Deliverable D6.2

Project Title:	Developing an efficient e-infrastructure, standards and data-flow for metabolomics and its interface to biomedical and life science e-infrastructures in Europe and world-wide.	
Project Acronym:	COSMOS	
Grant agreement no.:	312941	
Work Package 6 description	FP7-INFRASTRUCTURES-2012-1	
Deliverable title:	Establishment of an NMR metabolomics working group between COSMOS and BioMedBridges	
WP No.	6	
Lead Beneficiary:	10: CIRMMP	
WP Title	Coordination with BioMedBridges and biomedical ESFRI infrastructures	
Contractual delivery date:	01 10 2013	
Actual delivery date:		
WP leader:	Prof. Claudio Luchinat	CIRMMP
Contributing partner(s):	*Claudio Luchinat, Antonio Rosato, Leonardo Tenori, Paola Turano*	

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Content

1. Executive summary

This deliverable describes establishing a NMR working group between the NMR metabolomics working group of COSMOS and BioMedBridges. Crucially, during the first year of COSMOS activity it has became apparent that a meaningful working group is required and that it should not be restricted to partners from the two aforementioned projects. Instead, it deemed appropriate and timely in regards to prospect of the Horizon 2020 programme, to put together a wider collaborative team.

Furthuremore, the requirements outlined previously within the deliverable **D.6.1** of the current workpackage indicated that the action of the working group should be oriented towards Biomedical Sciences in general and specifically in regards to biobanks.

Within the above framework, a working group has been established involving eight different research teams with expertise in metabolomics, mainly but not exclusively, focused on the NMR techniques.

2. Project objectives

With this deliverable, the project has reached or the deliverable has contributed to the following objectives:

No.	Objective	Yes	No
1	Coordinate with the activities of BiomedBridges regarding the standardization of metabolomic data	x	
2	Coordinate the activities of COSMOS, taking into account the requirements of Biobanks with respect to the association of NMR metabolic profiles to stored samples.	x	
3	Develop a strategy for the use of Metabolomics for Biobank sample monitoring and deposition of the metabolomics experiment data in COSMOS partner databases, particularly MetaboLights	X	

3. Detailed report on the deliverable

3.1 Background

The aim of WP6 is to foster the interaction between COSMOS and the biomedical infrastructures with a particular interest in metabolomics (BBMRI, Elixir, EU-Openscreen, EuroBioimaging and INSTRUCT) that are also participating in the BioMedBridges project. The idea is to obtain indications useful to focus and prioritize the various activities in COSMOS in order to effectively respond to the needs of the current large scale EU biomedical infrastructures.

The present document reports on the establishment of a working group on NMR metabolomics involving, among others, partners from the COSMOS, BioMedBridges and BBMRI projects.

3.2 Description of Work

3.2.1 Composition of the Working Group

The composition of the Working Group (WG hereafter) is as follows:

- CIRMMP/CERM, University of Florence, Florence, Italy - PI Claudio Luchinat
- Medical University of Graz, Graz, Austria - PI Kurt Zatloukal
- EMBL- European Bioinformatics Institute (EMBL-EBI), Hinxton, United Kingdom - PI Chris Steinbeck
- University of Birmingham, Birmingham, United Kingdom - PI Ulrich Günther
- University of Alberta, Edmonton, Canada - PI David Wishart
- TNO, Zeist, The Netherlands – PI Ben van Ommen
- Metanomics GmbH, Berlin, Germany - PI Beate Kamlage
- Helmholtz Zentrum München, Neuherberg, Germany - PI Rui Wang-Sattler

WG member no.1 (CERM/CIRMMP) is a project partner in both COSMOS and BioMedBridges, and the coordinator of the BIO-NMR I_3 (a comprehensive group including the top NMR research infrastructures providing access to NMR instrumentation in Europe as well as other

stakeholders in the field). WG 1, is also one of the core labs in the INSTRUCT. **WG member no. 2** is a project partner in BioMedBridges and the coordinator of BBMRI. **WG member no. 3** is a large institution that is coordinating, through different PI's, the COSMOS, BioMedBridges and ELIXIR projects (only the projects relevant to COSMOS are mentioned). **WG member no. 4** is a project partner in COSMOS and in Bio-NMR. **WG member no. 5** is a global expert in NMR metabolomics and has established the Human Metabolome Database (HMDB). **WG member no. 6** is a project partner in COSMOS, although represented by a different PI. **WG member no. 7** is a private company operating in the field of metabolomics. **WG member no. 8** is a partner in BioMedBridges, , although represented by a different PI.

The present WG composition has the advantage that not only involves partners from both the COSMOS and BioMedBridges projects, but also reaches out to a number of other initiatives allowing the WG to maximize its scientific network across multiple infrastructures and applications of NMR metabolomics, ultimately enhancing the impact of each individual initiative.

3.2.1 Scope of the Working Group

The members of the WG share a strong interest in the development and application (e.g. for human health studies) of metabolomics, particularly, but not exclusively, to make use of NMR spectroscopy as the main technique for these studies. These activities are framed within the worldwide growing interest in –omics sciences. The role of metabolomics in the context of biobanks is of particular focus and interest to this WG.

The WG members additionally recognized the need for a coordinated effort to provide state-of-the-art technology applied to metabolomics and the scientific support to enable the European scientific communities to push forward the frontiers of metabolomics through excellence in scientific research. This is expected to provide an impetus and opportunity for the

development of innovative technology, standards and approaches that will enhance the quality of research in Europe and help investment in biobank related research.

3.3 Next steps

To WG will explore the possibility to implement an expert center within the European BBMRI-ERIC infrastructure for the use of metabolomics in Biomedical Sciences and in particular within the context of biobanking.

4 Publications

N/A

5 Delivery and schedule

The delivery is delayed: ? Yes ☑ No

6 Adjustments made

No

7 Efforts for this deliverable

Institute	Person-months (PM)	Period
	actual	estimated
CIRMMP	5	6 9
EMBL-EBI	1	1
Total	6	

Appendices

None.

Background information

This deliverable relates to WP6; background information on this WP as originally indicated in the description of work (DoW) is included below.

WP6 Title: Coordination with BioMedBridges and biomedical ESFRI infrastructures
Lead: Claudio Luchinat
Participants: EBI-EMBL, LU-NMLC, CIRMMP, UOXF

This work package aims at maximizing communications with BioMedBridges and with its partner BMS infrastructures with an interest in metabolomics (Elixir, EU-Openscreen, BBMRI and Instruct), and helping steer the work of the other work packages to maximize the usefulness of the COSMOS activity for the current large scale EU biomedical infrastructures. The COSMOS consortium will actively participate in the concertation activities and meetings related with the e-Infrastructures area. We will help to optimise synergies between projects by providing input and receiving feedback from working groups addressing activities of common interest (e.g. from clusters and projects). If requested we will offer advice and guidance and be receptive for any information relating to 7th Framework programme implementation, standardisation, policy and regulatory, EU Member States initiatives or relevant international initiative.
Description of work and role

Work package number	WP6	**Start date or starting event:**			month 1			
Work package title	Coordination with BioMedBridges and biomedical ESFRI infrastructures							
Activity Type	COORD							
Participant number	1: EMBL/EBI	2: LU/NMC	10:CIRMMP	14: UOXF				
Person-months per participant	6	2	12	2				

Objectives

1. maximizing communications with BMS infrastructures with an interest in metabolomics
2. helping steer the work of the other work packages to maximize the usefulness of the COSMOS activity for the current large scale EU biomedical infrastructures.

Description of work and role of participants

Task 1: Gather metabolomics requirements for BioMedBridges, BBMRI, ELIXIR and EU-OPENSCREEN CIRMMP will coordinate the gathering of requirements regarding the use of metabolomics data as a molecular phenotyping technique with the above-mentioned e-infrastructures. The University of Florence as a third party of CIRMMP will contribute to this task. EBI as coordinator of ELIXIR, BioMedBridges and responsible for database and standards development in EU – OPENSCREEN will contribute use cases from its on-going integration efforts. UOX is leading the development of the ISA infrastructure, which assists in the annotation, and local management of experimental metadata from high-throughput studies employing one or a combination of omics and other technologies, and will work toward integrating the findings from Task 1 in the ISA development.

Task 2: Coordinate with the activities of BioMedBridges regarding the standardization of metabolomics data WP 7 of the BioMedBridges grant will work in particular on NMR metabolomics data and towards a standardized description of sample donors, sample collection; pre-processing, analysis and evaluation will be established as a prerequisite for the inter-species comparison of metabolomics results. In this task all contributors to this task will ensure the appropriate coordination of the developments in WP2 of COSMOS and WP7 of BioMedBridges.

Task 3: Coordinate the activities of COSMOS versus the needs of Biobanks with respect to the association of NMR profiles to stored samples. The primary objective of biobanks is not merely archiving, but also distributing conserved and documented biological samples for research, and so they represent an irreplaceable support for all those studies in which the impact of the results is linked to the large number of the collected samples. The quality of stored biological samples is crucial for the outcome of subsequent studies. The molecules constituting the metabolic fingerprint are generally very sensitive to handling procedures and storage conditions, so metabolomics is a useful tool for checking and assessing the quality of stored samples. The NMR profile of a sample allows its evaluation in entrance (to decide its acceptance) and in exit (to decide if it is still good to be distributed), so it is important to associate each stored sample to the respective NMR metabolic profile. The aim of this task is to coordinate the activities of COSMOS, taking into account the requirements of Biobanks with respect to the association of NMR metabolic profiles to stored samples. BBMRI (Biobanking and Biomolecular Resources Research Infrastructure) was one of the first European Research Infrastructure projects funded by the European Commission (EC). The EC-funded preparatory phase of BBMRI came to its end in January 2011. During the past 3 years BBMRI has grown into a 53-member consortium with over 280 associated organisations (largely biobanks) from over 30 countries, making it the largest research

infrastructure project in Europe (http://www.bbmri.eu/). In this task we will interface with BBMRI and develop a strategy for the use of Metabolomics for Biobank sample monitoring and deposition of the sample status data in COSMOS partner databases.

Deliverables

No.	Name	Due month
D6.1	Document describing requirements for relevant biomedical infrastructures with regard to Metabolomics	6
D6.2	Establishment of an NMR metabolomics working group between COSMOS and BioMedBridges	12
D6.3	Joint consensus document between COSMOS and BioMedBridges	18
D6.4	Joint consensus document between COSMOS and BioMedBridges (Updated)	36
D6.5	Report on the recommendations of the use of Metabolomics of Biobank sample monitoring	24