, built around the Research Resource Identifier (RRID) and the FAIR data principles (Findable, Accessible, Interoperable, Re-usable).

# https://dknet.org





# Hypothesis Center - A Powerful FAIR Platform for Biomedical Researchers

- Lowering the barrier of entry to bioinformatics resources and workflows
- Provide information to the DK community on computational resources
- A hub for big data and hypothesis generation, bringing together a collection of online tools
- Detailed tutorials guide researchers in using these resources (Am I using the tools correctly? feedback from ASCB)





# Hypothesis Center - Signaling Pathways Project

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### The Signaling Pathways Project

A multi-omics knowledgebase for cellular signaling pathways

Consenso	me						L D	ownload	Results		
Category: Receptors Class: Nuclear receptors Family: Thyroid hormone receptors Species: House Mouse Physiological System: All Organ: All		Consensomes are list of genes ranked according to a meta-analysis of their differential expression in publicly archived transcriptomic datasets involving perturbations of a specific signaling pathway in a given biosample category. Consensome are intended as a guide to identifying those genes most consistently impacted by a given pathway in a given tissue context.									
	ss X data points from Y experiments in Z dat ntries	Regulation Report Transcriptomics									
Target	🛊 Gene Name	Display by: Category	<mark>⊘</mark> Down	v	Up				Currently display	Downloa ying 300 out of	
Bcl3	B cell leukemia/lym					Transcript Rel	ative Abundanc	e (Fold Chang	le)	=	Export Gr
Idh3a	isocitrate dehydrogenase 3		-7.5	-5	-2.5	0	2.5	5	7.5	10	12
Mmd	monocyte to macrophage differ	Receptors   Catalytic receptors Collagen receptor family NILOT					•				
Stat5a	signal transducer and activator	Enidermal growth factor recentors					•				
Ndrg1	N-myc downstream regu	EGF						•			
		ERBB2			•		•	•			
Trp53inp2	transformation related protein 53 in	EGF Fibroblast growth factor receptors					•				
Ces1f	carboxylesteras	ECE10					•				
	carboxytesteras	Hepatocyte growth factor receptors									
Ephx1	epoxide hydrolase 1, m	PHA665 HGF									
		IL1 receptor family									
		IL1B					•				

SPP simplifies data mining of 'omics data, connects bench researchers to FAIR data to allow them to easily interrogate the data to generate hypotheses

- Find genes with important roles in receptors, enzymes, organs and tissues
- **Define signaling pathways** relevant to a single gene or a regulation

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# **STRIDES Goals**

The Hypothesis Center allows researchers to extract information across transcriptomic and ChIP-Seq datasets, providing a powerful meta-analysis platform that surveys across millions of FAIRly biocurated omics data points to make high-confidence connections between genomic targets, their upstream regulatory pathways, and disease states. Future plans include expansion to more data types. The HC is comprised of two primary components: 1) The Signaling Pathways Project (SPP) knowledgebase and 2) Research resource information and resolution services. Through the tools in the HC, a researcher can find a list of target genes for receptors, enzymes and transcription factors, obtain a snapshot of the dynamic regulatory programs of the cells under study, and utilize this information to formulate new hypotheses. Researchers can then further, for example, prioritize molecules and design experiments to test the novel hypothesis by targeting these molecules. The HC is designed to be user-friendly for a wide spectrum of scientists including hench scientists with little computer programming skills. It is currently ho Medicine. The application seeks support to mi **Initial Phase:** Transition of SPP database and allow the investigators of dkNET to further enh application server to cloud environment and to make it more finable and accessible to t

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## **Signaling Pathways Project**

# SCIENTIFIC DATA

#### OPEN The Signaling Pathways Project, an ARTICLE integrated 'omics knowledgebase for mammalian cellular signaling pathways

Scott A. Ochsner<sup>1</sup>, David Abraham<sup>1,8</sup>, Kirt Martin<sup>1,8</sup>, Wei Ding<sup>2</sup>, Apollo McOwiti<sup>2</sup>, Wasula Kankanamge<sup>2</sup>, Zichen Wang<sup>3</sup>, Kaitlyn Andreano<sup>4</sup>, Ross A. Hamilton<sup>1</sup>, Yue Chen<sup>1</sup>, Angelica Hamilton<sup>5</sup>, Marin L. Gantner<sup>6</sup>, Michael Dehart<sup>2</sup>, Shijing Qu<sup>2</sup>, Susan G. Hilsenbeck<sup>2</sup>, Lauren B. Becnel<sup>2</sup>, Dave Bridges<sup>7</sup>, Avi Ma'ayan<sup>3</sup>, Janice M. Huss<sup>5</sup>, Fabio Stossi<sup>1</sup>, Charles E. Foulds<sup>1</sup>, Anastasia Kralli<sup>6</sup>, Donald P. McDonnell<sup>4</sup> & Neil J. McKenna<sup>1</sup><sup>1</sup>

# SCIENTIFIC DATA

#### OPEN Consensus transcriptional ANALYSIS regulatory networks of coronavirusinfected human cells

Scott A. Ochsner<sup>1</sup>, Rudolf T. Pillich<sup>2</sup> & Neil J. McKenna <sup>[]</sup><sup>1⊠</sup>

Establishing consensus around the transcriptional interface between coronavirus (CoV) infection and human cellular signaling pathways can catalyze the development of novel anti-CoV therapeutics. Here, we used publicly archived transcriptomic datasets to compute consensus regulatory signatures, or consensomes, that rank human genes based on their rates of differential expression in MERS-CoV-(MERS), SARS-CoV-1 (SARS1) and SARS-CoV-2 (SARS2)-infected cells. Validating the CoV

Check for updates

Research article Ô JHEP|Reports

# A human liver chimeric mouse model for non-alcoholic fatty liver disease

#### Authors

Beatrice Bissig-Choisat, Michele Alves-Bezerra, Barry Zorman, Scott A. Ochsner, Mercedes Barzi, Xavier Legras, Diane Yang, Malgorzata Borowiak, Adam M. Dean, Robert B. York, N. Thao N. Galvan, John Goss, William R. Lagor, David D. Moore, David E. Cohen, Neil J. McKenna, Pavel Sumazin, Karl-Dimiter Bissig

Correspondence karldimiter.bissig@duke.edu (K.-D. Bissig).

### **An NIDDK Resource**

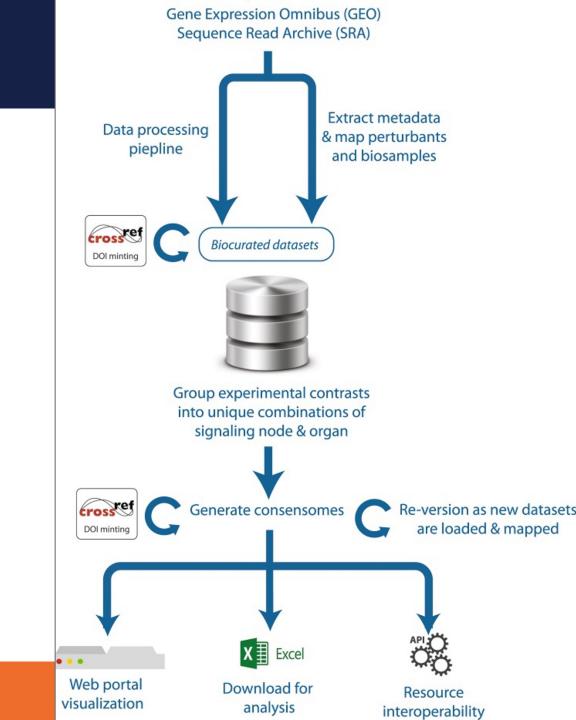
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**An NIDDK Resource** 

# **SPP FAIR Curation**

- Curation of existing datasets to improve FAIRness
- Enhanced datasets can be preprocessed to populate database
- Database content used to drive SPP
   web application





# **Current dkNET Cloud Experience**

- Familiarity with AWS administration
- Foundry data aggregation pipeline deployed to AWS
  - Utilizes EC2, S3, RDS (MariaDB)
  - Data processing takes advantage of AWS auto-scaling with spot instances







# **SPP STRIDES Migration**

### Typical systems administration:

- SPP Application
  - Standard Java application server
  - Basic AWS administration
  - Java application development and deployment

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- Data Processing
  - Basic AWS administration
  - Knowledge of Amazon S3



# **SPP STRIDES Migration**

Need for specialized AWS knowledge:

- SPP Data (Oracle Database)
  - AWS "variant" of Oracle database
  - Special AWS commands for data transfer (via data pump)
  - Deeper knowledge of AWS configuration and security

Utilized AWS Support Center to complete migration

- STRIDES provides Enterprise support plan
- Provide information to navigate AWS specific Oracle implementation

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# **Benefits of SPP STRIDES Migration**

- Collaborative Development
  - Ability to provide access to cloud resources for developers from multiple sites (e.g. UCSD, BCM)
- Ability to use built-in AWS features
  - Automated backups and snapshots
  - Load balancing and fault tolerance (currently investigating)
- More options to tailor service capacity
  - Development versus Production
  - EC2 compute nodes
  - Oracle RDS options





# **Current SPP STRIDES Costs Overview**

- Amazon RDS (Oracle)
  - 72% of total monthly cost
  - Largest cost driver due to Oracle database license [60% of RDS cost]
- Amazon EC2 (Web Application & Data Transfer nodes)
  - Expect increased cost (2-3X with fault tolerant deployment and additional processing

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• Other Costs (e.g. detailed monitoring, data transfer)





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