SEEK

openBIS
Biology Information System

FAIRDOM

SIB
Swiss Institute of Bioinformatics

ERASys APP
ERA-Net for Applied Systems Biology

# FAIRDOM Data and Model Management for ERASysAPP

## Combining SEEK and openBIS for ERASysApp and beyond

MANCHESTER
1824
The University of Manchester

HITS

Federal Ministry of Education and Research

SystemsX.ch
The Swiss Initiative in Systems Biology

BBSRC
bioscience for the future

# FAIRDOM

- **F**indable
- **A**ccessible
- **I**nteroperable
- **R**eusable

- **D**ata
- **O**perations
- **M**odels

- **FAIRDOM** is a separately and independently funded data and model management project, a joint action of ERA-Net EraSysAPP and European Research Infrastructure ISBE to establish a data and model management service facility for Systems Biology.

FAIRDOM
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1824
The University of Manchester


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Rostyslav
Kuzyakiv


Jakub
Straszewski


Chandrasekhar
Ramakrishnan


Caterina
Barillari

- Our prime mission is to support researchers students, trainers, funders and publishers by enabling Systems Biology projects to make their Data, Operating procedures and Models, Findable, Accessible, Interoperable and Reusable (FAIR).

- **FAIRDOM** offers
  - Software, Services, Curation support
- **Working closely together with users** and pre-existing resources, platforms and tools
  - PALs , DMG

# Always keep in mind:

**You** define and do the science

**We** do services, consulting, training,

tools to simplify managing the data/models/SOPs in the process, tailored to **your** requirements

**We do not** interfere with how you do your science

# The FAIRDOM Platform

## Front end: Science Commons

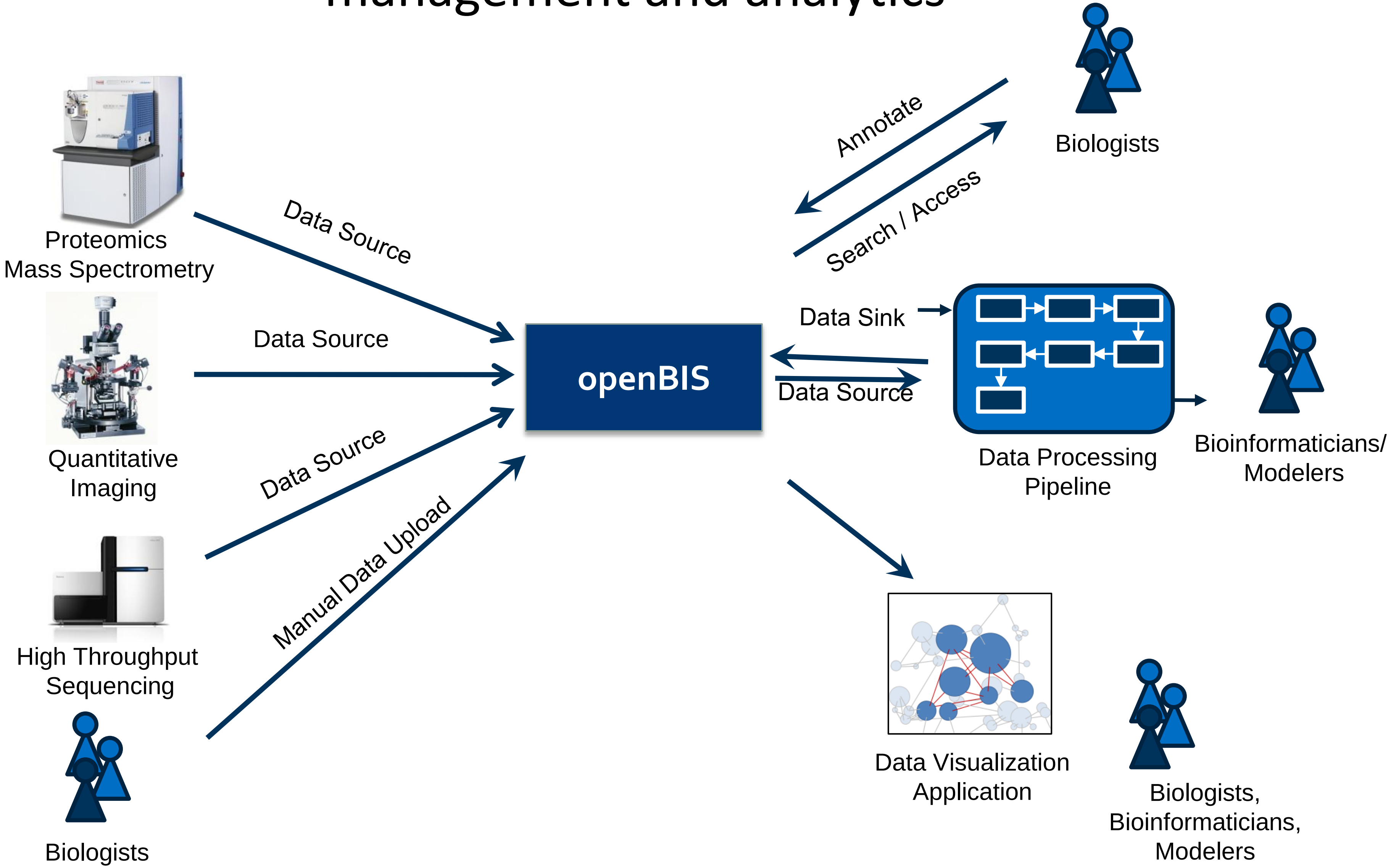
Web-based Cataloguing and Rich web interface for describing, finding, linking and promoting ongoing research and outcomes. Small files, aggregates across data archives.

## Back end: Scaled local LIMS and analytics

Extract, Transform and Load tooling  direct from the instrumentation, data analysis pipelines. Automatic archiving. Handles large data.

# openBIS in a nutshell

## management and analytics



Proteomics
Mass Spectrometry

Quantitative
Imaging

High Throughput
Sequencing

Biologists

Data Source

Data Source

Data Source

Manual Data Upload

openBIS

Annotate

Search / Access

Biologists

Data Sink

Data Source

Data Processing
Pipeline

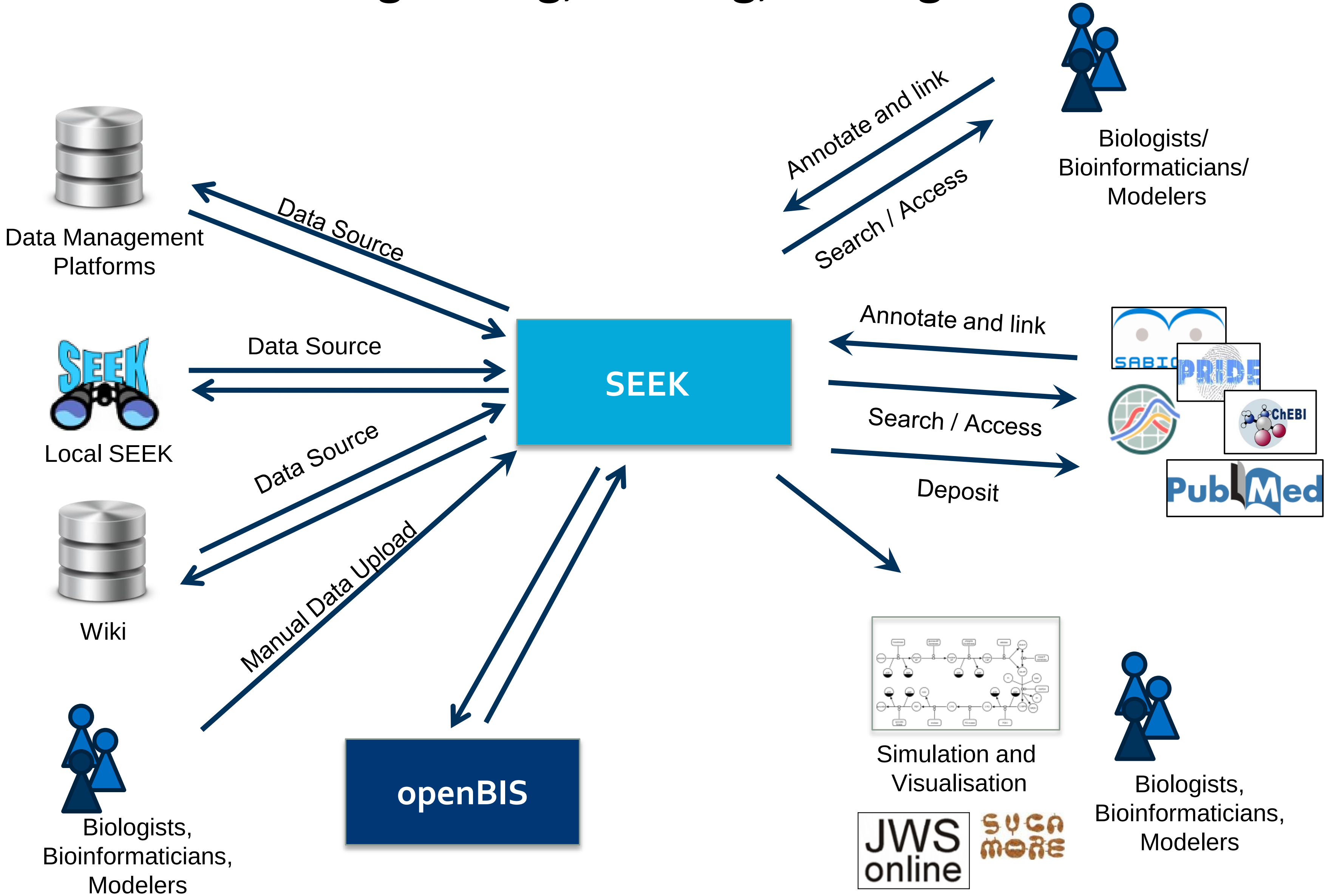
Bioinformaticians/
Modelers

Data Visualization
Application

Biologists,
Bioinformaticians,
Modelers

# SEEK in a nutshell

## organising, sharing, finding



Data Management Platforms

Data Source

Local SEEK

Data Source

Data Source

Wiki

Manual Data Upload

Biologists, Bioinformaticians, Modelers

SEEK

openBIS

Annotate and link

Search / Access

Biologists/ Bioinformaticians/ Modelers

Annotate and link

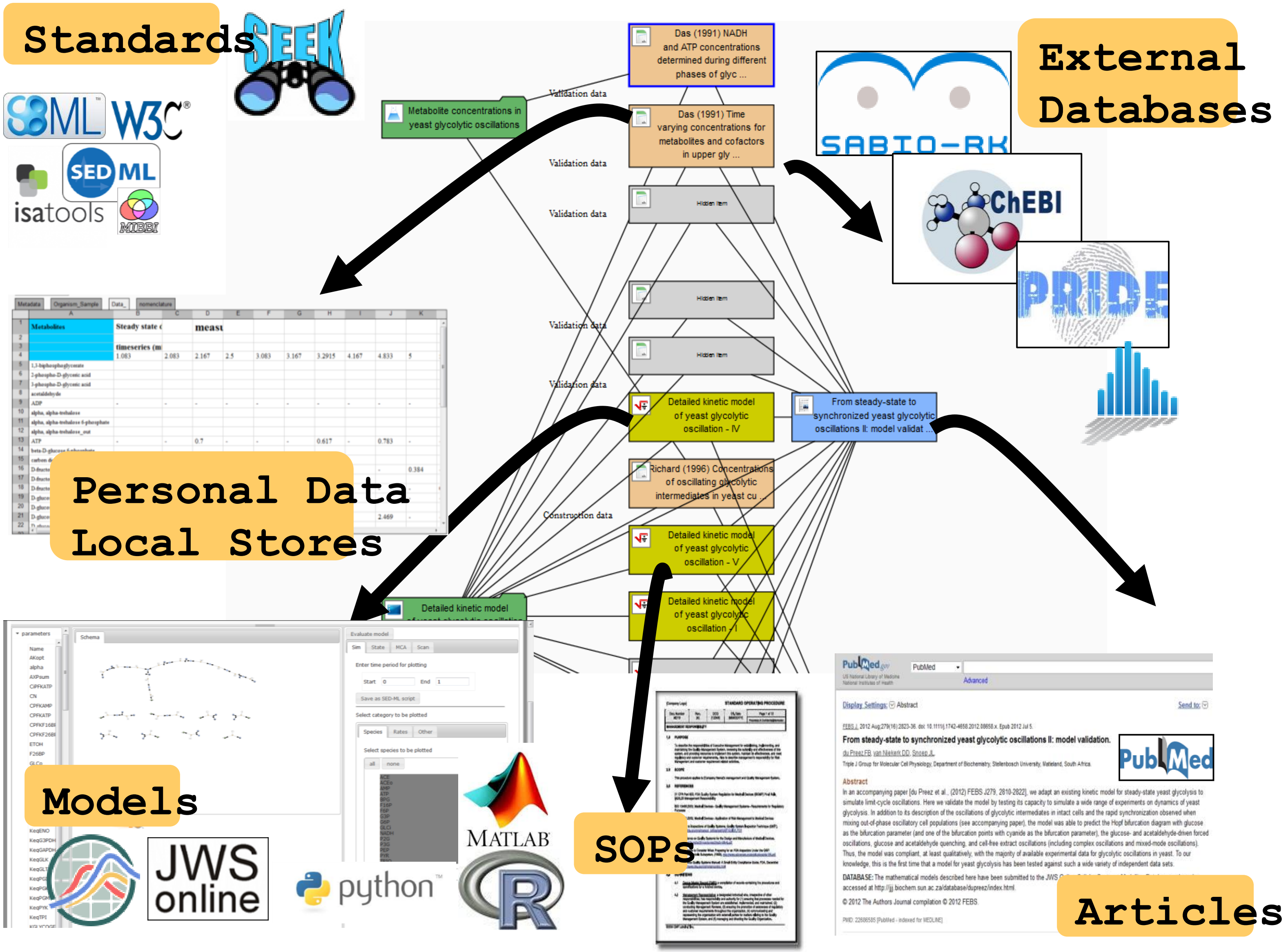
Search / Access

Deposit

Simulation and Visualisation

Biologists, Bioinformaticians, Modelers

# Aggregated Content



**Standards**

**External Databases**

**Personal Data Local Stores**

**Models**

**SOPs**

**Articles**

FEBS J. 2012 Aug;279(16):2823-36. doi: 10.1111/j.1742-4658.2012.08658.x. Epub 2012 Jul 5.

**From steady-state to synchronized yeast glycolytic oscillations II: model validation.**

du Preez FB, van Niekerk DD, Snoep JL.

Triple J Group for Molecular Cell Physiology, Department of Biochemistry, Stellenbosch University, Matieland, South Africa.

Abstract

In an accompanying paper [du Preez et al., (2012) FEBS J279, 2810-2822], we adapt an existing kinetic model for steady-state yeast glycolysis to simulate limit-cycle oscillations. Here we validate the model by testing its capacity to simulate a wide range of experiments on dynamics of yeast glycolysis. In addition to its description of the oscillations of glycolytic intermediates in intact cells and the rapid synchronization observed when mixing out-of-phase oscillatory cell populations (see accompanying paper), the model was able to predict the Hopf bifurcation diagram with glucose as the bifurcation parameter (and one of the bifurcation points with cyanide as the bifurcation parameter), the glucose- and acetaldehyde-driven forced oscillations, glucose and acetaldehyde quenching, and cell-free extract oscillations (including complex oscillations and mixed-mode oscillations). Thus, the model was compliant, at least qualitatively, with the majority of available experimental data for glycolytic oscillations in yeast. To our knowledge, this is the first time that a model for yeast glycolysis has been tested against such a wide variety of independent data sets.

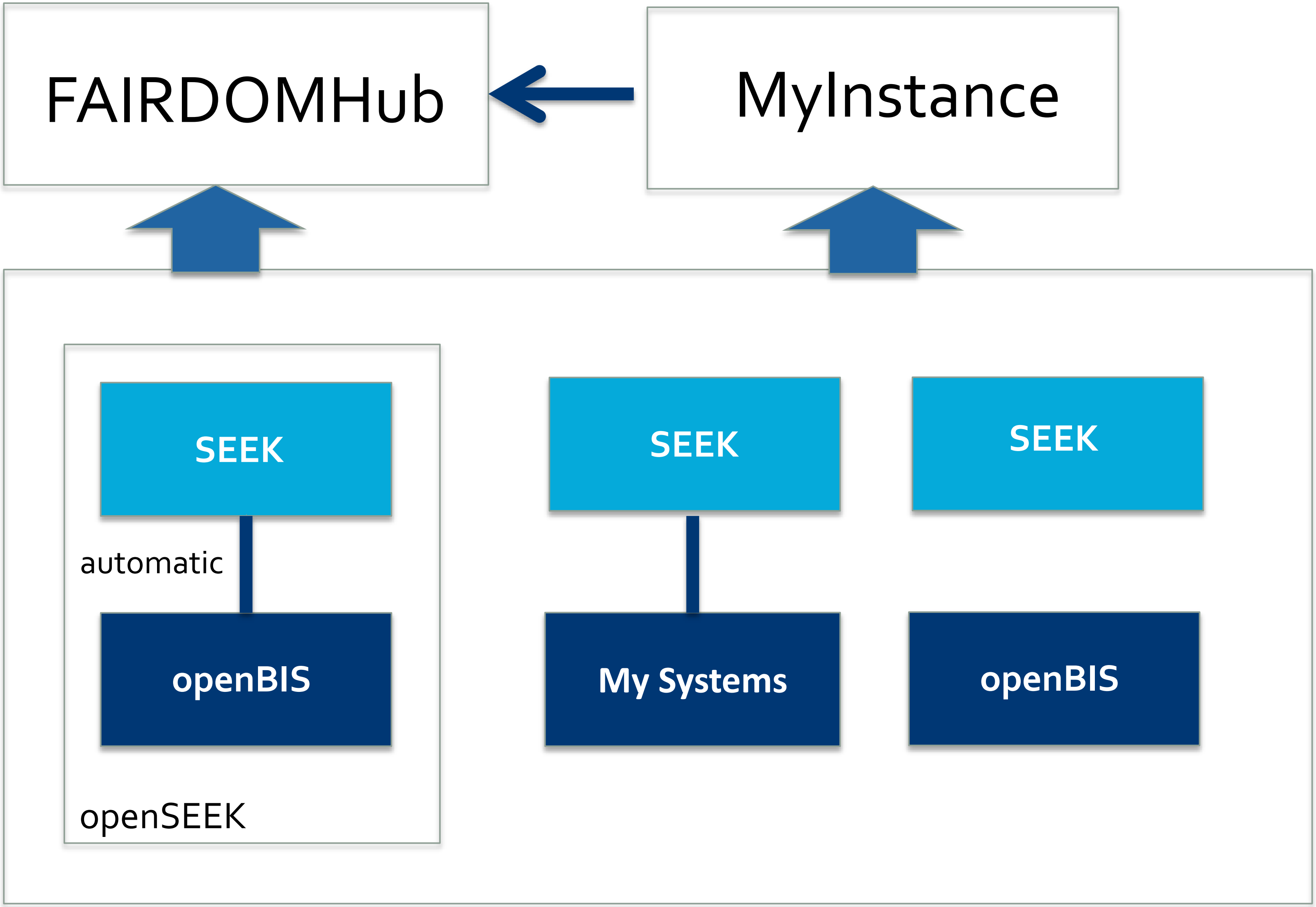
**DATABASE:** The mathematical models described here have been submitted to the JWS

accessed at http://jjj.biochem.sun.ac.za/database/dupreez/index.html.

© 2012 The Authors Journal compilation © 2012 FEBS.

PMID: 22686585 [PubMed - indexed for MEDLINE]

# The FAIRDOM Platform


FAIRDOMHub

MyInstance

SEEK

automatic

openBIS

openSEEK

SEEK

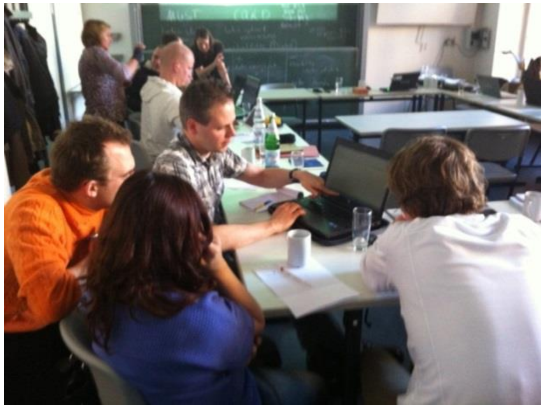
My Systems

SEEK

openBIS

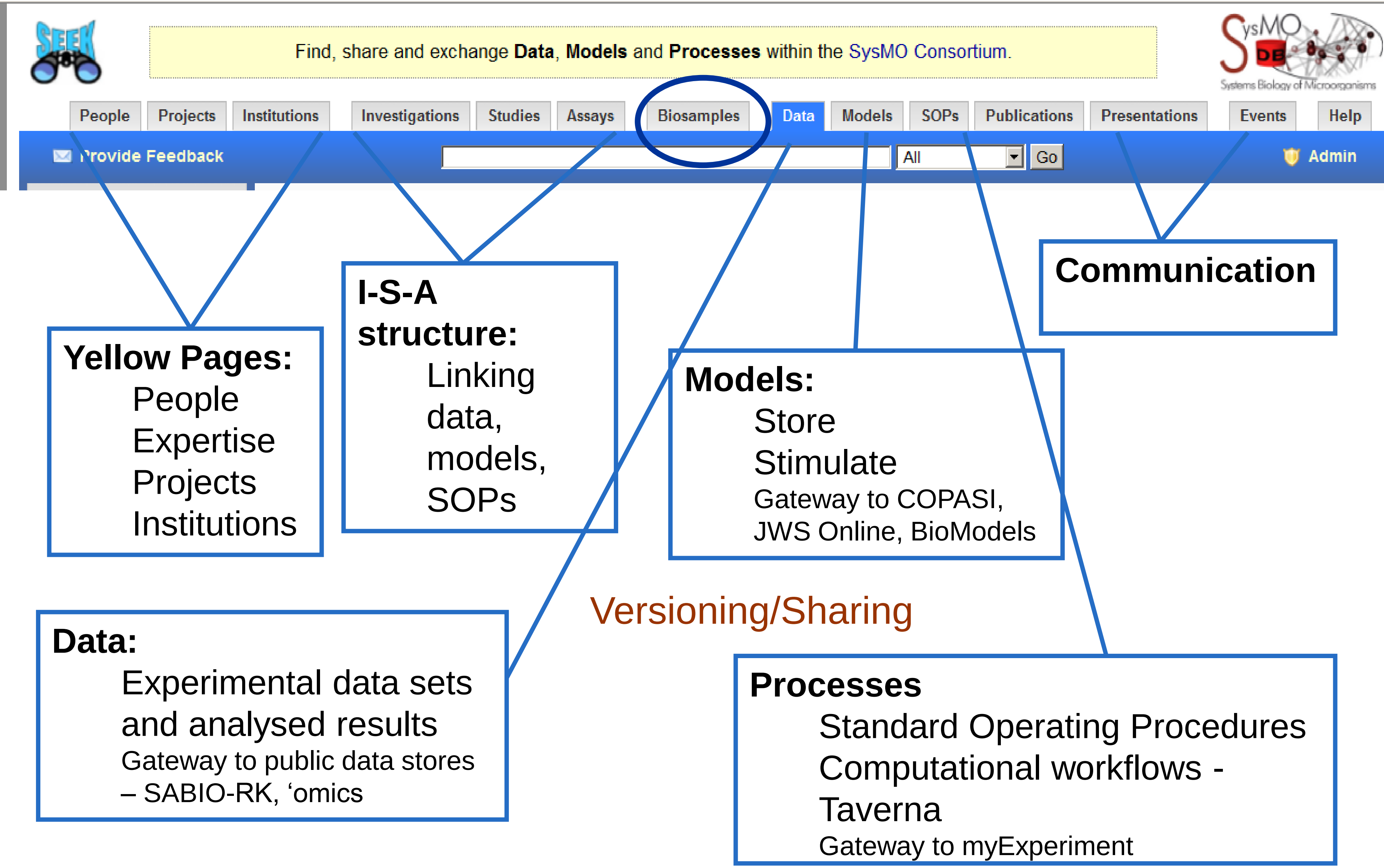
# Working together: EraSysAPP PALs

- Representatives of projects
- Post-docs, Postgrads
- Co-designers
- Bridge modellers-experimentalists
- Big training/engagement
- Workshops, meetings, Visits



***Tell me and I forget,***
***teach me and I may remember,***
***involve me and I learn.***
*(Benjamin Franklin)*

# Assets Catalogue. Archive. Social Network.



Find, share and exchange **Data**, **Models** and **Processes** within the SysMO Consortium.

**Yellow Pages:**
- People
- Expertise
- Projects
- Institutions

**I-S-A structure:**
- Linking data, models, SOPs

**Models:**
- Store
- Stimulate
- Gateway to COPASI, JWS Online, BioModels

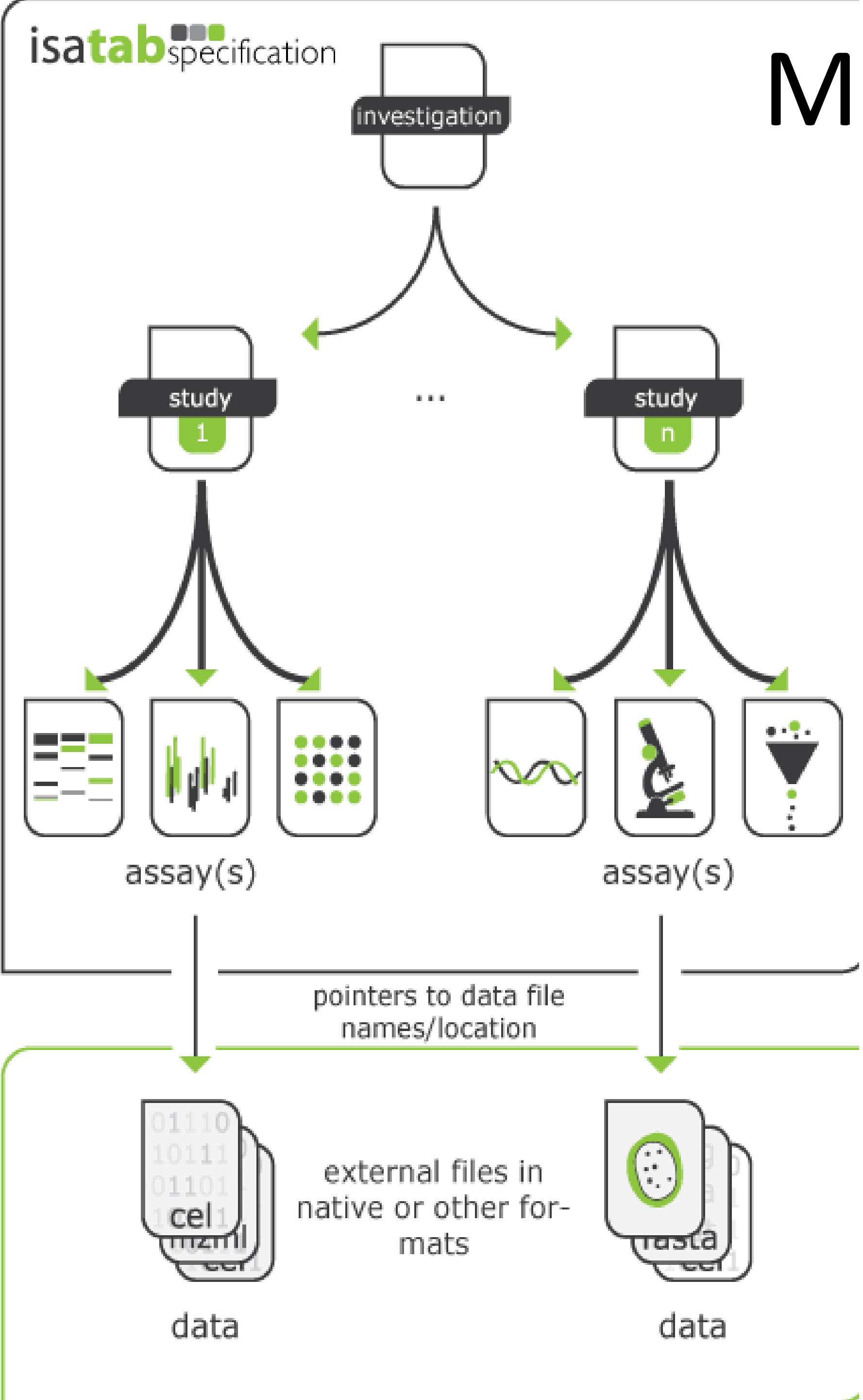
**Communication**

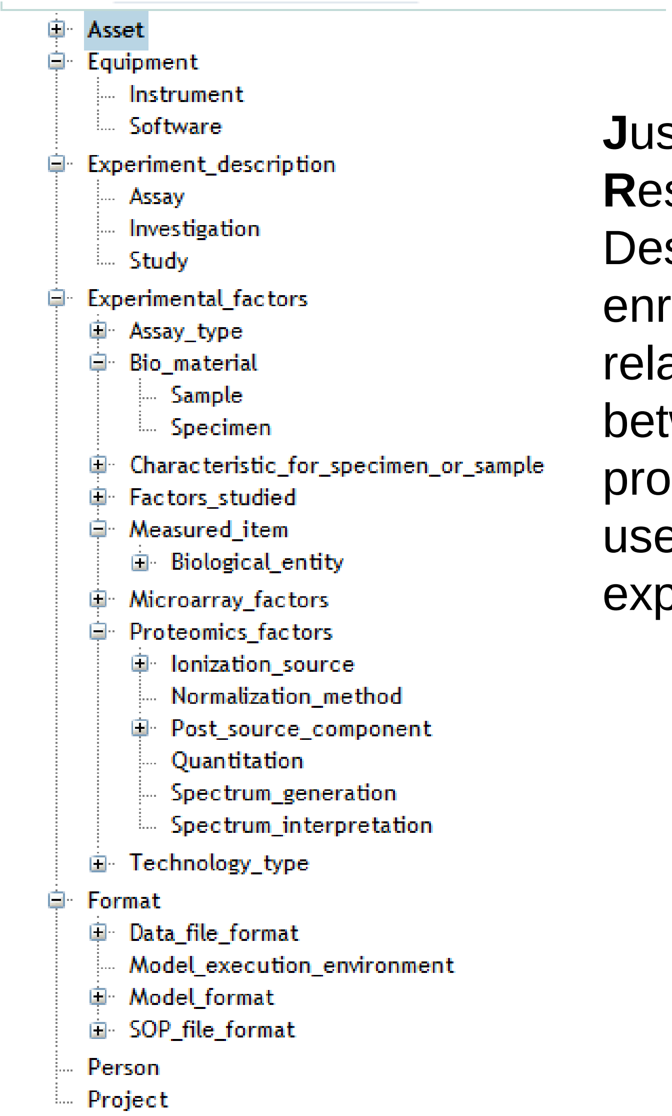
Versioning/Sharing

**Data:**
- Experimental data sets and analysed results
- Gateway to public data stores – SABIO-RK, ‘omics

**Processes**
- Standard Operating Procedures
- Computational workflows - Taverna
- Gateway to myExperiment

# Metadata standards & templates

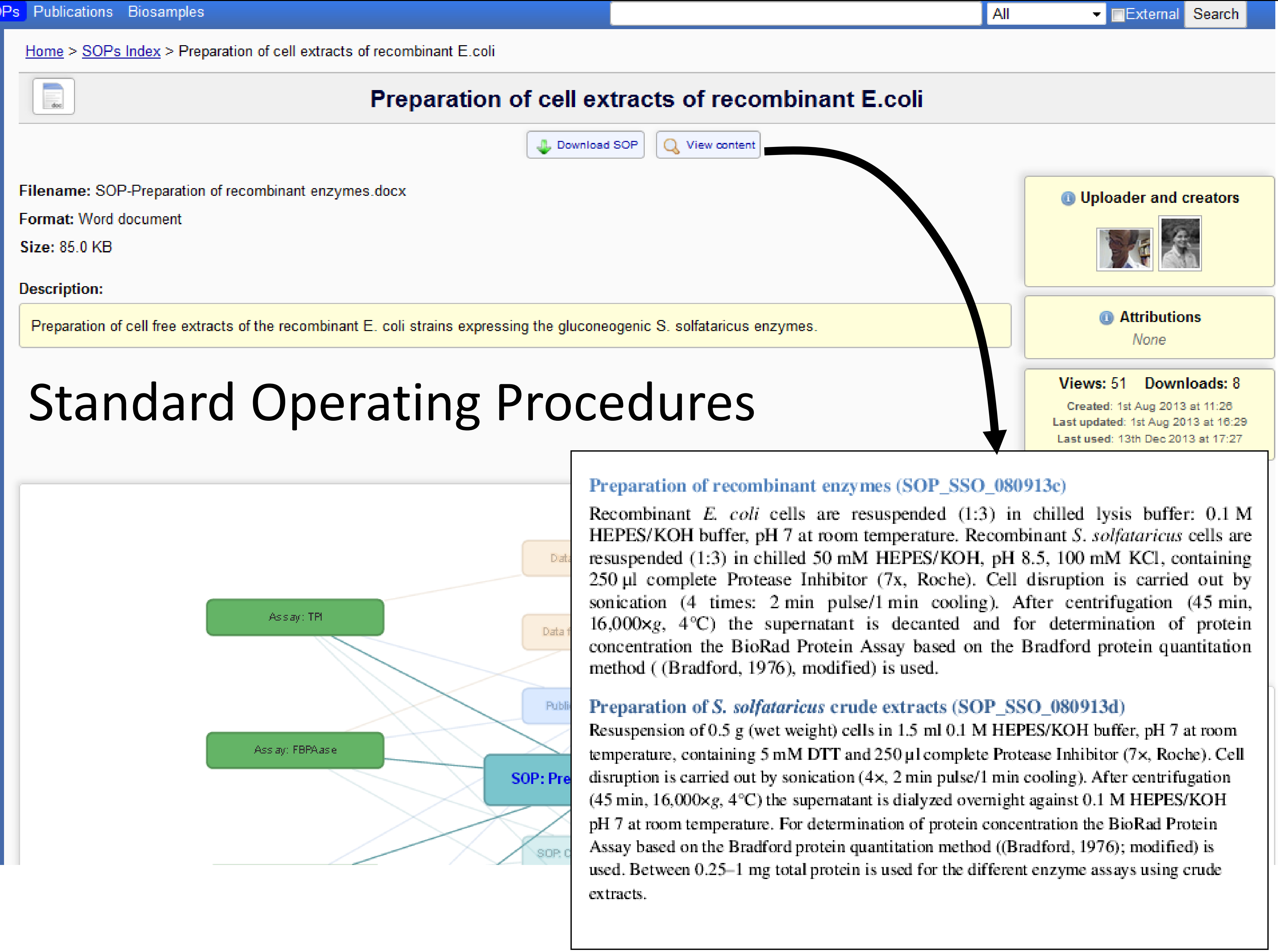




- Asset
- Equipment
  - Instrument
  - Software
- Experiment_description
  - Assay
  - Investigation
  - Study
- Experimental_factors
  - Assay_type
  - Bio_material
    - Sample
    - Specimen
  - Characteristic_for_specimen_or_sample
  - Factors_studied
  - Measured_item
    - Biological_entity
  - Microarray_factors
  - Proteomics_factors
    - Ionization_source
    - Normalization_method
    - Post_source_component
    - Quantitation
    - Spectrum_generation
    - Spectrum_interpretation
  - Technology_type
- Format
  - Data_file_format
  - Model_execution_environment
  - Model_format
  - SOP_file_format
- Person
- Project

**J**ust **E**nough **R**esults **M**odel Describes and enriches the relationships between things produced and used in experiments.

# Standard Operating Procedures



Home > SOPs Index > Preparation of cell extracts of recombinant E.coli

## Preparation of cell extracts of recombinant E.coli

**Filename:** SOP-Preparation of recombinant enzymes.docx

**Format:** Word document

**Size:** 85.0 KB

**Description:**

Preparation of cell free extracts of the recombinant E. coli strains expressing the gluconeogenic S. solfataricus enzymes.

**Uploader and creators**

**Attributions**

*None*

**Views:** 51 **Downloads:** 8

**Created:** 1st Aug 2013 at 11:26

**Last updated:** 1st Aug 2013 at 16:29

**Last used:** 13th Dec 2013 at 17:27

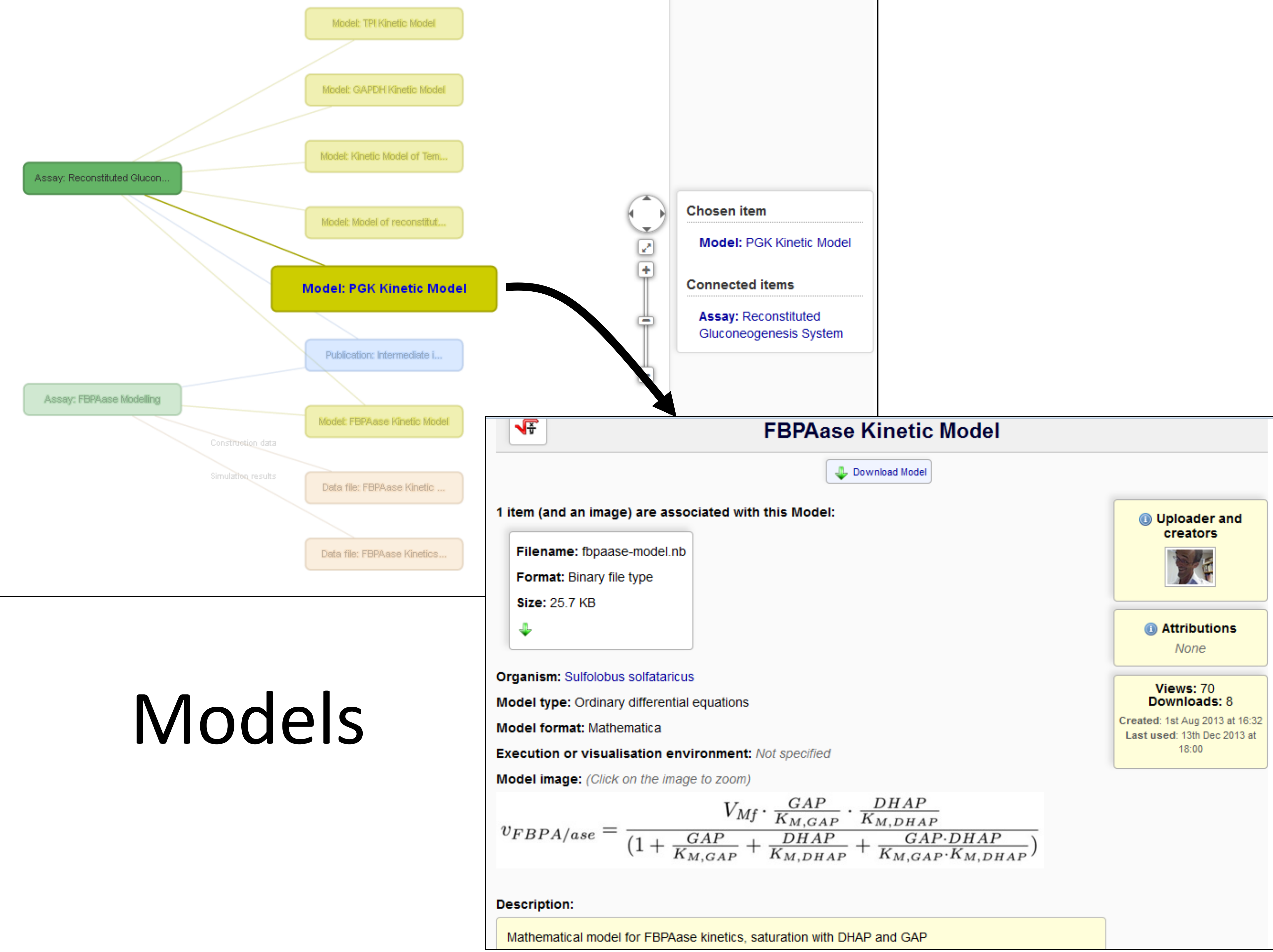
### Preparation of recombinant enzymes (SOP_SSO_080913c)

Recombinant *E. coli* cells are resuspended (1:3) in chilled lysis buffer: 0.1 M HEPES/KOH buffer, pH 7 at room temperature. Recombinant *S. solfataricus* cells are resuspended (1:3) in chilled 50 mM HEPES/KOH, pH 8.5, 100 mM KCl, containing 250 µl complete Protease Inhibitor (7x, Roche). Cell disruption is carried out by sonication (4 times: 2 min pulse/1 min cooling). After centrifugation (45 min, 16,000×*g*, 4°C) the supernatant is decanted and for determination of protein concentration the BioRad Protein Assay based on the Bradford protein quantitation method ( (Bradford, 1976), modified) is used.

### Preparation of *S. solfataricus* crude extracts (SOP_SSO_080913d)

Resuspension of 0.5 g (wet weight) cells in 1.5 ml 0.1 M HEPES/KOH buffer, pH 7 at room temperature, containing 5 mM DTT and 250 µl complete Protease Inhibitor (7×, Roche). Cell disruption is carried out by sonication (4×, 2 min pulse/1 min cooling). After centrifugation (45 min, 16,000×*g*, 4°C) the supernatant is dialyzed overnight against 0.1 M HEPES/KOH pH 7 at room temperature. For determination of protein concentration the BioRad Protein Assay based on the Bradford protein quantitation method ((Bradford, 1976); modified) is used. Between 0.25–1 mg total protein is used for the different enzyme assays using crude extracts.

# Models



**Chosen item**

**Model:** PGK Kinetic Model

**Connected items**

**Assay:** Reconstituted Gluconeogenesis System

## FBPAase Kinetic Model

**1 item (and an image) are associated with this Model:**

**Filename:** fbpaase-model.nb

**Format:** Binary file type

**Size:** 25.7 KB

**Organism:** Sulfolobus solfataricus

**Model type:** Ordinary differential equations

**Model format:** Mathematica

**Execution or visualisation environment:** *Not specified*

**Model image:** *(Click on the image to zoom)*

$$v_{FBPA/ase} = \frac{V_{Mf} \cdot \frac{GAP}{K_{M,GAP}} \cdot \frac{DHAP}{K_{M,DHAP}}}{\left(1 + \frac{GAP}{K_{M,GAP}} + \frac{DHAP}{K_{M,DHAP}} + \frac{GAP \cdot DHAP}{K_{M,GAP} \cdot K_{M,DHAP}}\right)}$$

**Description:**

Mathematical model for FBPAase kinetics, saturation with DHAP and GAP

**Uploader and creators**

**Attributions**

*None*

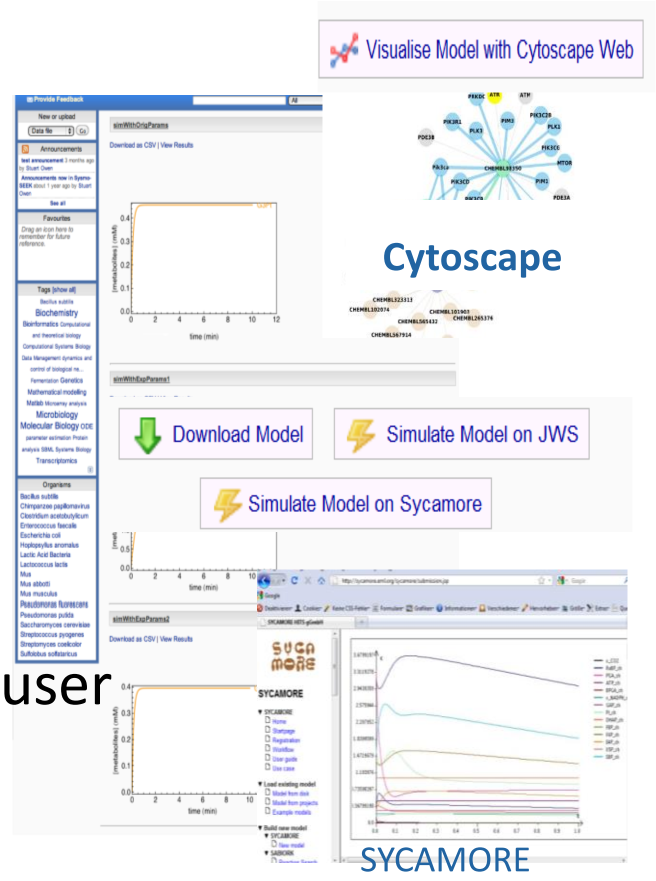
**Views:** 70
**Downloads:** 8

**Created:** 1st Aug 2013 at 16:32
**Last used:** 13th Dec 2013 at 18:00

# Models

- Model storage, model reuse and actual simulation.
- Interlinking of data used for construction/validation with models
- Versioning

- Integrated simulation
- Sycamore, Cytoscape, (COPASI, MatLab?)
- JWS Online Simulator
  - Auto generation of SBGN schemas for user models
  - SED-ML export
  - SBML support to simulate majority of BioModels

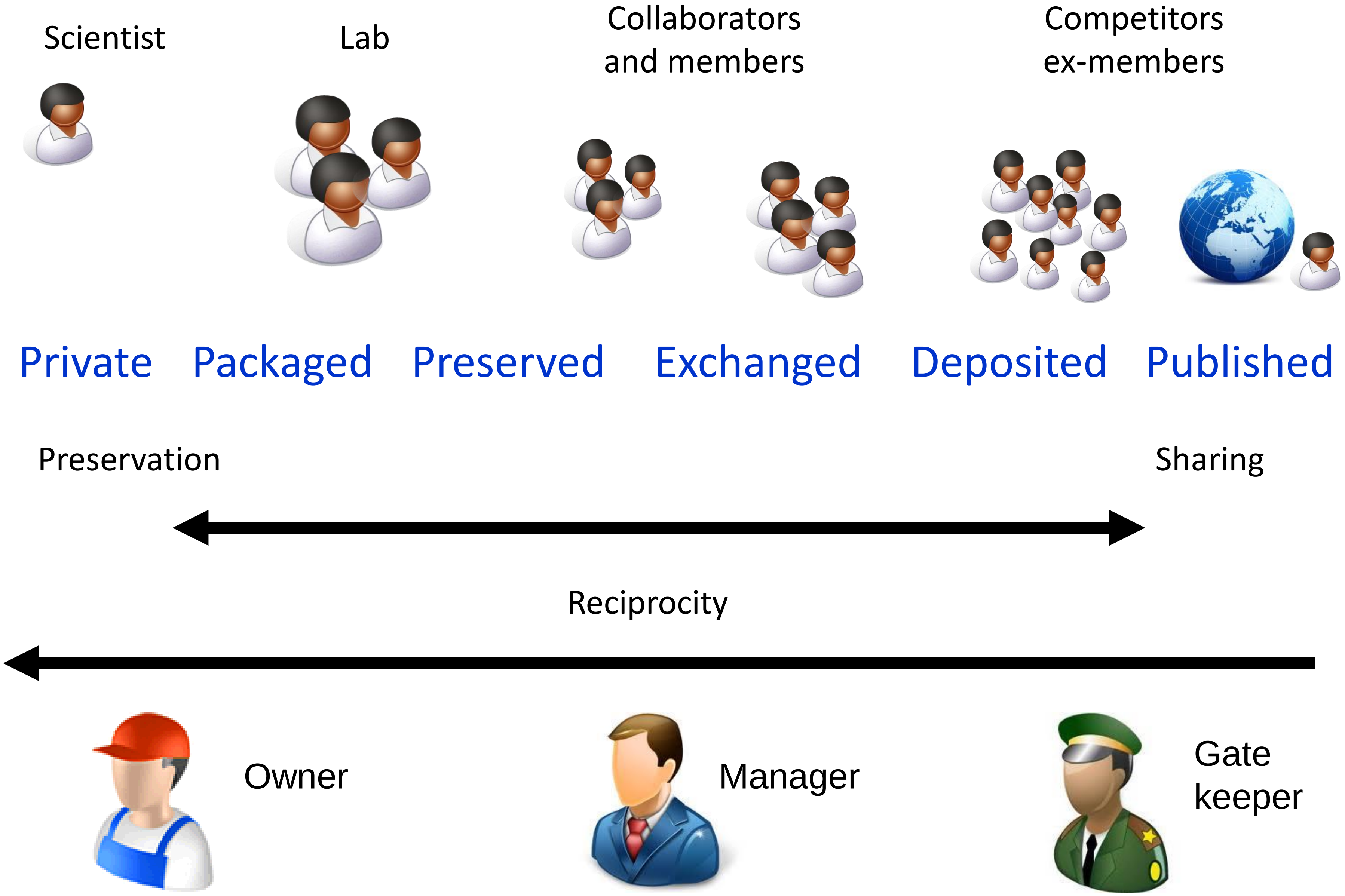


# Publication, Citing, Credit

- Publishing data in formats and with DOIs (Fixed, citeable identifier for data) suitable for inclusion in peer-review journals -> Credit & visibility
- Assistance publishing data to community repositories (GEO, PRIDE, SABIO-RK)
- Links with PubMed
- Project-managed access permissions to content
- Temp. links for peer review

# Content Sharing Creep, Self-Interest

## Blurred Boundaries



Scientist

Lab

Collaborators
and members

Competitors
ex-members

Private Packaged Preserved Exchanged Deposited Published

Preservation

Sharing

Reciprocity

Owner

Manager

Gate
keeper

Contact mail

- fairdom@fair-dom.org

Web site

- http://fair-dom.org

FAIRDOMHub

- http://fairdomhub.org/