CIMR: *In vivo* Context

Metabolomics Standards Initiative (MSI)

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Authors: Clare Daykin, Nottingham, UK <clare.daykin@nottingham.ac.uk>
Jules Griffin, Cambridge, UK <jlg40@mole.bio.cam.ac.uk>
Sarah Heald, Bayer, USA <sarah.heald.b@bayer.com>
Hector Keun, Imperial College London, UK <h.keun@imperial.ac.uk>
Andrew Nicholls, GSK, UK <andrew.w.nicholls@gsk.com>
Don Robertson, Pfzier, UK <Donald.Robertson@pfizer.com>
Ina Shuppe, Astra Zeneca, Sweden <ina.schuppe-koistinen@astrazeneca.com>
John Griffiths, St. George's Hospital, London, UK <sgbc100@sghms.ac.uk>
Leo Cheng, Harvard Medical School & MGH, Boston, USA <cheng@nmr.mgh.harvard.edu>
Philippe Rocca-Serra, European Bioinformatics Institute <rocca@ebi.ac.uk>
Edited by Nigel Hardy

Credits: *Chair*: Jules Griffin

Table of Contents

1. This document

This document forms part of the the standards for reporting metabolomics experiments developed under the Metabolomics Society (http://www.metabolomicssociety.org/ Metabolomics Standards Initiative (MSI). It should be read in the context of top level document for those standards ??? .

The current version of the document is work in progress. ???.

2. Required information

All information is required unless marked *thus*[†] in which case it is recommended further information.

3. Standards for Mammalian Functional Genomic

and Toxicology Studies

Sources:

- SOPs from Pfizer, Bayer HealthCare and GlaxoSmithKline.
- [1],[2],[3],[4]

3.1. Experimental Subject Description

Species/Strain Designation	For rat/mouse http://www.informatics.jax.org/mgihome/nomen/strains.shtml
Generation of mixed strain†	
Model Description	Other species ? (if different than Species/Strain.) surgical/pharmacological/feeding manipulation
Animal Supplier	Company/location/*colony designation*†/*wild caught*†
Age range (*DOBs*†)	as well as age at time of experiment
Weight range	(*individual weights*†)

3.2. Husbandry

3.2.1. Housing

group or individual	
Cage type†	(shoe box/metabolic/wire mesh, etc)
Cage change/cleaning frequency†	
Environmental enrichment†	

3.2.2. Light Cycle

3.2.3. Feed

Type/manufacturer	(or reference to composition if custom diet)
ad lib or restricted	(e.g. 25 g/day)
Diet supplements†	("treats") if any (what treats/how often/how much)

3.2.4. Water

Bottle or automated	
Tap or purified	*(qualified - e.g. distilled, 18 MΩ, etc*†*)*

3.2.5. *Veterinary treatments if any and exercise regimen (large animals)*†

3.2.6. *Use of anesthesia (e.g. for blood collection or physicals)*†

Type of anesthetic†	/formulation/ time of administration/dose of anesthetic

3.2.7. *Acclimation*†

Acclimation duration†	to experimental facility
Acclimation duration†	to diet (if experimental diet differs).
Acclimation duration†	to metabolic cages (if used).
Acclimation duration†	to repeat procedures

3.3. Experimental Design

3.3.1. Number of groups

animals/sex/group

3.3.2. *Inclusion criteria*†

(e.g. physical exams or normal metabolomic model screen)

3.3.3. Treatments

Compound
Route
Dose
Dose volume
Duration of dosing
Vehicle

3.3.4. Fasting

(when relative to metabonomic sample collection and *duration of fast in hours*†)

3.3.5. End Points

Euthanasia method
Tissue collection list
Tissue processing method (e.g snap freezing)

Clinical signs (*time of observation relative to dose*†)
Body weights/food consumption† (*how often measured*)
Blood chemistries, hematology, histopathology, special assays

3.4. Metabolomics-related Sample Collection

3.4.1. Blood

Volume collected
Location of collection
Time of collection relative to dose and *light cycle*†
Serum or plasma (anticoagulant or presence of serum separator)

3.4.2. Urine

How collected (metabolic cage, cystocentesis, catheterization)
Frequency of collection
Duration of collection
Time of collection (if less than 24 hrs) relative to dose and light cycle
Bacteriostatic agent or any other additive (final concentration)
Urine volume† (for 24 hour collections)
Temperature of urine collection tube† (on ice or room temp?)

3.4.3. Tissues

Identification
Approximate quantity taken
Tissue processing method (e.g snap freezing, time from kill to snap freezing)

4. Standards for Mammalian Clinical Trials and Human Studies

Sources:

- SOPs from Pfzier, Bayer HealthCare and GlaxoSmithKline.
- [5], [6], [7], [8], [9], [10]
- Orla Teahan, Simon Gamble, Elaine Holmes, Jonathan Waxman, Jeremy K. Nicholson, Charlotte Bevan, and Hector C. Keun. Impact of Analytical Bias in Metabonomic Studies of Human Blood Serum and Plasma. *Anal Chem* (in press).

4.1. Experimental Subject Description

Was ethical approval sought?	
Geographical	location/hospital/ethnic background (based on FDA and Office of National statistics criteria)
Medical History	(disease or clinical symptoms; criteria for disease presence (all volunteers should not have factors in their medical history which confound the study). e.g. surgical or pharmacological manipulation, medication (may be referenced)
Age range	
Weight range and Height	and/or BMI
Gender	
Trial type	(e.g. randomized trail? Disease biomarker, Phase I-IV?)
Dietary restrictions	(if applicable) and relevant control groups for such dietary restrictions.
Further descriptors	*Smoking, blood pressure, anomalies in habitual diet (e.g. vegetarian, vegan etc), habitual alcohol consumption*[†]

4.2. Experimental Design

4.2.1. Number of groups

subjects/gender/group

4.2.2. Inclusion criteria

4.2.3. Exclusion criteria

4.2.4. Treatments/Fasting

Compound
Route
Dose
Dose volume
Duration of dosing
Vehicle

4.2.5. End Points

Clinical chemistries, blood chemistry and haematology[†]	(Urea, creatinine, glucose, total cholesterol, HDL-cholesterol, LDL-cholesterol, triglycerides, total protein, albumin, erythrocyte count, hemoglobin, hemocrit, platelets, white blood count, sodium, potassium, bilirubin, ALT, ALP, -GT.)

Urine chemistry[†]	(osmolality, ketones, pH, protein, glucose, bilirubin, blood, sediment and colour)

4.3. Metabolomics-related Sample Collection

4.3.1. Blood

Volume collected.	
Location of collection.	
Serum or plasma	(anticoagulant); *(Separation: if serum, time allowed for clotting and temperature, for plasma and serum temperature of centrifugation, time and speed of centrifugation)*[†]
Arterial or venous blood collected[†]	
Observations of haemolysis[†]	in samples and reporting of whether samples were used in subsequent analysis

Time from separation to freezing/freezing process.[†]

4.3.2. Urine

Frequency of collection	
Duration of collection	
Bacteriostatic agent	or any other additive (final concentration)/*mid flow?*[†]

4.3.3. Tissues

Identification	
Approximate quantity taken	
post mortem tissues	(hours after death, storage conditions)

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