



# The nutritional phenotype database A real data structure for systems biology

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A paper based on this presentation will soon be published in Genes and Nutrition: <http://dx.doi.org/10.1007/s12263-010-0190-x>

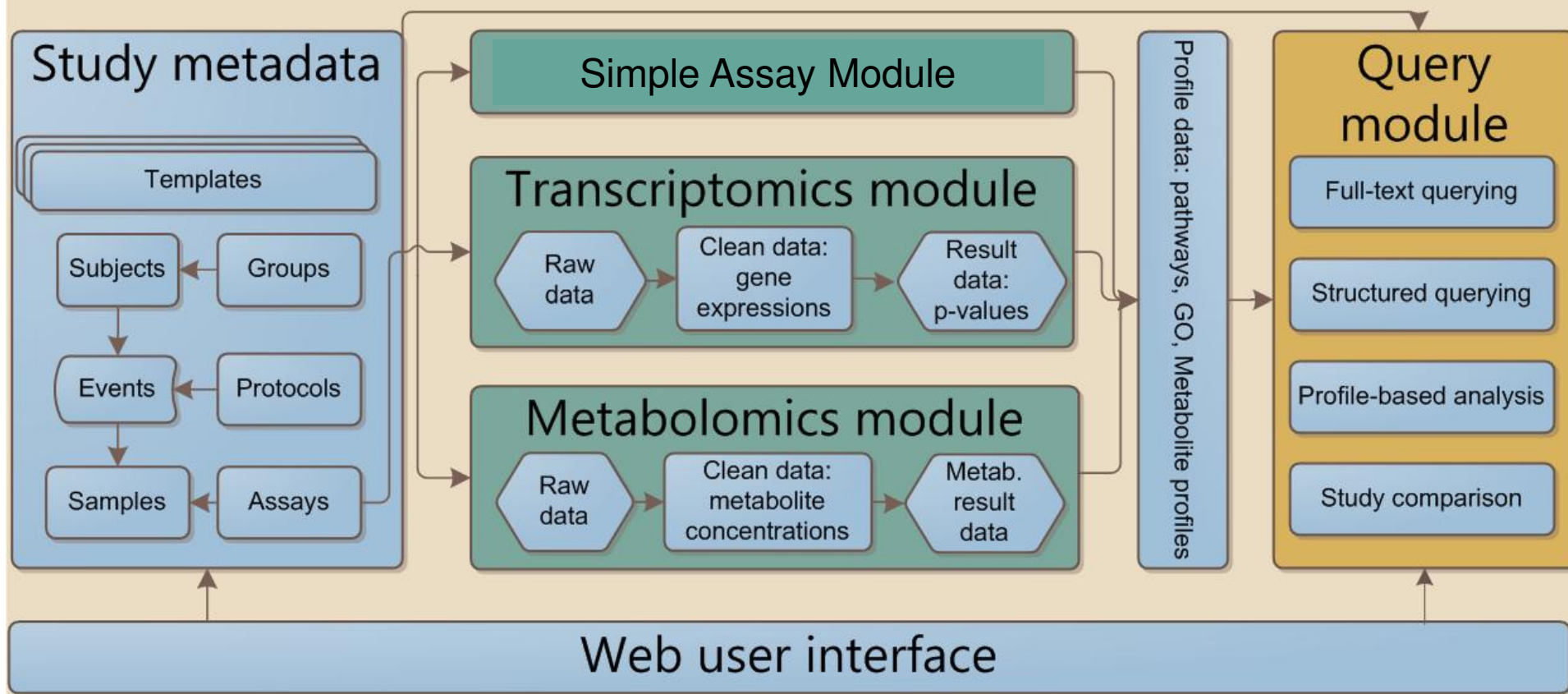


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the European Nutrigenomics Organisation

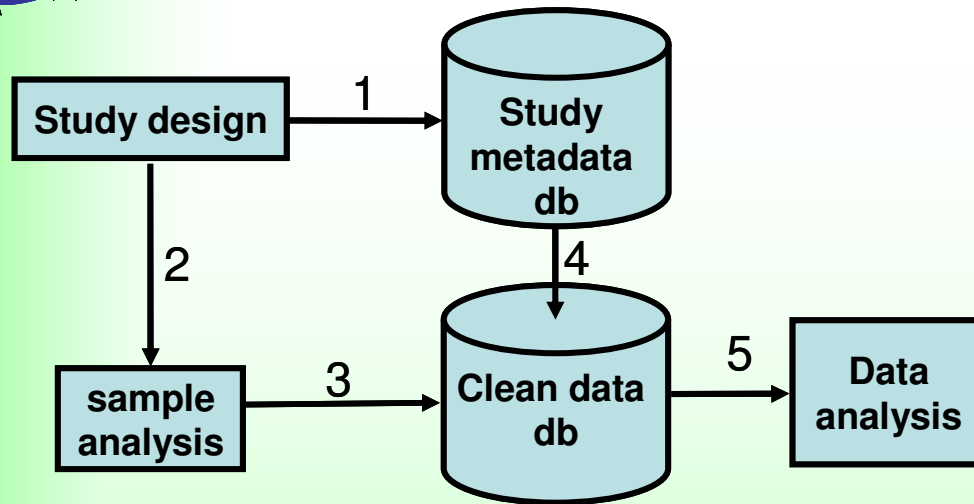


# DbNP architecture





# The basic structure

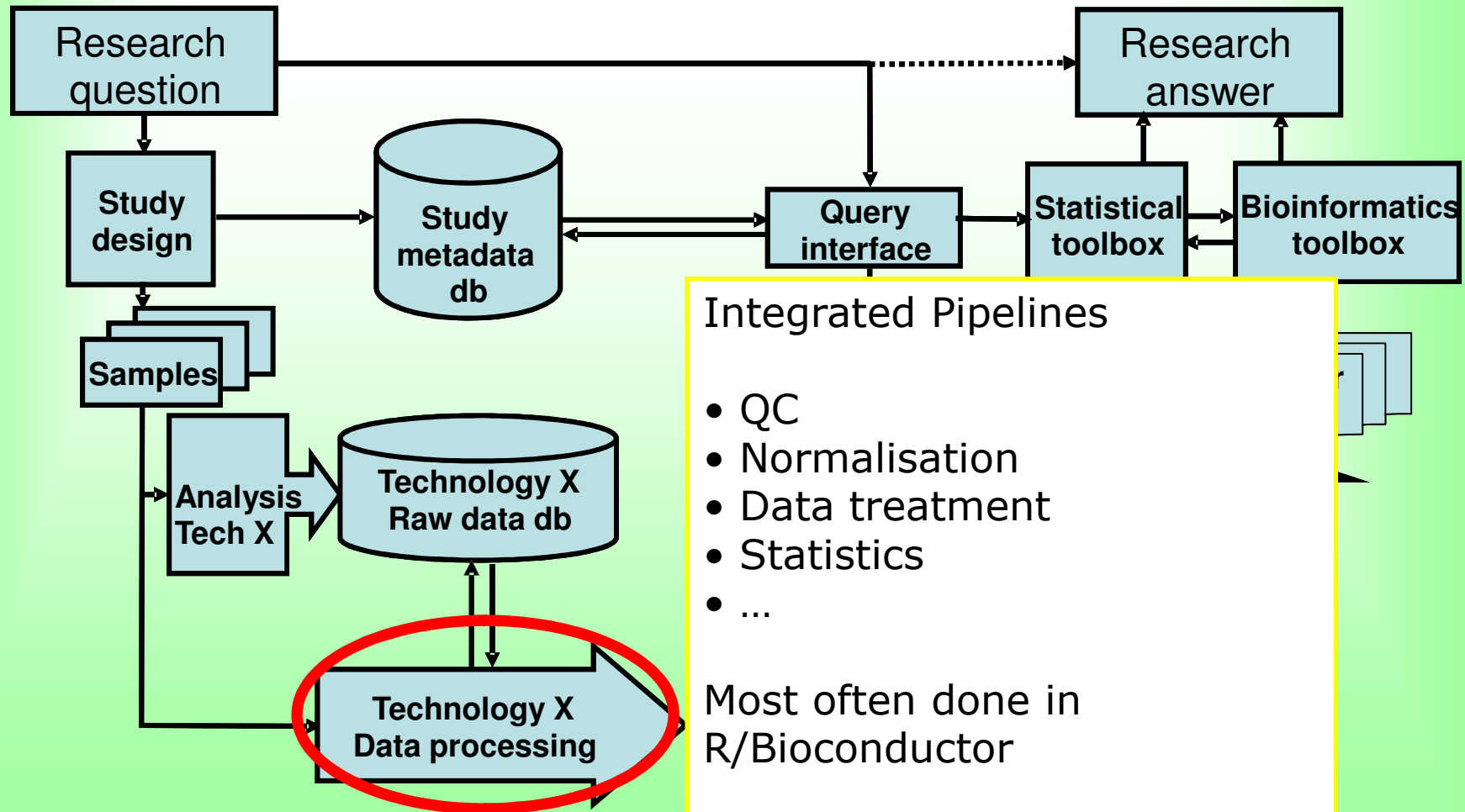


- 1) *Protocols are stored in the study metadata database.*
- 2) *Analytical procedures on study samples*
- 3) *Processing to 'clean data'*
- 4) *By interrogating the study metadata database, data subsets of multiple studies can be selected*
- 5) *and analyzed by statistical and bioinformatics tools.*





# The overall structure



## Integrated Pipelines

- QC
- Normalisation
- Data treatment
- Statistics
- ...

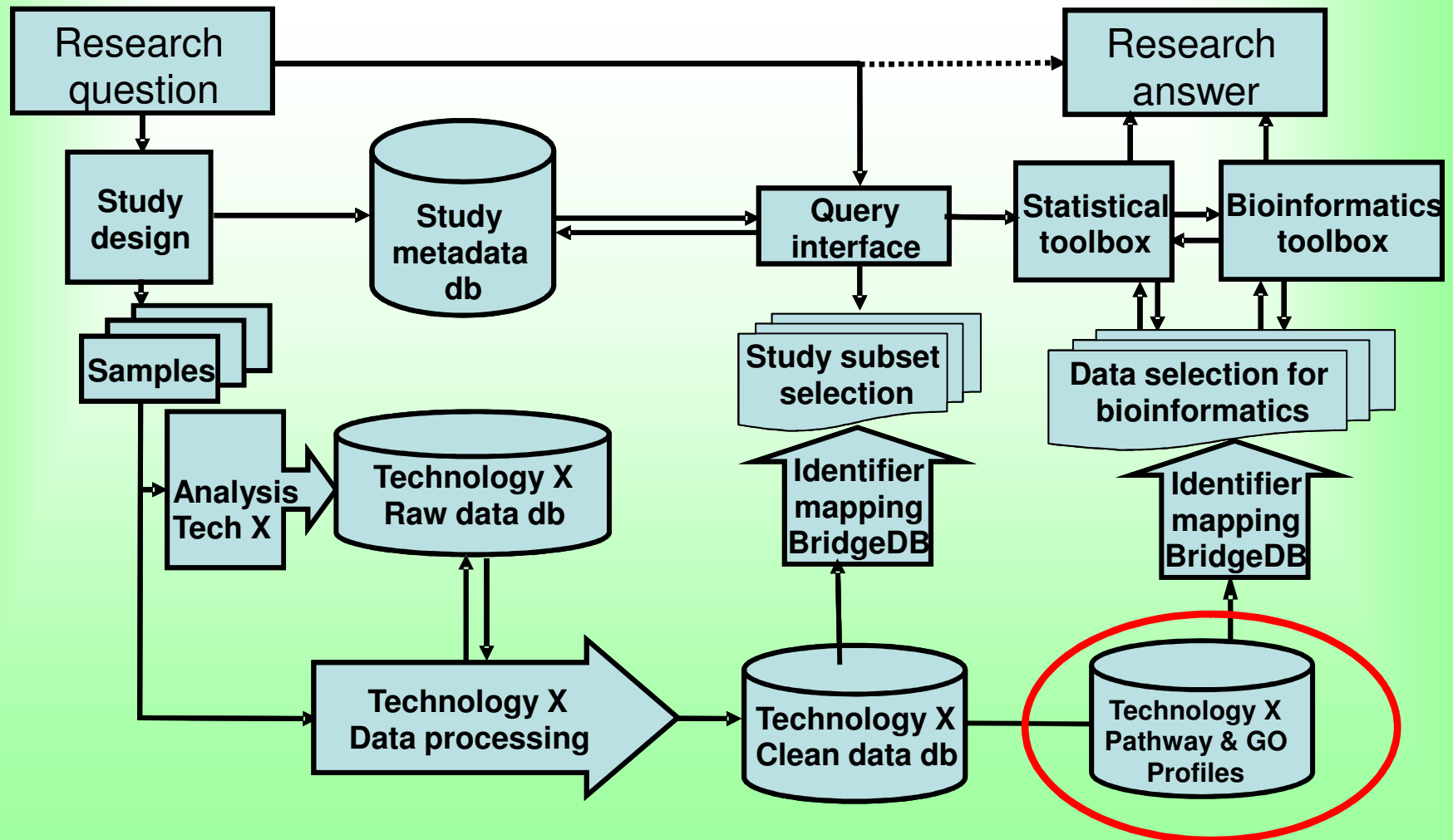
Most often done in R/Bioconductor

Using NuGO R-servers or Grid





# The overall structure





## Biological processes in duodenal mucosa affected by glutamine administration



Pathway	number of genes			Measured	Total	Z Score
	Changed	Up	Down			
<a href="#">Hs Mitochondrial fatty acid betaoxidation</a>	6	6	0	16	16	4.456
<a href="#">Hs Electron Transport Chain</a>	17	17	0	85	105	4.278
<a href="#">Hs Fatty Acid Synthesis</a>	5	5	0	21	22	2.757
<a href="#">Hs Fatty Acid Beta-Oxidation</a>	6	6	0	31	32	2.424
<a href="#">Hs mRNA processing Reactome</a>	16	6	10	118	127	2.402
<a href="#">Hs Unsaturated Fatty Acid Beta Oxidation</a>	2	2	0	6	6	2.342
<a href="#">Hs HSP70 and Apoptosis</a>	4	4	0	18	18	2.299
<a href="#">Hs Oxidative Stress</a>	5	5	0	27	28	2.097
<a href="#">Hs Fatty Acid Omega Oxidation</a>	3	3	0	14	15	1.915
<a href="#">Hs Proteasome Degradation</a>	8	8	0	60	61	1.629
<a href="#">Hs RNA transcription Reactome</a>	5	5	0	38	40	1.25
<a href="#">Hs Irinotecan pathway PharmGKB</a>	2	1	1	12	12	1.154
<a href="#">Hs Synthesis and Degradation of Ketone Bodie</a>						
<a href="#">s_KEGG</a>	1	1	0	5	5	1.023





## Find the relevant pathways



- And ask what other studies contain high z-scores in these pathways
- Essentially asking questions like:  
“What studies showed an effect on e.g. Apoptosis”

Querying pathway by pathway  
instead of gene by gene







## Biological processes in duodenal mucosa affected by glutamine administration



Pathway	number of genes			Measured	Total	Z Score
	Changed	Up	Down			
<a href="#">Hs Mitochondrial fatty acid betaoxidation</a>	6	6	0	16	16	4.456
<a href="#">Hs Electron Transport Chain</a>	17	17	0	85	105	4.278
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<a href="#">Hs Synthesis and Degradation of Ketone Bodie</a>						
<a href="#">s_KEGG</a>	1	1	0	5	5	1.023







# Biological processes in duodenal mucosa affected by glutamine administration



Pathway	Pathway ID	Z Score
<a href="#">Hs Mitochondrial fatty acid betaoxidation</a>	XXXX	4.456
<a href="#">Hs Electron Transport Chain</a>	....	4.278
<a href="#">Hs Fatty Acid Synthesis</a>		2.757
<a href="#">Hs Fatty Acid Beta-Oxidation</a>		2.424
<a href="#">Hs mRNA processing Reactome</a>		2.402
<a href="#">Hs Unsaturated Fatty Acid Beta Oxidation</a>		2.342
<a href="#">Hs HSP70 and Apoptosis</a>		2.299
<a href="#">Hs Oxidative Stress</a>		2.097
<a href="#">Hs Fatty Acid Omega Oxidation</a>		1.915
<a href="#">Hs Proteasome Degradation</a>		1.629
<a href="#">Hs RNA transcription Reactome</a>		1.25
<a href="#">Hs Irinotecan pathway PharmGKB</a>		1.154
<a href="#">Hs Synthesis and Degradation of Ketone Bodie</a>		1.023

That's a  
vector!

s KEGG

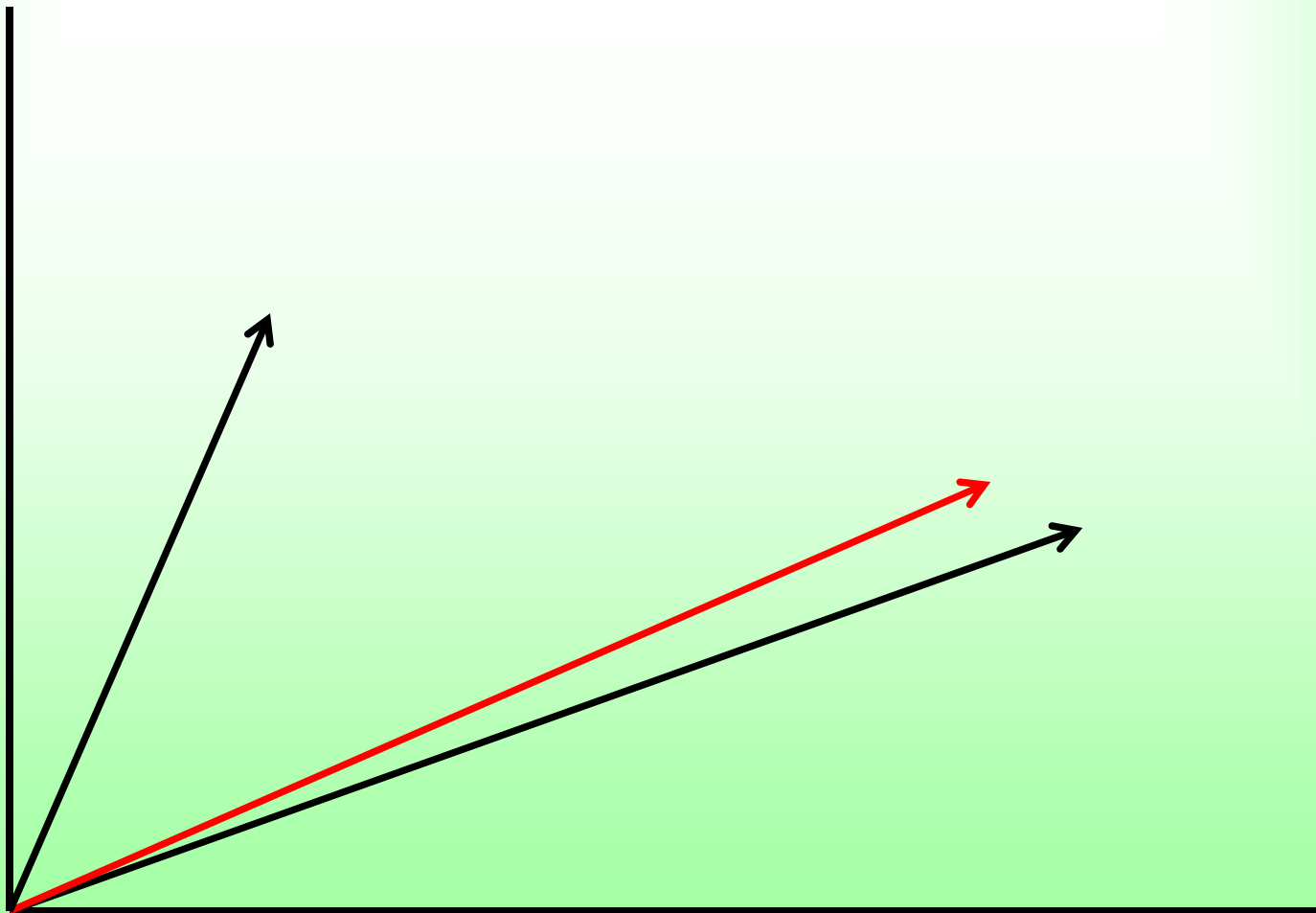




# Find a nearby vector



Z-score 2



Z-score 1

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## Vectors look alike?



- 1 study is a vector
- So 2 studies is 2 vectors
- And we can calculate the distance
- And find the other vector closest
- So we can ask questions like:

“What other studies showed an overall biological effect like this one”




# www.dbNP.org

The Nutritional Phenotype Database - dbNP - Mozilla Firefox

File Edit View History Delicious Bookmarks Tools Help

Back Forward Reload Stop New Window New Tab Home Delicious Tag FireFTP AutoPager http://www.dbnp.org/

The Nutritional Phenotype Data...



Search the entire project  Search [Advanced search](#)

Log In [New Account](#) **nbic** netherlands bioinformatics centre

Home My Page Project Tree Code Snippets Project Openings Nutritional Phenotype Database

Summary Wiki Forums Tracker Lists Tasks News SCM Files

The Nutritional Phenotype Database (dbNP) project's page

- Development Status: 1 - Planning
- Intended Audience: Developers
- License: GNU General Public License (GPL)
- Natural Language: English
- Operating System: Linux
- Topic: Database Engines/Servers

Registered: 2009-09-30 11:33  
Activity Percentile: 0%  
View project activity [statistics](#).  
View list of [RSS feeds](#) available for this project

**Developer Info**

Project Admins:  
[Adem Bilican](#)  
[Ben van Ommen](#)  
[Chris Evelo](#)  
[Jildau Bouwman](#)  
[Kees van Bochove](#)

Developers:  
[Jahn-Takeshi Saito](#)  
[Martijn van Iersel](#)  
[Robert Kerkhoven](#)

[\[View Members\]](#)  
[\[Request to join\]](#)

**Latest File Releases**

Package	Version	Date	Notes / Monitor	Download
dbnp	Nutritional Phenotype Database Paper	October 14, 2009		<a href="#">Download</a>

[\[View All Project Files\]](#)

**Public Areas**

- [Project Home Page](#)
- [Tracker](#)
  - [Bugs](#) ( 0 open /0 total )  
Bug Tracking System
  - [Support](#) ( 0 open /0 total )  
Tech Support Tracking System
  - [Patches](#) ( 0 open /0 total )  
Patch Tracking System
  - [Feature Requests](#) ( 0 open /0 total )  
Feature Request Tracking System
- [Public Forums](#) ( 2 messages in 2 forums )
- [Mailing Lists](#) ( 2 public mailing lists )
- [Task Manager](#)
  - [Next Release](#)
  - [To Do](#)

**Latest News**

- Generic Study Capturing Framework**  
*Adem Bilican - 2009-10-16 11:03* (0 Comment) [\[Read More/Comment\]](#)
- An interesting paper about Nutritional Phenotype**  
*Adem Bilican - 2009-10-07 11:23* (0 Comment) [\[Read More/Comment\]](#)
- dbNP on NuGO**  
*Adem Bilican - 2009-10-05 13:36* (0 Comment) [\[Read More/Comment\]](#)
- NMC-DSP project**  
*Adem Bilican - 2009-09-30 11:43* (0 Comment) [\[Read More/Comment\]](#)
- ISAweb project**  
*Adem Bilican - 2009-09-30 11:42* (0 Comment) [\[Read More/Comment\]](#)

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Start | RuneScape - the... | The Nutrition... | Calculator | Skype™ - chris\_... | Search Desktop | EN | 5:36 PM



The real thing...



Nature Precedings : doi:10.1038/npre.2010.5141.1 : Posted 27 Oct 2010

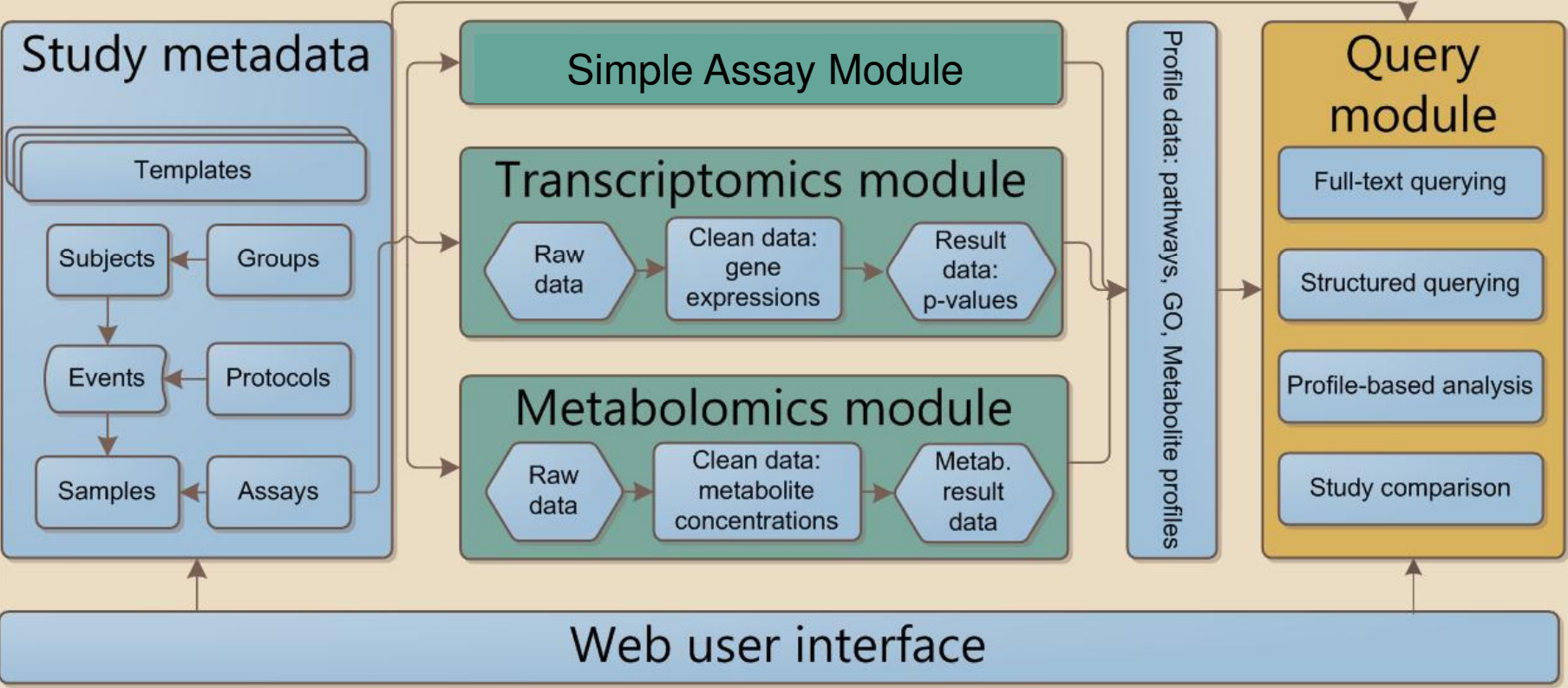


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# DbNP architecture





# Browsing the GSCF

The screenshot shows a Mozilla Firefox browser window titled "Generic Study Capture Framework - Mozilla Firefox". The address bar contains the URL "http://test.dbnp.org/gscf-0.4.3/?execution=e3s1". The browser's menu bar includes "File", "Edit", "View", "History", "Delicious", "Bookmarks", "Tools", and "Help". The page content features a dark header with the title "Generic Study Capture Framework" in large blue letters, followed by the subtitle "a joint initiative of the NMC and NuGO, powered by NBIC". A navigation menu below the header includes "Home", "Studies", "Contacts", and "Publications". The main content area contains a welcome message: "Welcome to GSCF version 0.4.3. At this moment, there are 12 studies in the database." This is followed by a detailed paragraph describing the application's purpose and capabilities. A login/register section follows, with instructions for testing user functionality. The footer contains the copyright notice: "Copyright © 2008 - 2010 NMC & NuGO. All rights reserved." The browser's status bar at the bottom shows "Done" and various system icons.

Generic Study Capture Framework - Mozilla Firefox

File Edit View History Delicious Bookmarks Tools Help

http://test.dbnp.org/gscf-0.4.3/?execution=e3s1

Grails Generic Study Capture Fra...

Hello Guest! + Log In | Register

## Generic Study Capture Framework

a joint initiative of the NMC and NuGO, powered by NBIC

Home Studies Contacts Publications

Welcome to GSCF version **0.4.3**. At this moment, there are 12 studies in the database.

This application will facilitate systems biological research and collaboration between researchers at various locations. This application is a combined effort of the [Nutrigenomics Organization \(NuGO\)](#) the [Netherlands Metabolomics Centre \(NMC\)](#), [European Micronutrient recommendations Aligned \(Eurreca\)](#), the [Netherlands Organization for Applied Scientific Research \(TNO\)](#) and the [Netherlands Bioinformatics Centre \(NBIC\)](#) . The GSCF is part of the [Nutritional Phenotype Database](#) described by [van Ommen et al, 2010: The Nutritional Phenotype Database. Genes and Nutrition. DOI: 10.1007/s12263-010-0167-9](#) . This study capturing module can be easily linked to assay specific modules and therefore can be reused for new technologies. This application is built for the easy input/storage and retrieval of studies. Studies can be stored with high detail and the type for information being stored can be field (e.g. human, mouse, plant) specific. Complex designs like studies with multiple doses, sampling time points and challenge tests, can be stored in this system. Studies will only be accessible for people that are specified by the study owner.

To be able to create, view or search studies, please log on or register at the right top corner of this page. NB: For this (test) version it is not required to login, but if you login as administrator ( admin / admin123! ) or user ( user / user123! ) you can test user functionality.

Choose from the upper bar whether you would like to create, view or search studies

---

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Done



# Study overview

Hello Guest! | [+](#) [Log In](#) | [Register](#)

## Generic Study Capture Framework

a joint initiative of the NMC and NuGO, powered by NBIC

[Home](#) | [Studies](#) ▾ | [Contacts](#) ▾ | [Publications](#) ▾

### Study List

	Code	Title	Subjects	Events	Assays
<input type="checkbox"/>	<a href="#">add/modify</a>	add/modify	1 Bos taurus	Diet treatment, Diet treatment (4-fold)	-
<input type="checkbox"/>	<a href="#">2323</a>	Tomato fruit volatiles	94 Solanum lycopersicum , 20 Homo sapiens , 10 Mus musculus	Plant-material preparation	-
<input type="checkbox"/>	<a href="#">1000</a>	metabolite profile in tomatoseeds	1 Solanum lycopersicum	Plant-material preparation	-
<input type="checkbox"/>	<a href="#">PPS-H</a>	Human PPS: an intervention study	10 Homo sapiens	Fasting treatment	clinical measurements
<input type="checkbox"/>	<a href="#">5696</a>	Effects of a high-protein breakfast and gastric emptying on the postprandial ghrelin response	15 Homo sapiens	-	-
<input type="checkbox"/>	<a href="#">PPS2</a>	Evaluation of the acute whole-body response to glucose stress in C57BL/6J mice	102 Mus musculus	Fasting treatment, Compound challenge, Food intake measurement, Euthanasia, Liver isolation, Body weight measurement, Blood sampling, Diet treatment (general)	-
<input type="checkbox"/>	<a href="#">PPS1, VP9 mouse phase 3</a>	Development of insulin resistance on a high fat diet in ApoE3 mice	75 Mus musculus	Diet treatment, Food intake measurement, Euthanasia, Compound challenge, Liver isolation, Area Under Curve (AUC) estimation, White Adipose Tissue (WAT) isolation, Subcutaneous Adipose Tissue isolation, Skeletal Muscle isolation, Visceral Adipose Tissue isolation, Fasting treatment, Body weight measurement, Blood sampling, Epididymal Adipose Tissue isolation	-
<input type="checkbox"/>	<a href="#">OM06001</a>	MTX	10 Homo sapiens	General drug treatment	-
<input type="checkbox"/>	<a href="#">6374</a>	Relation Between Reduction of the Inflammatory Status and Glucose Metabolism in Healthy Overweight Men	19 Homo sapiens	-	-
<input type="checkbox"/>	<a href="#">6957</a>	Effect of Nutritional Interventions on Inflammatory Status in Healthy Overweight Men	35 Homo sapiens	-	-

# Example view: event time line

The screenshot displays the 'Generic Study Capture Framework' interface. At the top, it says 'Hello Guest!' with a '+' icon and links for 'Log In' and 'Register'. Below the header, there are navigation links: 'Home', 'Studies', 'Contacts', and 'Publications'. The main content area is titled 'Show Study' and has several tabs: 'Study Information', 'Subjects', 'Events timeline' (which is selected), 'Events table', 'Assays', 'Samples', 'Persons', and 'Publications'. The 'Events timeline' view shows a study titled 'Human PPS: an intervention study' with a timeline from Sep 6 to Sep 22. The timeline is divided into two groups: 'Group 1' (subjects 1, 11, 2, 3, 4, 5, 6, 7, 8, 9) and 'No group'. Events are represented by blue dots with text labels and descriptions. For Group 1, there are 'Fasting treatment' events on Sep 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, and 22, and 'Blood sampling' events on Sep 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, and 22. For the 'No group' section, there are 'Urine sampling' events on Sep 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, and 22. At the bottom left, there are icons for 'Edit', 'Delete', and 'Back to list'.

# Web flow for creating studies

Hello Guest! [Log In](#) | [Register](#)

## Generic Study Capture Framework

a joint initiative of the NMC and NuGO, powered by NBIC

Home Studies ▼ Contacts ▼ Publications ▼

### Study wizard

1. Start ▶ 2. Study ▶ 3. Subjects ▶ 4. Events ▶ 5. Groups ▶ 6. Samples ▶ 7. Confirmation ▶ 8. Done

#### ④ Add subjects to your study

Describe the subjects studied with all details available. Use the template that contains the necessary fields. New templates can be defined (based on existing templates). To add subjects to the study, select the correct species and template, input the number of subjects you want to add, and click 'Add'. They will appear below the 'Add' button. As multiple species may be studied within one study, there is no hard link between the template and the species.  
*Note that you can edit multiple subjects at once by selecting multiple rows by either ctrl-clicking them or dragging a selection over them in the space between the fields.*  
*Note that depending on the size of your browser window and the template, additional fields can be reached by the slider at the bottom of the page.*

Number of subjects to add:  ⓘ

of species:  ⓘ

with template:  ⓘ

#### Human template

#	Name ⓘ	Species ⓘ	Gender	Age (years) ⓘ	DOB ⓘ	Height (m)	Weight (kg)
1	<input type="text" value="Subject 1"/>	<input type="text" value="Homo sapi"/>	<input type="text" value="Male"/>	<input type="text" value="34"/>	<input type="text" value="21/09/2010"/>	<input type="text" value="1,84"/>	<input type="text" value="90"/>
2	<input type="text" value="Subject 2"/>	<input type="text" value="Homo sapi"/>	<input type="text" value="Male"/>	<input type="text" value="27"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
3	<input type="text" value="Subject 3"/>	<input type="text" value="Homo sapi"/>	<input type="text" value="Male"/>	<input type="text" value="34"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
4	<input type="text" value="Subject 4"/>	<input type="text" value="Homo sapi"/>	<input type="text" value="Male"/>	<input type="text" value="35"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>



# Assays and modules in dbNP

## Assay module

Assay PPSH\_Lipids\_Before

Sample token	LDL-C	HDL-C	TG
1_B	145.3	55.3	170.8
2_B	198.3	46.2	212.3
3_B	203.5	58.7	204.6

## GSCF

Studies

Assays

Samples

- Modules store and process types of assays
- Simple Assay (SAM)
- Transcriptomics assay (Transcriptomics module)
- Metabolomics assay (NMC-DSP)

# Example Module: SAM

The screenshot shows a web browser window titled "SAM - Simple Assays List - Mozilla Firefox". The address bar contains the URL "http://sam.dbnp.org/sam-0.1/simpleAssay/list". The page header features the title "Simple Assay Module" in red, with a subtitle "a joint initiative of the NMC and NuGO, powered by NBIC". A navigation menu includes "Home", "Simple Assays List", "Import data to SAM", and "Measurement Types List".

The main content area is titled "Simple Assays List" and displays three assay entries:

- Name :** PPS-H-antigen panel (proteins)  
**Samples :** []  
**Types :** []
- Name :** clinical chemistry  
**Samples :** [5\_BloodSampling\_4w1d, 11\_BloodSampling\_3w, 5\_BloodSampling\_3w, 3\_BloodSampling\_4w1d, 4\_BloodSampling\_4w1d, 1\_BloodSampling\_2w, 8\_BloodSampling\_1w, 11\_BloodSampling\_2w, 11\_BloodSampling\_4w1d, 8\_BloodSampling\_4w1d, 2\_BloodSampling\_4w, 3\_BloodSampling\_1w, 4\_BloodSampling\_2w, 2\_BloodSampling\_3w, 9\_BloodSampling\_4w1d, 7\_BloodSampling\_3w, 5\_BloodSampling\_1w, 8\_BloodSampling\_2w, 7\_BloodSampling\_4w1d, 2\_BloodSampling\_2w, 4\_BloodSampling\_3w, 6\_BloodSampling\_3w, 1\_BloodSampling\_4w1d, 8\_BloodSampling\_3w, 6\_BloodSampling\_1w, 9\_BloodSampling\_2w, 6\_BloodSampling\_4w, 3\_BloodSampling\_3w, 7\_BloodSampling\_1w, 4\_BloodSampling\_1w, 2\_BloodSampling\_4w1d, 9\_BloodSampling\_1w, 5\_BloodSampling\_4w1d, 1\_BloodSampling\_3w, 2\_BloodSampling\_1w, 11\_BloodSampling\_4w, 1\_BloodSampling\_4w, 4\_BloodSampling\_4w1d, 7\_BloodSampling\_4w, 5\_BloodSampling\_2w, 9\_BloodSampling\_3w, 11\_BloodSampling\_1w, 6\_BloodSampling\_4w1d, 7\_BloodSampling\_2w, 8\_BloodSampling\_4w1d, 9\_BloodSampling\_4w1d, 3\_BloodSampling\_4w1d, 6\_BloodSampling\_2w, 3\_BloodSampling\_2w, 1\_BloodSampling\_1w]  
**Types :** [sodium (Na+), potassium (K+), total carbon dioxide (tCO), chloride (Cl-), glucose, total calcium (Ca), blood urea nitrogen, creatinine, alkaline phosphatase, alanine-aminotransferase, aspartate-aminotransferase, total bilirubin, albumin, total protein, ammonia , urea, 3-hydroxybutyrate , free fatty acids , glycerol , lactate]
- Name :** PPS-H-haematological analysis  
**Samples :** [7\_BloodSampling\_4w, 9\_BloodSampling\_3w, 1\_BloodSampling\_4w1d, 5\_BloodSampling\_4w1d, 2\_BloodSampling\_1w, 4\_BloodSampling\_4w1d, 1\_BloodSampling\_2w, 2\_BloodSampling\_4w1d, 4\_BloodSampling\_1w, 7\_BloodSampling\_3w, 1\_BloodSampling\_1w, 3\_BloodSampling\_1w, 3\_BloodSampling\_1w, 2\_BloodSampling\_4w, 5\_BloodSampling\_1w, 3\_BloodSampling\_4w, 6\_BloodSampling\_1w, 7\_BloodSampling\_1w, 8\_BloodSampling\_3w, 4\_BloodSampling\_2w, 8\_BloodSampling\_2w, 3\_BloodSampling\_2w, 4\_BloodSampling\_4w, 6\_BloodSampling\_4w1d, 9\_BloodSampling\_2w, 9\_BloodSampling\_1w, 4\_BloodSampling\_3w, 6\_BloodSampling\_3w, 7\_BloodSampling\_2w, 1\_BloodSampling\_3w, 11\_BloodSampling\_2w, 8\_BloodSampling\_4w1d, 11\_BloodSampling\_3w, 9\_BloodSampling\_4w, 11\_BloodSampling\_4w, 5\_BloodSampling\_4w, 6\_BloodSampling\_4w, 2\_BloodSampling\_2w, 2\_BloodSampling\_3w, 6\_BloodSampling\_2w, 8\_BloodSampling\_1w, 5\_BloodSampling\_3w, 8\_BloodSampling\_4w, 7\_BloodSampling\_4w1d, 3\_BloodSampling\_4w1d, 5\_BloodSampling\_2w, 9\_BloodSampling\_4w1d, 3\_BloodSampling\_3w, 11\_BloodSampling\_4w1d, 11\_BloodSampling\_1w, 1\_BloodSampling\_4w]  
**Types :** []

At the bottom of the page, there is a "Create" button and a "Done" status indicator.

# Simple Assay Module

a joint initiative of the NMC and NuGO, powered by NBIC

[Home](#) [Simple Assays List](#) [Import data to SAM](#) [Measurement Types List](#)

## Import Assays

1. Select Study 2. Select Assay 3. Input Assay Data 4. Choose Samples 5. Matching Subjects 6. Done

### Select Attributes

Column name:	Subject name	Sample name	Sample material	SamplingEvent name	Sampling Event time
Time :	Subjects	4 weeks, 1 day	4 weeks, 1 day	3 weeks	4 weeks, 1 day
Type :	-	total carbon dioxide (tCO)	total carbon dioxide (tCO)	total carbon dioxide (tCO)	total carbon dioxide (tCO)
Value	1209-31	1209-31_Blood sampling_1w	blood		1w
Value	1222-32	1222-32_Blood sampling_1w	blood		1w
Value	...	and so on for group 2a			
Value	1391-47	1391-47_Blood sampling_2w	blood		2w
Value	1392-48	1392-48_Blood sampling_2w	blood		2w

- total carbon dioxide (tCO)
- total carbon dioxide (tCO)
- sodium (Na+)
- potassium (K+)
- chloride (Cl-)
- glucose
- total calcium (Ca)
- blood urea nitrogen
- creatinine
- alkaline phosphatase
- alanine-aminotransferase
- aspartate-aminotransferase
- total bilirubin
- albumin
- total protein
- ammonia
- urea
- 3-hydroxybutyrate
- free fatty acids
- glycerol
- lactate

[« prev](#) | [next »](#)



# Querying assays from SAM in GSCF

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Home Studies **▼** Contacts **▼** Publications **▼**

### Simple Query

#### Search term

Search term (e.g. 'paracetamol')

Species (e.g. 'rattus norvegicus')

Organ (e.g. 'liver')

#### Simple Assays (optional)

Compound

Operator

Value

Add compound

#### Transcriptomics (optional)

List of Gene IDs or pathway IDs

Type of regulations



# Many people involved

## **Challenges of molecular nutrition research 6: The Nutritional Phenotype database to store, share and evaluate nutritional systems biology studies.**

Ben van Ommen, Jildau Bouwman, Lars Dragsted, Christian A. Drevon, Ruan Elliott, Philip de Groot, Jim Kaput, John C. Mathers, Michael Müller, Fre Pepping, Jahn Saito, Augustin Scalbert, Marijana Radonjic, Philippe Rocca-Serra, Tony Travis, Suzan Wopereis and Chris Evelo. *Genes and Nutrition*, 2010

Developers on dnNP.org lead by Kees van Bochove

Pathway profiling: Martijn van Iersel, Martina Kutmon, Jahn Saito

Investments (time) by: NuGO, NMC, NBIC, FDA

Many more to come...(including innovative medicine initiative FP7)

A paper based on this presentation will soon be published in *Genes and Nutrition*: <http://dx.doi.org/10.1007/s12263-010-0190-x>