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Data publishing and archival

Alexey Kolodkin and Olga Krebs

Training on "Best practices in research data management and stewardship"

17 June 2021

FAIR publishing and archival (outline)

- Data Publishing in Open Science
- How to choose right discipline-specific data repository (examples)
- CoreTrustSeal concept
- Introduction to Zenodo and FAIRDOMHub (and interoperable publishing)
- Practicum using FAIRDOMHub and Zenodo for FAIR data and results publishing



Transformation to Open Science

ELIXIR All Hands meeting, June 9th, 2021

“Driving the paradigm shift towards Open Science”, Kostas Glinos, Head of unit for Open Science / Directorate-General for Research and Innovation European Commission:

Current System (dominant)		Open Science	
Excellence defined largely on the basis of <i>where</i> scientists publish		Composite definition of excellence	
Incentivises researchers to produce specific outputs (<i>mainly publications</i>) and to publish as much and as fast as possible (<i>publish or perish!</i>)	Use of quantitative metrics	Incentivises researchers to share knowledge/data early and openly, to collaborate, and to increase quality and impact; While considering diversity of outputs and research cultures	Use of qualitative and quantitative metrics
Rewarding individual competing scientists - gaining scientific prestige		Rewarding team work, collaboration and sharing to achieve societal impact (e.g. Covid-19)	



Publishing for Open Science and Reproducibility

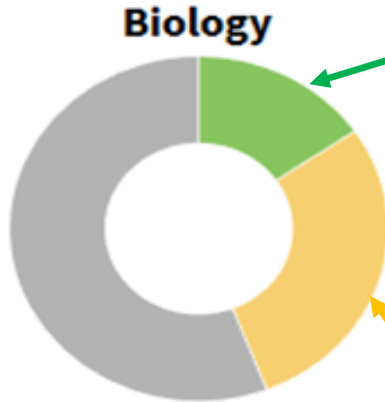
- no papers without data
- preferences for open access papers, open access code, etc.
- FAIR data publishing



Still, many researches are not familiar with FAIR ☹️

Open Data Survey, 2019

never heard of the FAIR principles before



familiar with the FAIR principles (15% !)

previously heard of the FAIR principles but not familiar with them

<https://www.natureindex.com/news-blog/what-scientists-need-to-know-about-fair-data>

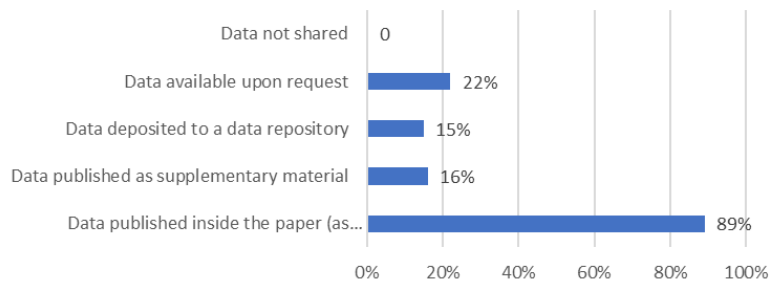
European commission published that we waste €26bn/yr in Europe by not having FAIR research data:



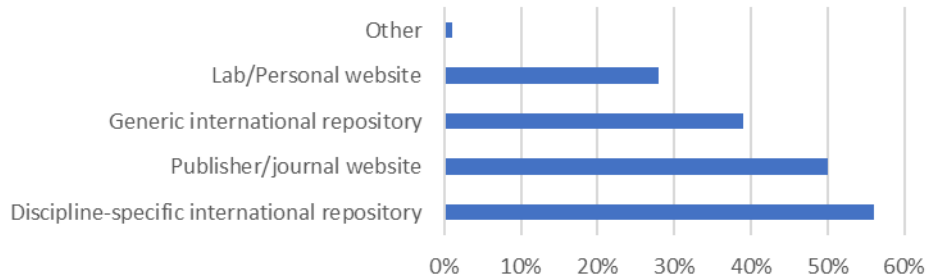
<https://dx.doi.org/10.2777/02999>

You are exception 😊

Please select the top 3 approaches you adopt to data availability when publishing your research



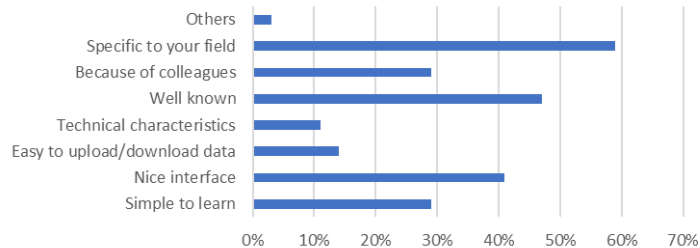
Where your data are shared



Most popular platforms (number of people, from 18 participants)

Zenodo (13, 76.5%)	FairdomHub (3, 17.6%)
European Nucleotide Archive (ENA) (6, 35.3%)	Metabolights (3, 17.6%)
Gene Expression Omnibus (GEO) (5, 29.4%)	Genbank (3, 17.6%)
European Genome-Phenome Archive (EGA) (4, 23.5%)	PRIDE (2, 11.8%)
Dryad (6, 35.3%)	Figshare (2, 11.8%)
DNA Data Bank of Japan (DDBJ) (2, 11.8%)	GitHub (2, 11.8%)
	SYNAPSE (2, 11.8%)

Why do you use a certain platform?



Discipline-specific repositories. How to choose the right one? How to do the right things?

Nucleic acid sequence data:

- [European Nucleotide Archive \(ENA\)](#)
- [GenBank](#)
- [dbSNP](#)
- [European Variation Archive \(EVA\)](#)
- [DNA DataBank of Japan \(DDBJ\)](#)
- [dbVar](#)
- [MGnify](#)
- [NCBI Trace Archive](#)
- [NCBI Sequence Read Archive \(SRA\)](#)
- [NCBI Assembly](#)

Mathematical & modelling resources:

- [BioModels Database](#)
- [Kinetic Models of Biological Systems \(KiMoSys\)](#)
- [The Network Data Exchange \(NDEX\)](#)

Protein sequence:

- [UniProtKB](#)

Molecular & supramolecular structure:

- [Protein Circular Dichroism Data Bank \(PCDDDB\)](#)
- [Crystallography Open Database \(COD\)](#)
- [Coherent X-ray Imaging Data Bank \(CXIDB\)](#)
- [Biological Magnetic Resonance Data Bank \(BMRB\)](#)
- [Electron Microscopy Data Bank \(EMDB\)](#)
- [Worldwide Protein Data Bank \(wwPDB\)](#)
- [Structural Biology Data Grid](#)

[PRIDE](#) (required for publishing structural data)

Neuroscience:

- [NeuroMorpho.org](#)
- [OpenNeuro](#) (formerly OpenfMRI)
- [EBRAINS](#)

Metabolomics & Proteomics

- [MassIVE](#)
- [MetaboLights](#)

- [Gene Expression Omnibus \(GEO\)](#)
- [ArrayExpress](#)
- [GenomeRNAi](#)
- [dbGAP](#)
- [The European Genome-phenome Archive \(EGA\)](#)
- [Database of Interacting Proteins \(DIP\)](#)
- [IntAct](#)
- [Japanese Genotype-phenotype Archive \(JGA\)](#)
- [Biological General Repository for Interaction Datasets](#)
- [Genomic Expression Archive \(GEA\)](#)
- [NCBI PubChem BioAssay](#)



<https://www.nature.com/sdata/policies/repositories>



Discipline-specific repositories. How to choose the right one? How to do the right things?

- FAIR-suitable data repository
- standardized file format
- minimal required information (metadata), in standardized form, machine readable

FAIRsharing.org
standards, databases, policies

<https://www.nature.com/sdata/policies/repositories>

DNA DataBank of Japan (DDBJ)	view FAIRsharing entry
European Nucleotide Archive (ENA)	view FAIRsharing entry
GenBank	view FAIRsharing entry
dbSNP	view FAIRsharing entry
European Variation Archive (EVA)	view FAIRsharing entry
dbVar	view FAIRsharing entry
MGnify	view FAIRsharing entry
NCBI Trace Archive	view FAIRsharing entry
NCBI Sequence Read Archive (SRA)	view FAIRsharing entry
NCBI Assembly	

Protein sequence →

UniProtKB	view FAIRsharing entry
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Examples: ENA (European Nucleotide Archive)



Name	Abbreviation	Related Database
------	--------------	------------------

ENA Sequence XML Schema

ENA EMBL XSD

ENA

minimal required information

ENA Sequence Flat File Format

ENA Sequence Flat File Format

ENA Sequence Flat File Format is a standardised plain text format for nucleotide sequences. This format was previously called the EMBL Sequence Flat File Format.



Examples: PRIDE (Proteomics IDentification Database)



Project PXD026560

PRIDE Assigned Tags: Sars-cov-2 Covid-19

Summary

Title

Analysis of SARS-CoV-2 S protein by LC-MS

Description

Analysis of disulfide bonds for SARS-Cov-2 S protein by LC-MS

Sample Processing Protocol

Cross-linked peptides generated by digesting SARS-Cov-2 S protein using alpha lytic protease, or a combination of trypsin,

Data Processing Protocol

Byonic (v3.8.13, Protein Metrics Inc.) was used for database searches with mass tolerance set as 20 ppm for both precurs

Contact

Peng Zhao, University of Georgia

Lance Wells, Univeristy of Georgia (lab head)

Submission Date

08/06/2021

Publication Date

08/06/2021

Name	Type	Size (M)	Download
checksum.txt	OTHER	732 bit	FTP
LZ-20200501-Chen-S-CC-TASVc-AV5pmol.raw_20200505(1).byrsIt	SEARCH	516	FTP
LZ-20200501-Chen-S-CC-TASVc-AV5pmol.raw.byspec2	SEARCH	753	FTP
LZ-20200501-Chen-S-CC-TASVc-AV5pmol.raw	RAW	4139	FTP
LZ-20200501-Chen-S-CC-KREc-AV5pmol.raw_20200505(1).byrsIt	SEARCH	602	FTP



Examples: GEO (Gene Expression Omnibus)

Series GSE175450		Query DataSets for GSE175450
Status	Public on Jun 08, 2021	
Title	Complement activation induces excessive T cell cytotoxicity in severe COVID-19	
Organism	Homo sapiens	
Experiment type	Expression profiling by high throughput sequencing	
Summary	We performed single cell transcriptomics in 13 acute and convalescent mild versus severe COVID-19 subjects, in healthy controls and in subjects with flu-like-illness and HBV infection to assess COVID-19-specific T cell populations und function.	
Overall design	Blood from 13 COVID-19 patients at acute and convalescent phases, from 5 healthy controls as well as from 5 patients with flu-like disease and 4 patients with chronic HBV infection was collected and PBMC prepared. From part of the PBMC CD38+ CD4+ an CD8+ were purified and both, total PBMC and enriched CD38+ T cells were subjected to 5' GEX scRNA- and 5'-VDJ library preparation. For many samples, both all PBMCs and enriched CD38+ T-cells were sequenced. Samples were pooled with Antibody-based Hashtags and demultiplexed. based on both Hashtags and SNPs.	
Contributor(s)	Sawitzki B, Astaburuaga-García R, Blüthgen N, Obermayer-Wasserscheid B,	

Submission date	May 24, 2021
Last update date	Jun 10, 2021
Contact name	Nils Blüthgen
E-mail(s)	nils.bluehngen@charite.de
Organization name	Charite Universitätsmedizin Berlin
Department	Institute of Pathology
Street address	Chariteplatz 1
City	Berlin
ZIP/Postal code	10117
Country	Germany
Platforms (1)	GPL24676 Illumina NovaSeq 6000 (Homo sapiens)
Samples (57)	GSM5333722 C19-CB-0029_acute_CD38-T-cells
More...	GSM5333723 C19-CB-0029_acute_PBMC
	GSM5333724 C19-CB-0029_convalescent_CD38-T-cells
Relations	
BioProject	PRJNA732416

Download family		Format	
SOFT formatted family file(s)		SOFT	?
MINIML formatted family file(s)		MINIML	?
Series Matrix File(s)		TXT	?
Supplementary file	Size	Download	File type/resource
GSE175450_RAW.tar	235.5 Mb	(http)(custom)	TAR (of TSV)
GSE175450_cell_metadata_table.tsv.gz	1.5 Mb	(ftp)(http)	TSV
<i>Raw data not provided for this record</i>			
<i>Processed data provided as supplementary file</i>			



CoreTrustSeal future



COAR – Confederation of Open Access Repositories , CoreTrustSeal, the European University Association, Science Europe and the World Data System have published a joint position statement on “Data Repository Selection – Criteria That Matter”.

DSA (Data Seal Approval) and WDS (World Data System)

Core Trustworthy Data Repositories Requirements and procedures:

- universal catalogue of requirements that reflects the core characteristics of trustworthy data repositories
- certification to any interested data repository



Generalist repositories



<https://about.zenodo.org>

Data repository that allows to deposit research papers, data sets, research software, reports, and any other research related digital artifacts (provides DOI)



<http://www.fairdomhub.org>

<http://www.fair-dom.org>

Open-source software and services that allows to deposit and catalogue data, SOPs, models, visualizations (provides DOI)

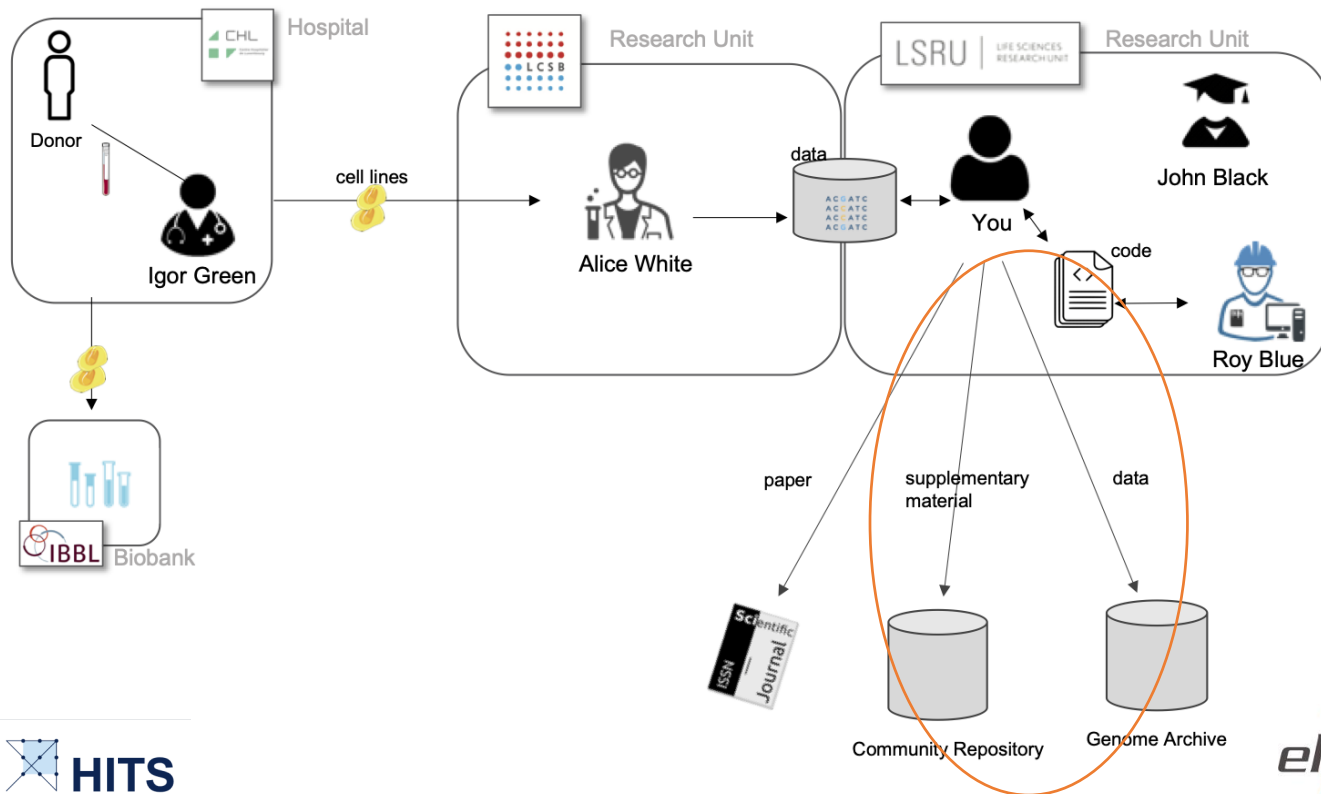
Not just repositories, but FAIR project-oriented platforms to integrate data, SOPs, codes, visualizations, publications...and research communities..

FAIRDOMHub and Zenodo can talk to each other using same language (Interoperable)

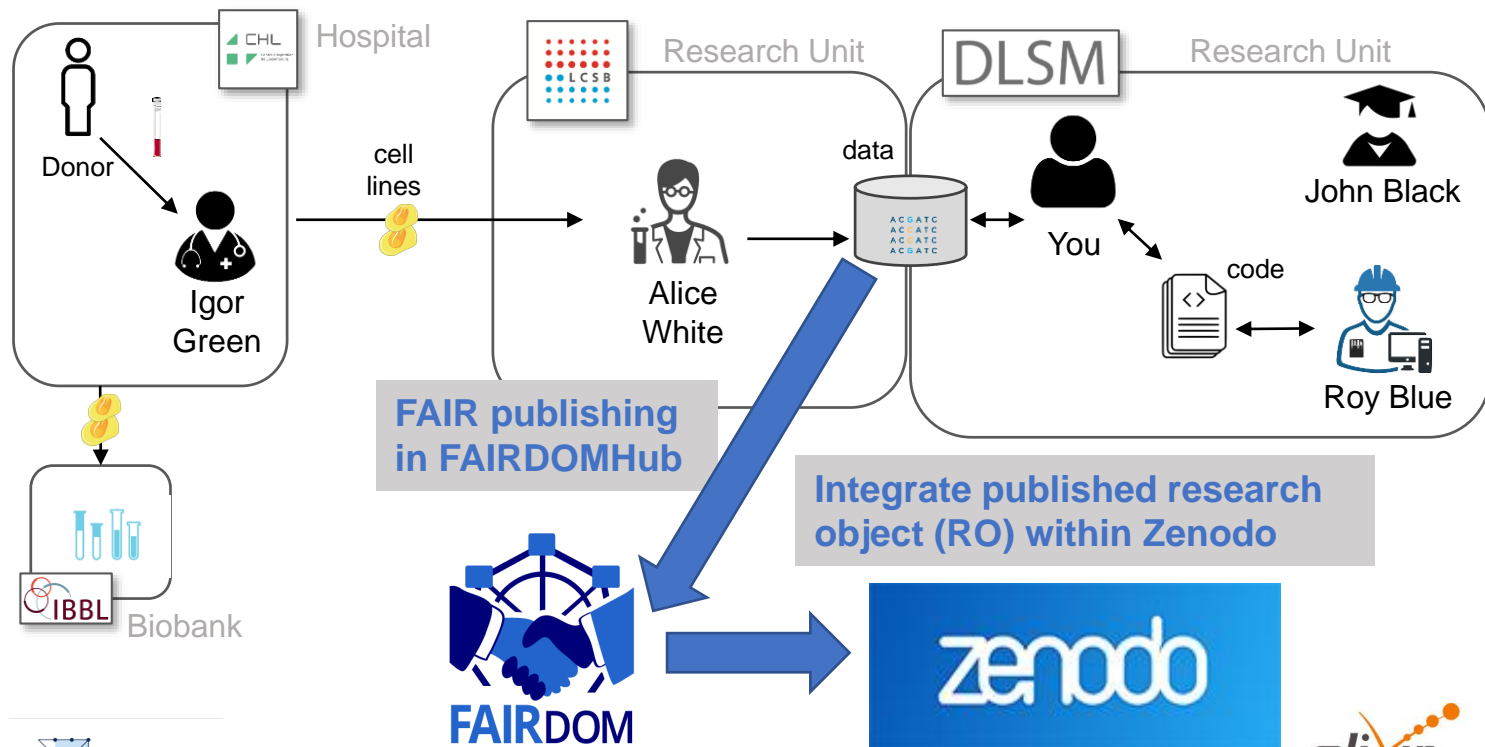
...you will see it on the example



Practicum using FAIRDOMHub and Zenodo for FAIR data and results publishing



Practicum using FAIRDOMHub and Zenodo for FAIR data and results publishing



One can publish various things in Zenodo, easily search and organize

File Type	Keywords	Type
<input type="checkbox"/> Pdf (922741)	<input type="checkbox"/> Taxonomy (658312)	<input type="checkbox"/> Publication (1053896) +
<input type="checkbox"/> Jpg (367879)	<input type="checkbox"/> Biodiversity (657049)	<input type="checkbox"/> Image (612242) +
<input type="checkbox"/> Png (250679)	<input type="checkbox"/> Animalia (377029)	<input type="checkbox"/> Dataset (90605)
<input type="checkbox"/> Html (109493)	<input type="checkbox"/> Arthropoda (290929)	<input type="checkbox"/> Software (56151)
<input type="checkbox"/> Zip (89258)	<input type="checkbox"/> Terrestrial (270732)	<input type="checkbox"/> Presentation (22134)
<input type="checkbox"/> Xml (16484)	<input type="checkbox"/> Herbarium (270653)	<input type="checkbox"/> Poster (8853)
<input type="checkbox"/> Hdf5 (15142)	<input type="checkbox"/> Insecta (196335)	<input type="checkbox"/> Other (7383)
<input type="checkbox"/> Docx (14456)	<input type="checkbox"/> Coleoptera (54916)	<input type="checkbox"/> Video (3679)
<input type="checkbox"/> Xlsx (14403)	<input type="checkbox"/> Arachnida (46335)	<input type="checkbox"/> Lesson (2705)
<input type="checkbox"/> Txt (13597)	<input type="checkbox"/> Chordata (44654)	<input type="checkbox"/> Physicalobject (69)

Communities created and curated by Zenodo users

Search communities

Showing 0 to 10 out of 10463 communities. Sort by ▾

Coronavirus Disease Research Community - COVID-19 Featured

This community collects research outputs that may be relevant to the Coronavirus Disease (COVID-19) or the SARS-CoV-2. Scientists are encouraged to upload their outcome in this collection to facilitate sharing and discovery of information. Although Open Access articles and datasets are recommended, also closed and restricted access material are accepted. All types of research outputs can be included in this Community (Publication, Poster, Presentation, Dataset, Image, Video/Audio, Software, Lesson, Other).

zenodo Search Upload Communities Log in Sign up

October 6, 2020 Presentation Open Access

Practicalities of Data Handling

Vilém Déd

Project leader(s)
Roland Krause

Project member(s)
Pinar Alper

Slides used for the practical data handling session of training on "Best practices and Data Management and Stewardship" held by ELIXIR Luxembourg on 6 October 2020.

Preview

71 views 71 downloads See more details...

Indexed in **OpenAIRE**

Publication date: October 6, 2020

DOI: [10.5281/zenodo.4998228](https://doi.org/10.5281/zenodo.4998228)

Keyword(s):



Entering metadata when publishing in Zenodo

zenodo Search Upload Communities alexey.kolodkin@uni.lu

Delete Save Publish

New upload

Instructions: (i) Upload minimum one file or fill-in required fields (marked with a red star). (ii) Press "Save" to save your upload for editing later. (iii) When ready, press "Publish" to finalize and make your upload public.

Files Choose files Start upload

Filename (1 files)	Size	Progress	Delete
Data_Publishing_AK_2021-06-14_v10.ppt	6.1 MB		

Upload type required

Publication Poster Presentation Dataset Image Video/Audio Software Lesson Physical object Other

Publication type Journal article

Publication type.

Publication date * 2021-06-17

Required. Form

Title *

Required.

Authors * Family name

+ Add another

Description *

..and so on...



<https://sandbox.zenodo.org/>





F
A
I
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D
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M

Findable
Accessible
Interoperable
Reusable

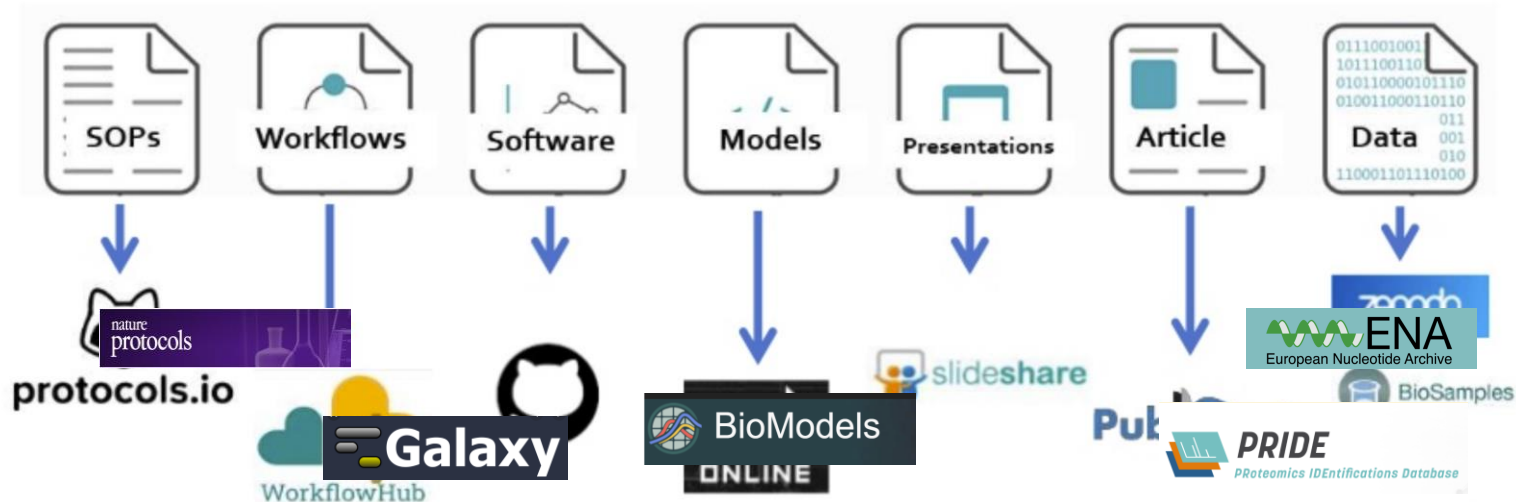
Data
SOPs
Models

} Assets

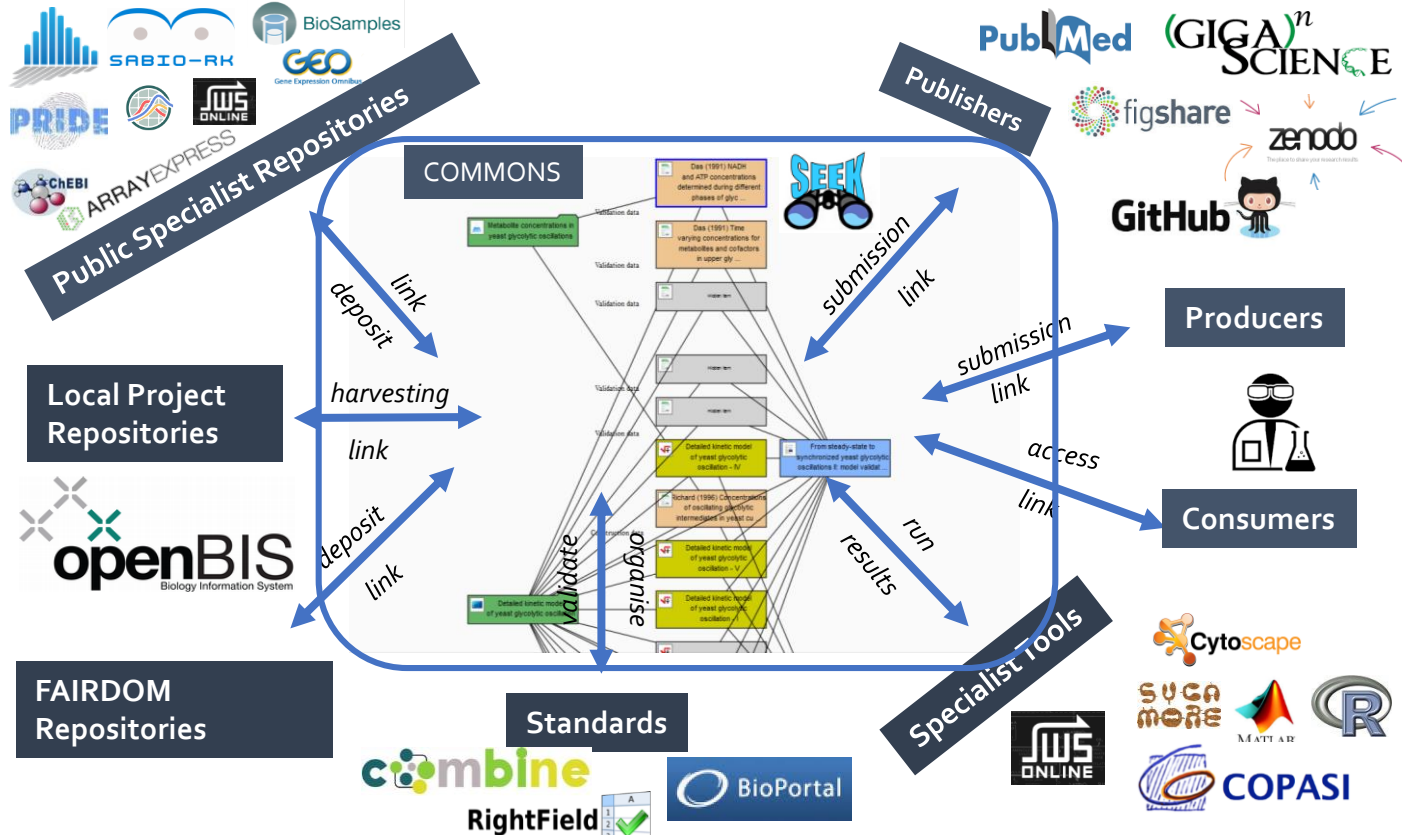
Many Objects are the Outcomes of Research

All are first class citizens and are required to make research FAIR+R

Each object has its own metadata and repositories

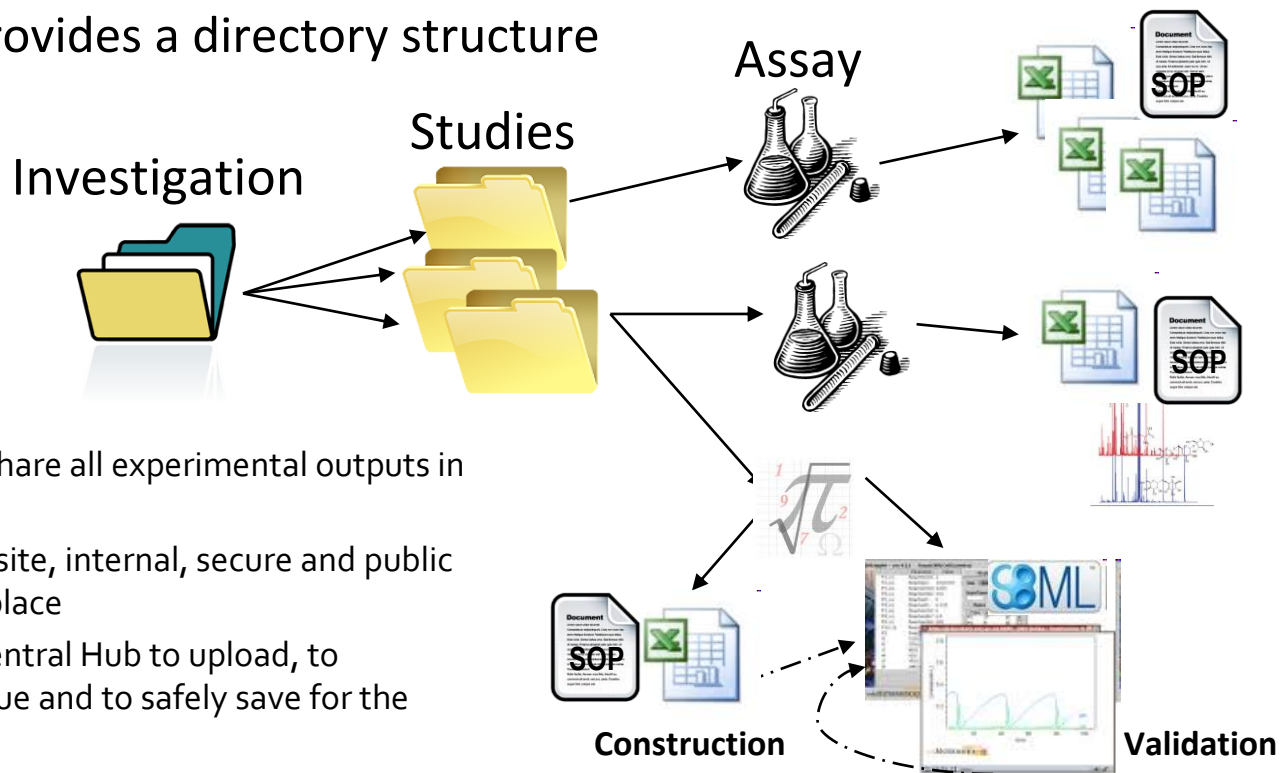


FAIRDOM Platform: Catalogue, Commons, Collections, Project-centric Data Management



Organising and Linking Assets

ISA infrastructure provides a directory structure for experiments



- Organise, find and share all experimental outputs in one place
- Organise across on-site, internal, secure and public stores all from one place
- Use our managed central Hub to upload, to organise, to catalogue and to safely save for the long-term
- Use national or institutional data storage infrastructure

Project centric approach

[Home](#) > [Projects Index](#) > MOSES

MOSES (Micro Organism Systems biology: Energy and *Saccharomyces cerevisiae*) develops a new Systems Biology approach, which is called 'domino systems biology'. It uses this to unravel the role of cellular free energy ('ATP') in the control and regulation of cell function. MOSES operates through continuous iterations between partner groups through a new systems-biology driven data-management workflow. MOSES also tries to serve as a substrate for three or more other SYSMO programs.



Programme: SysMO

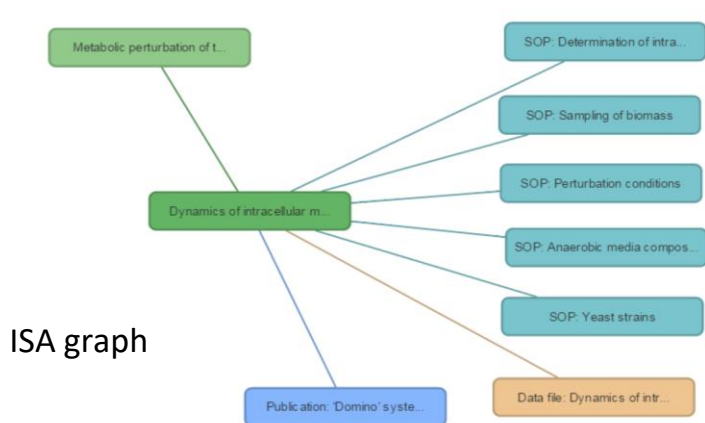
Public web page: <http://www.moses.sys-bio.net/>

Organisms: *Saccharomyces cerevisiae*

FAIRDOM PALS: Femke Mensonides, Maksim Zakhartsev, Walter Glaser

Related items

People (20) Institutions (6) Investigations (3) Studies (8) Assays (12+1) Samples (0+4) Cell cultures (0+4) Strains (1) Data files (9+1) Models (1+2) SOPs (7+4) Publications (5)



Experimental

Assay: Dynamics of intracellular metabolites during glucose pulse

Connected items

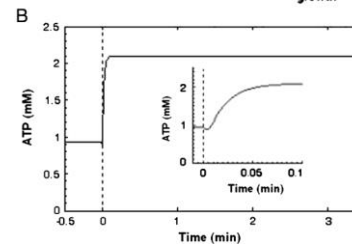
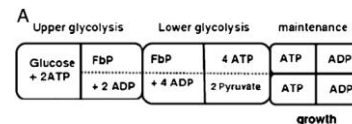
Data file: Dynamics of intracellular metabolites during glucose pulse

SOP: Yeast strains

SOP: Anaerobic media composition

SOP: Perturbation conditions

SOP: Sampling of biomass



FAIRDOMHub: Landing page



Q Browse ▾

+ Create ▾

i Help ▾

Search here

Search



- Yellow pages
- Programmes
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- People
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- Studies
- Assays
- Assets
- Data files
- Models
- SOPs
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- Documents
- Activities
- Presentations
- Events
- Samples
- Sample types
- Organisms

The FAIRDOMHub is a web platform for the FAIR Data and Model Management service to the European Systems Biology community. FAIRDOM is a joint action of ERA-Net EraSysAPP and European Research Infrastructure ISBE

Please cite us in your publications and reports. For more information about FAIRDOMHub, please visit <https://fair-dom.org>

FAIRDOMHub

FAIRDOM is an initiative to develop a community, and establish an internationally sustained Data and Model Management service to the European Systems Biology community. FAIRDOM is a joint action of ERA-Net EraSysAPP and European Research Infrastructure ISBE

For more information about FAIRDOM please visit <http://fair-dom.org>

If you are interested in using FAIRDOMHub within your own funding programme, or have any other questions related to FAIRDOMHub, including feedback, please contact us.

+ Create ▾

i DM- get

- Assets
- Data file
- Model
- SOP
- Publication
- Experiments
- Investigation
- Study
- Assay
- Activities
- Presentation
- Event
- Admin
- Programme
- Project
- Institution
- Profile

Get started

Who is using it?

Get

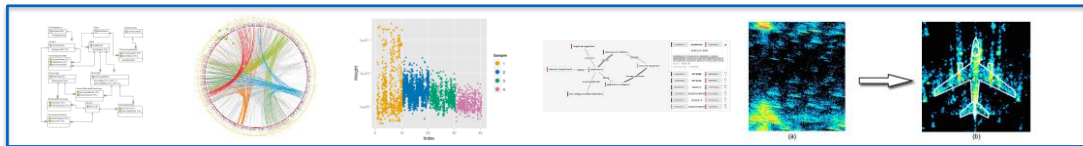
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- Provide feedback
- and model management

Data Generation

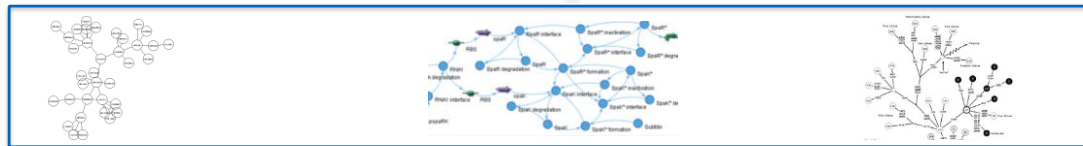
High-Performance
Analysis



Analysis transformation



FAIR (meta)data
(RDF, XML etc.)

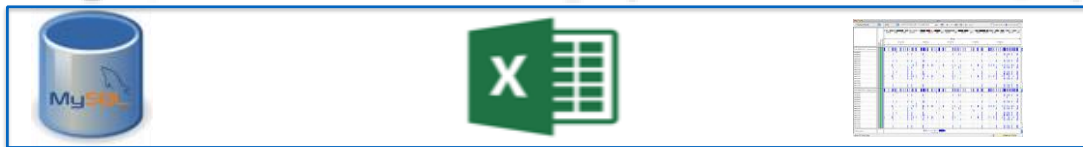


FAIR transformation

FAIR download
(in local format)



Processed data
(primary storage format)



Initial transformation

Provenance



Raw data
(many formats)



Standard Operating Procedures (SOP): Quality Control

[Home](#) > [SOPs Index](#) > Introduction of shRNAs, miRNAs or anti-miRNAs into primary human hepatocytes with lentivirus



Introduction of shRNAs, miRNAs or anti-miRNAs into primary human hepatocytes with lentivirus

Download SOP

View content

Here we used VSV-G-pseudotyped, EGFP-expressing lentiviral vectors to develop an efficient gene transfer protocol to modify gene expression in primary human hepatocytes (by RNAi). The protocol comprises the production of recombinant viruses as well as the steps for efficient delivery of short-hairpin RNA (shRNAs), microRNAs or anti-microRNAs to human hepatocytes. On average infection efficiencies of over 95% are achieved at relatively low multiplicity of infection (MOI), which effectively reduces the amount of preparative work required per experiment. Depending on the laboratory equipment available, we provide here two alternative workflows, which can be easily adapted in the lab. The procedure of virus production with subsequent titer determination takes approx. 6 to 10 working days. The procedure of viral infection of hepatocytes until effects can be measured takes approx. 3 to 5 days. This protocol should be helpful to study many aspects of functional genomics in primary human hepatocytes.

Contributors

[Maria Thomas]

Attributions

None

Scales

Filename: Lentiviral production and infection_SOP_04042011.pdf

Format: PDF document

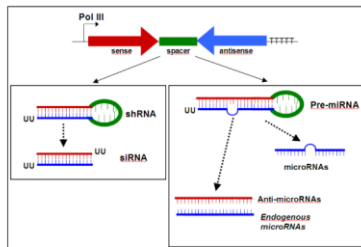


Fig.1: Schematic presentation of designed template sequences which are processed intracellularly into short hairpin RNAs, microRNAs or anti-microRNAs. The stem-loop structures consisting of both the sense and anti-sense strands of the targeted sequence are separated by a loop sequence.

MATERIALS

REAGENTS/KITS

BLOCK-iT™ Lentiviral RNAi Expression Kit (Invitrogen#49-4400)

ViraPower™ Lentiviral Gateway Expression Kit (Invitrogen#K49-6000)

miRZip™ Lentivector-based Anti- MicroRNAs (System Biosciences#MZIPxxxPA/AA-1)

Anti-miRNAs (System Biosciences#PMIRHxxxPA/AA-1)

PROCEDURE

NOTE: all the steps marked with "S" should be performed following recommended guidelines for working with BL-2 organisms (Germany; S2 lab).

1. Preparation of HEK293FT cells.

For cultivating HEK293FT cells, add G148 (Geneticin, final concentration 500 µg/ml) to the DMEM culture medium with components (see Reagent Setup). The cells should be passaged at least 1-2 times after thawing to adapt to the culture conditions. Three days prior to transfection, plate out the cells at a density of approximately 3.5×10^5 cells/per 1 T175 flask in 30 ml of medium with components and G148 to achieve optimal phase of cellular growth.

Reproducible models in FAIRDOM

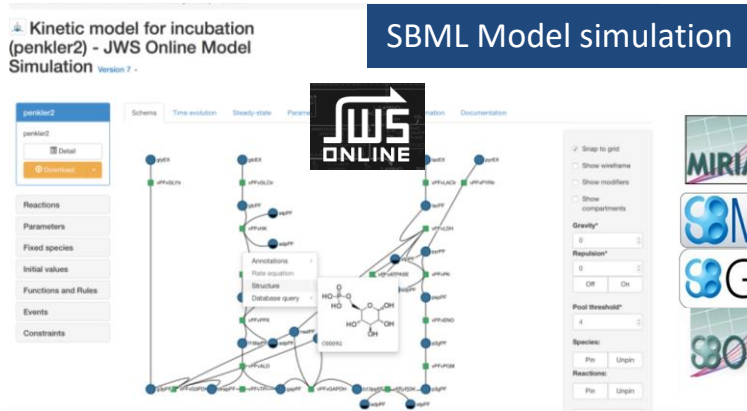
metadata annotation against standards
validation, comparison and simulation

JWS Online

Kinetic model for incubation (penkler2) - JWS Online Model Simulation

Version 7

SBML Model simulation



SBML Differences

Both documents have same Level/Version: L3V1

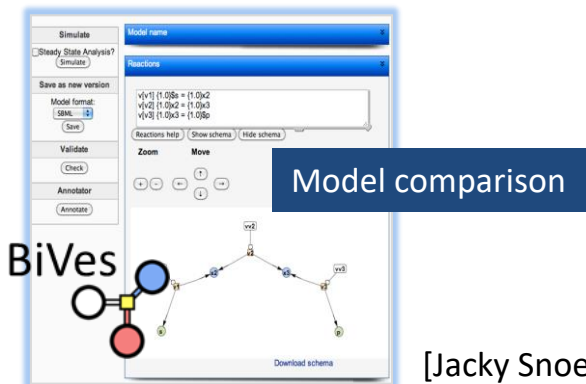
Model versioning

Parameters	Attributes
VappSPSPPP	Attribute value has changed: 797 → 500

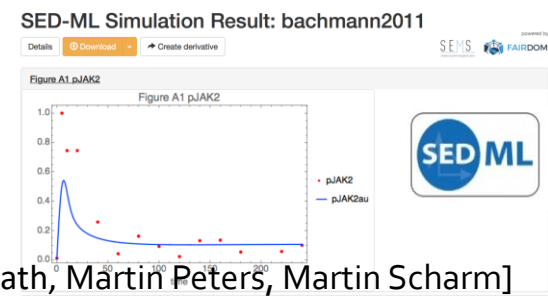
Compartments	Attributes
default_compartment → main	Attribute id has changed: default_compartment → main

Species	Attributes
Sucrose	Attribute compartment has changed: default_compartment → main
ADPGam	Attribute compartment has changed: default_compartment → main
PPam	Attribute compartment has changed: default_compartment → main
Pcvt	Attribute compartment has changed: default_compartment → main
F6Pcvt	Attribute compartment has changed: default_compartment → main
ADPam	Attribute compartment has changed: default_compartment → main
UDPcvt	Attribute compartment has changed: default_compartment → main
Glucoseam	Attribute compartment has changed: default_compartment → main
G6Pam	Attribute compartment has changed: default_compartment → main

Model comparison



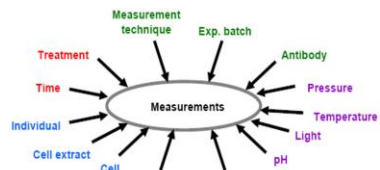
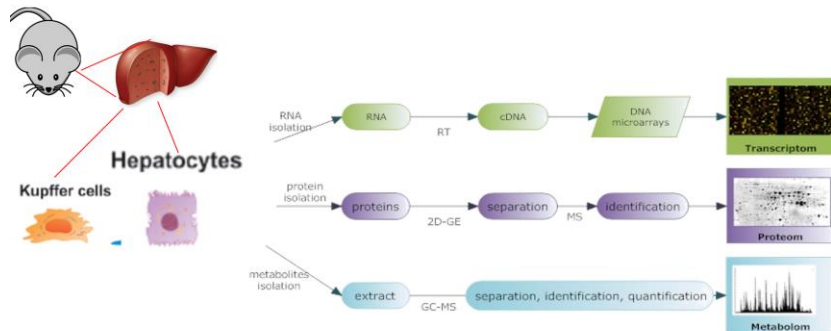
Reproducing simulations



[Jacky Snoep, Dagmar Waltemath, Martin Peters, Martin Scharm]



Biosamples



- Effects of interest
- Physical conditions
- Technical variations
- Biological variations

More examples here
https://fairdomhub.org/sample_types

Samples

UID	Name	DateOfBirth	Sex	Treatment1	Treatment1Route
MUS-200901ENG-1	19-1892	29 August 2019	F	saline	intraperitoneal
MUS-200901ENG-2	19-2135	19 September 2019	M	saline	intraperitoneal
MUS-200901ENG-3	19-2136	19 September 2019	M	saline	intraperitoneal
MUS-200901ENG-4	19-2137	19 September 2019	M	saline	intraperitoneal
MUS-200901ENG-5	19-2140	27 September 2019	F	saline	intraperitoneal
MUS-200901ENG-6	19-2141	27 September 2019	M	saline	intraperitoneal
MUS-200901ENG-7	19-2142	27 September 2019	M	saline	intraperitoneal
MUS-200901ENG-8	19-2143	27 September 2019	M	saline	intraperitoneal
MUS-200901ENG-9	19-2148	28 September 2019	F	saline	intraperitoneal
MUS-200901ENG-10	19-2149	28 September 2019	F	saline	intraperitoneal

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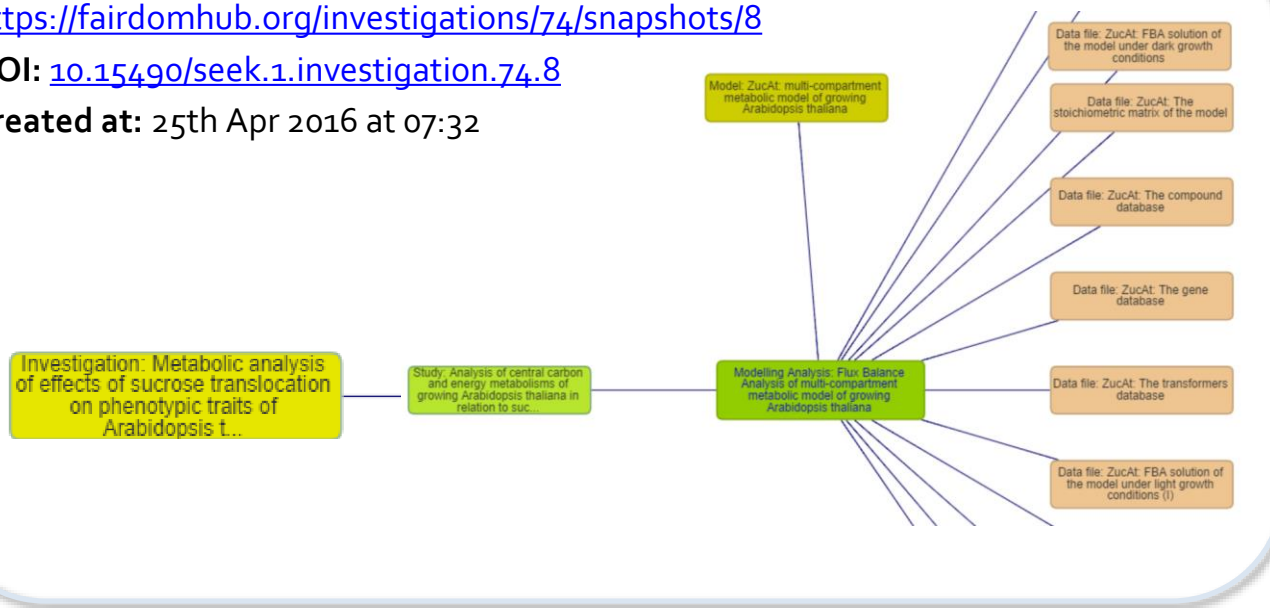
Snapshot 8 (25th Apr 2016) 

DOI: 10.15490/seek.1.investigation.74

<https://fairdomhub.org/investigations/74/snapshots/8>

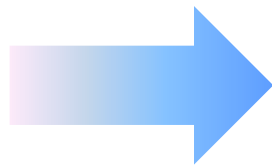
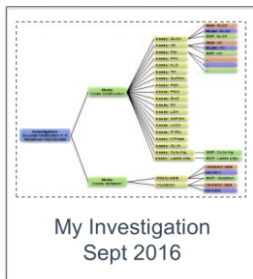
DOI: [10.15490/seek.1.investigation.74.8](https://doi.org/10.15490/seek.1.investigation.74.8)

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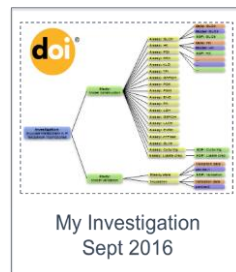


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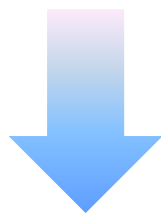
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G. Penkler, F. Du Toit, W. Adams, M.
Rautenbach, D. C. Palm, D. D. Van
Niekerk, & J. L. Snoep. (2014).
Glucose metabolism in Plasmodium
falciparum trophozoites. FAIRDOMHub.

<http://doi.org/10.15490/seek.1.investigation.56>

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