

# PoLiMeR data management



PoLiMeR

Polymers in the Liver - Metabolism and Regulation

Olga Krebs

Heidelberg Institute for Theoretical Studies

26 November 2019, Groningen



# Project Dashboard

Period last 12 months



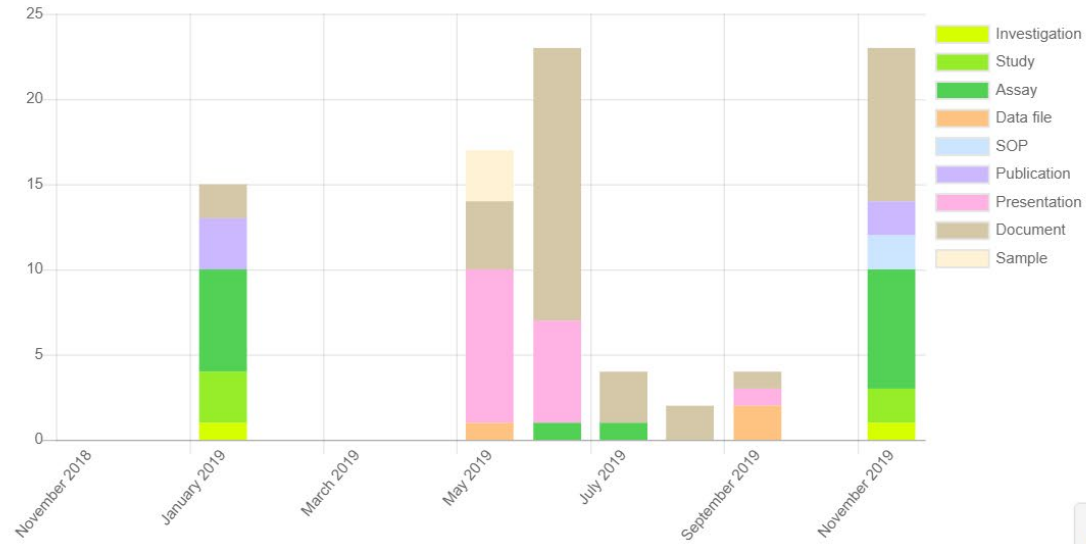
## Most viewed assets

Type All

- Hepatocytes contribute to residual glucose production... 802
- A systems study reveals concurrent activation of AMP... 761
- Translational Targeted Proteomics Profiling of Mitochondria... 731
- Python presentation by Adelaide Raguin, Friday May 3... 267
- Agenda for PoLiMeR kick-off meeting 28
- Model A 20
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- Assignments dynamic modelling 14
- Human cell cultures samples 13
- Lecture on Dynamic modelling and enzyme kinetics by ... 13

## Contributions

Interval Month



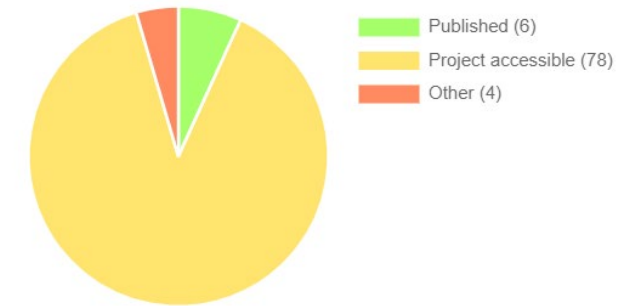
Mouse over a bar to see the breakdown of contributions for that month. Clicking on a type in the legend will hide it from the chart.

## Most active contributors

	Olga Krebs	81
	Karen Van Eunen	35
	Barbara Bakker	12
	Adelaide Raguin	6
	Oliver Ebenhöf	2
	Wolfgang Müller	1
	Maike H. Oosterveer	1

## Asset accessibility

Type All



## Related items

People (31)

Institutions (15)

Investigations (2)

Studies (5)

Assays (15)

Data files (3)

SOPs (2)

Publications (5)

Presentations (16)

Events (5)

Documents (37)

# PoLiMeR : Data Management Plan



Polymers in the Liver – Metabolism and Regulation  
GA N° 812616  
Start Date: 01/10/2018 – Duration: 48 months  
Coordinator: B.M. Bakker, UMCG

## D6.3 – “Data and model management plan(DMP)”

### WP6 – Data and model management

<b>Author (s):</b>	<b>Olga Krebs (HITS), Karen van Eunen (UMCG)</b>
<b>Reviewer(s):</b>	Barbara Bakker (UMCG)
<b>Identifier:</b>	D6.3_HITS_v1
<b>Dissemination level:</b>	CO
<b>Date:</b>	20190926
<b>Number of pages:</b>	17



# PhD at HITS Ghadir Mobasher



B.Sc. In Software Engineering of Computer and Information Sciences  
Master in Computer and Information at the British University in Egypt.  
Assistant lecturer and a Faculty of Informatics & Computer Science,  
The British University in Egypt in Cairo

- I am an enthusiastic, adaptive and fast learning person with a broad and acute interest in the discovery of new data mining and deep learning techniques
- I particularly enjoy collaborating with scientist from different disciplines to develop new skills and solve new challenges
- I have professional experience in the field of Data Science, technical expertise and collaboration skills needed to solve advanced problems related to Data Mining
- I use algorithmic approaches to solve the class imbalance problem generating the smallest most accurate decision tree.



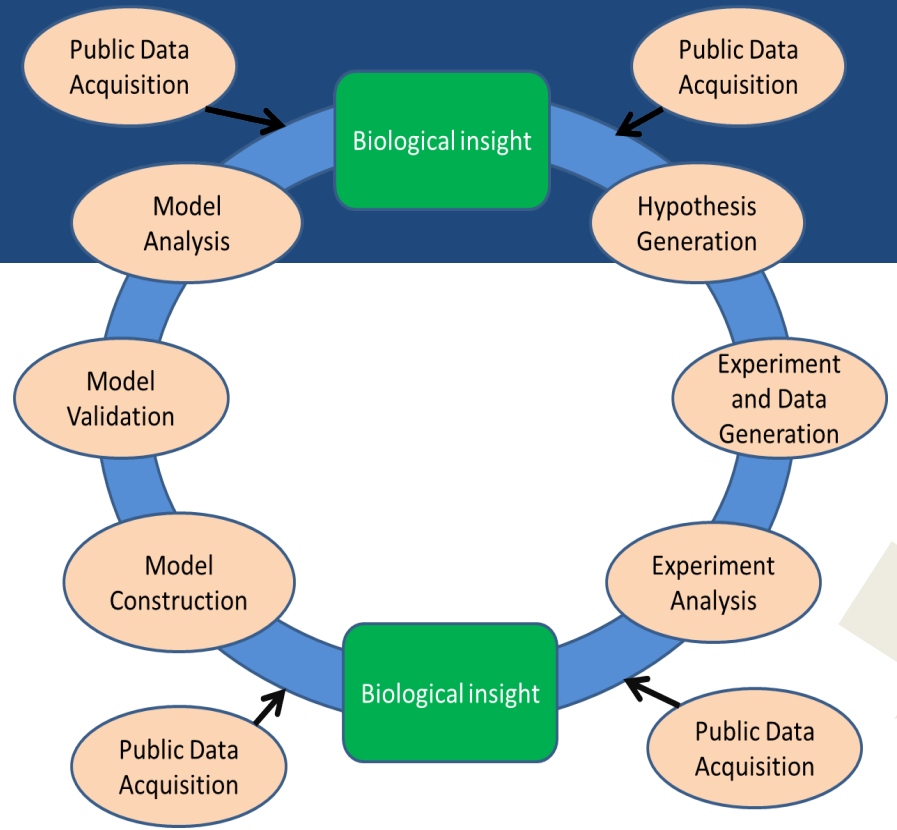
# PhD student 2 : Data and model management and information retrieval



- The PhD student will provide FAIR data management services to the PoLiMeR consortium based on the FAIRDOM Hub (the data sharing site hosted at HITS) and on GitLab.
- The PhD student will use the database generated in the PoLiMeR project together with pre-existing and public data in the to determine how changes in data collection, metadata quality and data feature extraction affect the information that can be found.
- The PhD student will seek to improve existing tools for data collection as well as querying at critical points.
- finding out how to tailor information retrieval and information storage algorithms such that they work best in combination?
- finding out the best combination of data enrichment/search algorithm in real life, in an exciting application area: The life sciences.



# Systems Biology



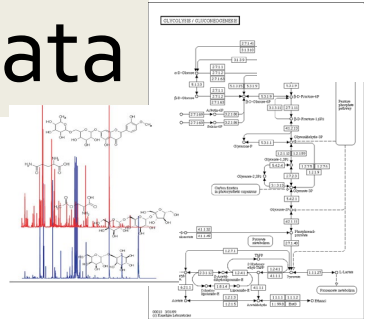
**SOPs**  
Not just experimental procedures

**Samples**

**Models**

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

**Data**



**Publications**

**IFBES**  
**Construction and validation of a detailed kinetic model of glycolysis in *Phanerochaete chrysosporium***  
Gang Li, Guohua Chen, and David A. Bruns

**Abstract**  
The kinetics in the Embden-Meyerhof-Parnas pathway of *Phanerochaete chrysosporium* were investigated and a detailed kinetic model was constructed. The model was validated by comparing the model results with experimental data. The model was used to study the effect of pH on the glycolysis rate and the effect of the inhibitor on the glycolysis rate. The model was used to study the effect of the inhibitor on the glycolysis rate. The model was used to study the effect of the inhibitor on the glycolysis rate.



# ....organised in an ISA (Investigation, Study, Assay/Analysis) format.



Browse ▾

- Yellow pages
- Programmes
- Projects
- Institutions
- People
- Experiments
- Investigations
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- Organisms

Browse ▾ Help ▾ Search here... Search

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Home / Investigations Index / Glucose metabolism in Plasmodium falciparum trophozoites

## Glucose metabolism in Plasmodium falciparum trophozoites

The investigation entails the construction and validation of a detailed mathematical model for glycolysis of the malaria parasite Plasmodium falciparum in the blood stage trophozoite form.

ID:56  
Projects: Whole body modelling of glucose metabolism in malaria patients

Selected item: Investigation: Glucose metabolism in Plasmodium falciparum trophozoites Full graph

### Study

Study Model construction

Study Model validation

Study Model analysis

Publication: Construction and validation of a detailed kinetic model of glycolysis in Plasmod...

### Related Items

People (1) Projects (1) Studies (3) Assays (24) Data files (16) Models (19) SOPs (13) Publications (1)

David Van Niekirk

Projects: SysMO DB, Whole body modelling of glucose metabolism in malaria patients

Institutions: University of Stellenbosch

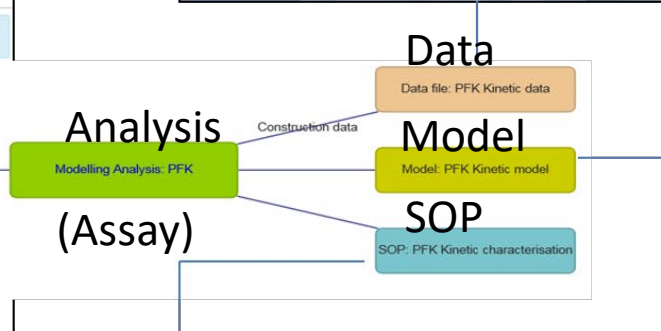
Disciplines: Mooster

Roles: Not specified

Expertise: Not specified

Tools: Not specified

Metadata		Values (example)			
Assay Title	PFK Kinetic Data				
Clipboard	Cheney van Niekirk				
Clipboard SEEK ID					
Project					
<b>Assay</b>					
Assay SEEK ID	0				
Assay Title	PFK				
Assay Type	microarrayAssay				
Technique_Type	metabolic experiment				
Description	Kinetic characterisation of PFK, Enzym				
ExperimentDate	Ceraid Pradhan				
Date					
SOP					
Publication (optional)					
<b>Experimental conditions</b>					
Temperature (of concentration)	temperature	pH	buffer	buffer	buffer
Component (of concentration)	ATP	HEPES	KCl	NaCl	
Unit	mM	mM	mM	mM	mM
Start_value (optional)	10	7.17	20	20	20
End_value (optional)					
Comments					
Other growth	Batch				
<b>FACTORS_PLUNED</b>					
Name	concentration	concentration	concentration	concentration	
Component (of concentration)	ATP	ATP	ATP	ATP	
Unit	mM	mM	mM	mM	
Start_value (optional)	0.21473	0	0	0	
End_value (optional)	10	5	5	60	
SD (optional)					



**REXSOP**

Specific activity of the glycolytic enzymes were measured in NADPH(NADP)<sup>+</sup> linked enzyme assays that were adapted from Tsai et al. [1] and measured at 350 nm in 96-well plates (Flat Bottom microplate, Greiner Bio-One, Kremsmünster, Austria) on a spectrophotometer (Biochrom, microplate reader, Thermo Electron Corporation, Waltham, Massachusetts, USA). The same buffer, (20 mM HEPES, 20 mM MgCl<sub>2</sub>, 10 mM KCl and 10 mM NaCl) was used for all assays, with a pH set to 7.17, matching the cytosolic pH of *P. falciparum* D10 [2]. All of the linking enzymes were used at a non-limiting, final concentration of 5 U/ml. All reagents and enzymes were obtained from Sigma-Aldrich, St. Louis, Missouri, USA.

For phosphofruktokinase (PFK) activity, the phosphorylation of F6P (0-30 mM) by ATP (0-5 mM) as well as inhibition by ADP (0-5 mM) was linked to the oxidation of NADPH (0.8 mM) via  $\alpha$ -ketoglutarate, TPi. Product inhibition by F16BP (0-60 mM) was assayed by linking the production of ADP to the oxidation of NADPH (0.8 mM) via LDH. PK in the presence of PFK (2 mM). Since PFK exhibited substrate inhibition, the enzyme rates could not be normalised to maximal specific activity at saturating substrate concentrations. A control rate was determined at 1.25 mM ATP and 1 mM F6P.

[1] Tsaiak B, Passarge J, Rejzinger C, Esgehadad E, van der Weijden C, et al. (2003) Can yeast glycolysis be understood in terms of its stoichiometry of the constituent enzymes? testing biochemistry. Eur J Biochem 267: 333-339.

[2] Wünsch S, Sanchez C, Gekle M, Gosse-Wortmann L, Wiesner J, et al. (1998) Differential stimulation of the Na<sup>+</sup>/H<sup>+</sup> exchanger determines chromosome uptake in Plasmodium falciparum. J Cell Biol 140: 335-345.

### PFK Kinetic model

Mathematica notebook for the parameterisation of the PFK rate equation based on SEEK ID

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

- PFK-SEEK ID Mathematics Notebook - 382 KB

Organism: Not specified

Model type: Ordinary differential equations

Model format: Mathematica

Execution or visualisation environment: Not specified

Model image: [Click on the image to zoom](#)

$$v_{PFK} = \frac{V_{PFK} \cdot \frac{atp}{K_{ATP}} \cdot \frac{f6p}{K_{F6P}}}{(1 + \frac{atp}{K_{ATP}}) \cdot (1 + \frac{f16bp}{K_{F16BP}}) \cdot (1 + \frac{atp}{K_{ATP}} + \frac{atp}{K_{ADP}})}$$

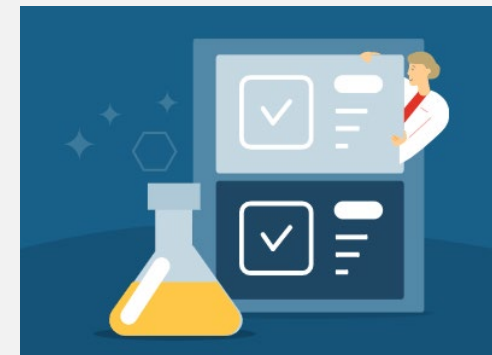
Selected item: Model: PFK Kinetic model



# Why SOPs



- Sharing experimental protocols
- Agreement within projects on strains and conditions
- Good scientific practice
- Understanding data, experiments and results for verification or for modifying for use in other experiments





# SOPs in SEEK

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



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

[Download SOP](#)

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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

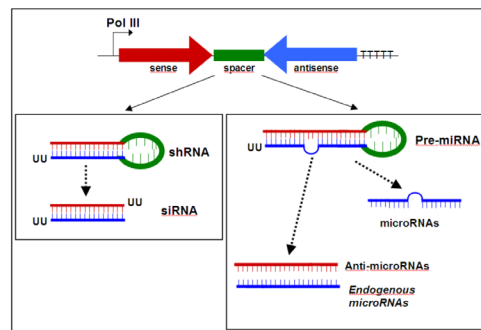
None

### Scales

Not Specified

**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)

miRZip™ Lentivector-based Anti-microRNAs (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  $3,5 \cdot 10^5$  cells/per 1 T175 flask in 30 ml of medium with components and G148 to achieve optimal phase of cellular growth.

# SOPs

 SOP for generating a Genome Scale Metabolic model of *M. hyopneumoniae*

MycoSynVac - Engineering *Mycoplasma pneumoniae* as a broad-spectrum animal vaccine



Standard Operating Procedure describing the process and software used in generating a Genome Scale Metabolic model of *M. hyopneumoniae*.

 Download

Used software:

Pathway tools

PathLogic

Cobrapy

the Cobra Toolbox

libSBML

**Creator:** [Niels Zondervan](#)

**Contributor:** [Niels Zondervan](#)

**Investigations:** [Modelling of \*M. pneumoniae\* metabolism](#)

**Studies:** [Genome-scale, constraint-based metabolic modeli...](#)

**Assays:** [Construction of a Genome Scale Metabolic mode...](#)

 DNA, RNA, Protein extraction from mineral samples

SysMetEx

SOP for extracting DNA, RNA and Proteins from the mineral pellet of a bioleaching culture using hot acidic phenol.

Current draft.

 Download

**Creators:** [Malte Herold](#), [Mario Vera](#), [Soeren Bellenberg](#)

**Contributor:** [Malte Herold](#)

**DOI:** [10.15490/fairdomhub.1.sop.249.2](https://doi.org/10.15490/fairdomhub.1.sop.249.2) 

**Investigations:** *1 hidden item*

**Studies:** *1 hidden item*

**Assays:** *2 hidden items*



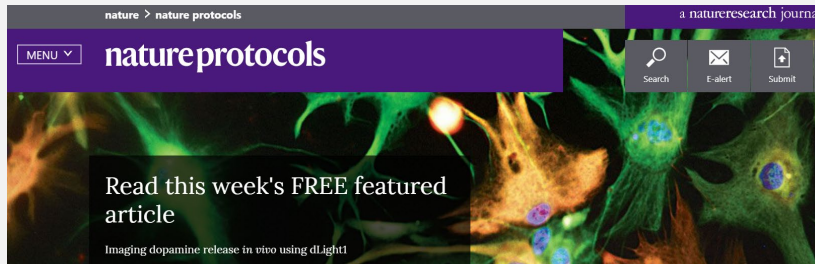
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All)

# Public Repositories



- Nature Protocols – published SOPs with links to publications – defined format
- Cold Spring Harbour Protocols – proprietary published SOPs – defined format
- Open Wetware – public access, no recommended format



protocolexchange | nature research

Protocol Exchange is an open repository of community-contributed protocols sponsored by Nature Research.



# Your Own SOPs



- Where are they now?
  - Wikis
  - Hard disks
  - Lab computers
  - Lab books
- FAIRDOM Hub
- Document store
- Indexed SOPs





# Standard Operating Procedures writing instructions



PoLiMeR

Polymers in the Liver - Metabolism and Regulation



# Nature protocol format (suggested)



**Protocol Title**

**Authors**

**Keywords**

**Abstract**

**Materials**

**Reagents**

**Reagent Set Up**

**Equipment**

**Time Taken**

**Procedure**

**Troubleshooting/ Critical Steps**

**Anticipated Results**

**References**





## Author checklist

- ✓ provide a list of keywords that can be used as search terms.
- ✓ indicate the corresponding author(s) and provide email address
- ✓ SOP version number, date of creation

## Abstract

- ✓ start by introducing the methods used in the protocol, including references to papers that catalogue their development and previous use.
- ✓ provide (all) information about the design of experiments that readers would need to adapt the protocol to apply to their own experimental situation.
- ✓ SOP for e.g. microarray experiments should adhere to the standards outlined in the MIAME guidelines . Please ensure relevant aspects are described in the Experimental Design and Procedure sections.
- ✓ include a sentence to explain how long the protocol takes to complete.





## Materials

- ✓ list reagents and pieces of equipment individually , (with supplier details and catalogue numbers?)
- ✓ indicate whether item should be made up fresh or can be stored and, if so, under which conditions and for how long.
- ✓ 13. **UNITS!!!** e.g. for % unit, state whether this is wt/vol or vol/vol, add a CAUTION note to any potentially harmful items and explain the danger plus precautions that should be taken when handling them.
- ✓ add a CAUTION note to any potentially harmful items and explain the danger plus precautions that should be taken when handling them.

## Procedure

- ✓ procedure can take the form of a continuously numbered set of steps (i.e. use 1, 2, 3, 4; not 1.1, 1.2 etc.), with numbering continuing from subsection to subsection.
- ✓ If there are any additional procedures that do not fit into the continuous flow of numbered steps, these can be referred (as e.g. web resource or another SOP in e.g. FAIRDOMHub)
- write the procedure steps in the active tense, e.g, “Add 50ml of solution X.”
- add timing information to all steps







include a **Troubleshooting** section. This should preferably take the form of a table with four columns, entitled 'Step', 'Problem', 'Possible reason' and 'Possible solution'.





## Anticipated results

- ✓ demonstrate the types of results that can be expected from the protocol and explain how they can be interpreted. Figures showing examples of good or poor quality results can also be referred to from this section.
- ✓ ensure data is fully explained (n values given, error bars defined, etc.). Graphs showing individual data points are often preferable to those showing means and error bars. If there are fewer than 6 data points, individual data points must be provided. Please ensure any statistics are applied appropriately

(**Know when your numbers are significant** <http://www.nature.com/nature/journal/v492/n7428/full/492180a.html>).

## Figures/Tables/Boxes

- | Figures/Tables/Boxes must be cited in the main text and should be numbered in the order in which the citations appear in the text.
- submit figures individually in one of our accepted file formats (preferably eps or tif).
- provide a title and figure legend for each figure. Individual panels cannot be cited from the title. Figures legends should fully explain the corresponding figure. Please include legends in the main manuscript.

## References

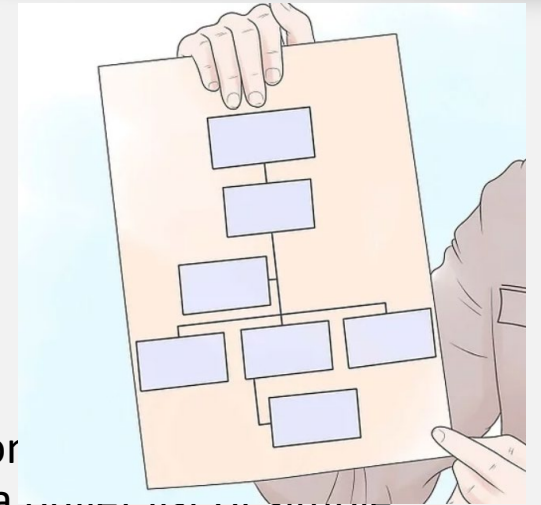


# Choose your format



There is no right or wrong way to write an SOP.  
Use the existing SOPs as a template.  
If not, you have a few options:

- A simple steps format. This is for routine procedures that are short, have few possible outcomes to the point. Apart from the necessary documentation and safety guidelines, it's really just a bullet list of simple sentences telling the reader what to do.
- A hierarchical steps format. This is usually for long procedures -- ones with more than ten steps, involving a few decisions to make, clarification and terminology. This is usually a list of main steps all with substeps in a very particular order.
- A flowchart format. If the procedure is more like a map with an almost infinite number of possible outcomes, a flowchart may be your best bet. This is the format you should opt for when results aren't always predictable



# Summary of useful rules



For the procedure itself, make sure you cover the following:

- Scope and applicability. In other words, describe the purpose of the process, its limits, and how it's used. Include standards, regulatory requirements, roles and responsibilities, and inputs and outputs.
- Methodology and procedures. The meat of the issue -- list all the steps with necessary details, including what equipment needed. Cover sequential procedures and decision factors. Address the "what ifs" and the possible interferences or safety considerations.
- Clarification of terminology. Identify acronyms, abbreviations, and all phrases that aren't in common parlance.
- Health and safety warnings. To be listed in its own section and alongside the steps where it is an issue. Do not gloss over this section.
- Equipment and supplies. Complete list of what is needed and when, where to find equipment, standards of equipment, etc.
- Cautions and interferences. Basically, a troubleshooting section. Cover what could go wrong, what to look out for, and what may interfere with the final, ideal product.
- Give each of these topics their own section (usually denoted by numbers or letters) to keep your SOP from being wordy and confusing and to allow for easy reference.
- This is by no means an exhaustive list; this is just the tip of the procedural iceberg. Your organization may specify other aspects that require attention.



## ... more useful rules



- **Make your writing concise and easy to read.** Odds are your audience isn't choosing to read this for fun. You want to keep it short and clear -- otherwise their attention will stray or they'll find the document formidable and hard to grasp. In general, keep your sentences as short as possible.

**Here's a bad example:** Make sure that you clean out all of the dust from the air shafts before you begin using them.

**Here's a good example:** Vacuum all dust from air shafts before use.

- **Break up large chunks of text with diagrams and flowcharts.** If you have a step or two that are particularly intimidating, make it easy on your readers with some sort of chart or diagram. It makes it easier to read and gives the mind a brief hiatus from trying to make sense of it all.
- In general, don't use "you." It should be implied. Speak in the active voice and start your sentences with command verbs.





# Upload to FAIRDOMEHub and share

## New SOP

### Upload

You can register a SOP by either directly uploading a file, or registering a URL to either another page or remote file. Please test the URL before submitting.

Local file

[Remote URL](#)

#### File to upload \*

Choose File

No file chosen

#### Title \*

Example of published SOP "Enzymatic in vitro test for the quantitative determination of glycogen"

#### Description

Enzymatic in vitro test for the quantitative determination of glycogen.  
Glycogen is a branched glucose polymer, in  $\alpha$ -1,4 linkage, with branching via  $\alpha$ -1,6 linkage. It is stored primarily in the liver, kidney and muscle cells, and forms an energy reserve that can be quickly mobilized to meet a sudden need for glucose. In this assay glycogen content is determined by using amyloglucosidase treatment and a glucose assay .

### Experimental assays and Modelling analyses ▾

The following Experimental assays and Modelling analyses are associated with this SOP:

SOPs collection for metabolomics data ✖

You may select an existing editable Experimental assay or Modelling analysis to associate with this SOP.

Select Experimental assay or Modelling analysis ... ▾

