Deliverable D1.2.1

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	
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Work Package 7 description	FP7-INFRASTRUCTURES-2012-1	
Deliverable title:	COSMOS Project Report	
WP No.	1	
Lead Beneficiary:	1:EMBL-EBI	
WP Title	Management	
Contractual delivery date:	01 04 2013	
Actual delivery date:	01 04 2013	
WP leader:	Christoph Steinbeck	EMBL-EBI
Contributing partner(s):	*Reza Salek, Christoph Steinbeck*	

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Contents

1 Executive summary

The aim of this deliverable is to summarise 6 months activity of WP1 and related work by COSMOS partners:

1. Report on coordination activity
2. Report outreach activity focused on workshops related to COSMOS and Partner exchange plan
3. COSMOS meetings and application development coordination

2 Project objectives

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

No.	Objective	Yes	No
1	Report on COSMOS coordination activities	X	
2	Report on COSMOS outreach, communication and Dissemination	X	
3	Report on COSMOS workshops and partner exchange	X	
4	Report on COSMOS application development coordination	X	

3 Detailed report on the deliverable

3.1 Background

This work package will provide the management infrastructure for the proposed work. It will make use of the existing electronic communication platforms of the Metabolomics Standards Initiative and the Metabolomics Society, and further develop them, in order to be used by the COSMOS consortium. We will also organize the annual COSMOS consortium and stakeholder meetings, as well as regular staff exchanges between the COSMOS partners. We will systematically document the decision-making process and decisions made in teleconferences, meetings and by email exchange. This will be compiled regularly into COSMOS consortium documentation.

3.3 Description of Work

3.3.1 Report on COSMOS coordination activities

COSMOS officially started its kickoff meeting in Barcelona, Spain organized by EMBL-EBI on 8 of October 2012. The two-day meeting included presentation by each work package (WP) leader and WP partner presenting his or her role in the project. DoW and CA were reviewed and discussed among WP leaders, currently no amendment is required. Additionally, COSMOS financial aspects were reviewed and discussed between WP leaders and partners for consultation. A brief discussion was carried out, regarding the upcoming annual COSMOS meeting, and a suitable location and approximate date was agreed, to be finalised in a subsequent online discussion. We also agreed on a tentative plan for stakeholder meetings and reviewing potential attendees to be invited, creating a tentative plan for the stakeholders meetings. Planning the initial 6-month of the work and deliverables, WP overview, creating a tentative planed staff exchange between partners was also discussed.

Other activities include selection of the scientific advisory board (SAB): After voting, we unanimously agreed to ask the following additions to the existing SAB (which includes; Prof. David Wishart, HMDB, Canada, Prof. Oliver Fiehn, UC Davis, USA, Prof. Masanori Arita, Tokio, Prof. Yulan Wang, The Chinese Academy of Sciences, Wuhan), from which the first two where invited subsequently and accepted to join the advisory board.

- **Kurt Zatloukal**- Coordinator of ESFRI Biomedical and Biobanking Resources Research
- **Richard Beger** - Branch Chief, Center for Metabolomics of Division of Systems Toxicology, USA
- **Sunil Kochhar** - Head of BioAnalytical Sciences, Geneva, Switzerland, Nestle (Not currently invited)

Election of the Steering Committee (SC): For the following year, all WP leaders agreed to be members of the SC, with monthly online meetings around the middle of the month, to discuss issues and progress related to COSMOS activity.

Another outcome of the kick-off meeting and subsequent Google hangout discussions was formation of two sub groups - one for nmrML development and a second group for mzML file format development. WP2 would be the lead organiser setting up biweekly online meetings which would involve invitation of the relevant stakeholders involved in development of NMR open standard extensible Markup Language (nmrML) file formats. These meetings involve more frequent technical teleconferences of the work package participants (including stakeholders) and likewise are extensively documented.

To date, as part of this deliverable, we have organized monthly teleconference meetings using Google hangout with the COSMOS SC. Discussions and decisions were minuted using a Google Document that could easily be shared within the SC participants with a final and a second copy of outcomes stored on the COSMOS website Internal pages (COSMOS-FP7.EU) and distributed among WP partners and announced via social media.

A list of potential stakeholders to be invited was discussed among participants and an initial list was suggested, to be further discussed in the next COSMOS annual meeting. We also agreed to schedule the stakeholder meeting during the Metabolomics Society meeting 2013 scheduled in Glasgow, July 1-4. Since most metabolomics researchers and stakeholders would participate in the metabolomic society meeting, this should save us on costing, logistics and the time required to arrange the meeting.

The first annual COSMOS meeting was held on 11-12th of March 2013 in Leiden hosted and organized by WP1 partner University of Leiden, Prof Thomas Hankemeier and Dr Theo Reijmers. Each WP leader and related WP partner presented an update of their work to date and planned the next steps ahead. This meeting included planning the next 6-month of the work, discussion on metabolomics standards and deliverables coordination, WP overview and finally creating additional plans for staff exchange between partners. Minutes of the meeting very distributed using Google document and is accessible on the COSMOS website. A copy of the presentation by WP leaders are kept in COSMOS website internal pages. In this meeting future partner exchange and workshops were discussed and planned, details below.

Another outcome of this meeting was agreement on setting up a metadata-focused group, primarily aiming to:

- Developing controlled terminology for supporting nmrML/mzML file formats
- Collect metabolomics application specific terminology for mass spectrometry and NMR for inclusion into PSI-MS vocabulary
- How to engage with MSI (Metabolomics standard initiative)
- Improving standards within MSI
- Refine MetaboLights configurations and templates based on community input for improving data collection and completeness

Other discussions include, agreement on location of the next annual meeting (2014) to be held in The Leibniz Institute of Plant Biochemistry (IPB), Germany.

3.3.2 Report COSMOS out reach and communication activity

Information on COSMOS that has appeared in news articles:

- **Metabonews:** on Issue 19 of March 2013 we published an article titled, MetaboLights - The new EBI Metabolomics database in which COSMOS is covered http://www.metabonews.ca/Mar2013/MetaboNews_Mar2013.htm
- EBI Press release: http://www.ebi.ac.uk/Information/News/press-releases/press-release-09102012-COSMOS.html
- COSMOS was also acknowledged in an ISA website: http://isatab.sourceforge.net/about.html

We have introduced COSMOS and actively promote via several social media sites, including:

- Blogger - http://metabolights.blogspot.co.uk

- Twitter - #cosmosfp7

- Facebook - http://www.facebook.com/cosmosfp7

PSI meeting April 2013 in Liverpool (http://www.psidev.info/) - This is an important opportunity where the members and stakeholders of HUPO Proteomics Standards Initiative (PSI) would gather annually. The aim of this meeting is to define community standards for data representation in proteomics and to facilitate data comparison, exchange and verification. Since there are lots of parallel development and common interest shared within the PSI and MSI community, it would be of great interest to have a presence and participation in this meeting. Therefore for the first time, the metabolomics community via COSMOS initiative will be actively participating in the meeting with an aim to establish long term collaboration and working participation with HUPO-PSI community.

3.3.3 Report on COSMOS Workshops and Partner Exchange

The workshops and scheduled meetings so far:

- COSMOS nmrML Workshop Florence , Italy 13-14 December 2012 M. Wilson (U. Alberta), R. Salek (EBI), C. Steinbeck (EBI), D. Schober (U. Freiburg), J. Hao (Imperial College), U. Guenther (U. Birmingham), C. Ludwig (U. Birmingham), C. Deborde (U. Bordeaux), A. Moing (U. Bordeaux), L. Mannina (U. Roma La Sapienza), F. Capozzi (U. Bologna), H. Schaefer (Bruker Biospin), A. Rosato (CIRMMP), C. Luchinat (CIRMMP), P. Turano (CIRMMP), L. Tenori (CIRMMP)
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- EMBL-EBI first Hackathon, April 8-14 2013.
    - Included invitation of Prof. David Wishart group member as one of the major stakeholders for development of nmrML file format.
    - Two representatives from BML-NMR Birmingham NMR group headed by Prof Mark Viant, another major stakeholder.
    - Hupo-PSI members developers based in the EMBL-EBI for contribution and feedback for development of mzML format and Spectra viewer
    - WP2 Daniel Schober developer which is leading the development
    - Bordeaux University WP partner for development of Spectra viewer
- Birmingham- EBI joint Workshop and meeting, 2 May 2013
- Staff Exchange Between University Bordeaux Segalen and Max Planck Institute Of Molecular Plant Physiology, April 22nd and May 3rd Benjamin Dartigues from Macha Nikolski's group
- 1 Day COSMOS Workshop, part of the We-NMR (http://www.wenmr.eu/) working groups, scheduled to take place in the ISMAR 2013, Brazil May 2013.
- Glasgow metabolomics society, 30 June 2013
    - Workshop on Metabolomics Data Dissemination, Standardization and Exchange (COSMOS/MetaboLights/NIH common funds Session)
    - *Organisers: Reza Salek, Marta Cascante, Christoph Steinbeck and the COSMOS consortium*
    - http://www.metabolomics2013.org/page/workshops
    - Background general metabolomics standards and data storage and data exchange in different standard formats (MSI, ontology, mzML, nmrML.
    - Hands on MetaboLights tools and data submission using ISACreator (Overview, Setting up ISAcreator and capturing metabolomics metadata, Study submission into MetaboLights).
    - Overview COSMOS (COordination Of Standards In MetabOlomicS) initiative on metabolomics standards.

COSMOS related websites setup by WP1 and WP leaders:

- **COSMOS website** with content management system, separate login for partners and work package leaders in production (http://www.cosmos-

fp7.eu)

- **nmrWiki page** This is a wiki based information portal where all the relevant links and documents relevant to development of nmrML file format and its deliverables will be kept. (http://cosmos-fp7.eu/nmrML/)
- **nmrML githhub** this is where the major development of the NMR mark-up language file formats will take place, documented and organized (https://github.com/nmrML/nmrML/)
- A free **sourceforge** site for storing documents and data related to software and tools development: http://sourceforge.net/projects/cosmos-fp7/
- Bordeaux Metabolome Facility Website: http://www.cgfb.u-bordeaux2.fr/en/metabolome
- The division of Analytical BioSciences, Leiden University website:http://analyticalbiosciences.leidenuniv.nl/research/projects/cosmos-coordination-of-standards-in-metabolomics
- Link to COSMOS within “about-crem” webpage under “EU project”: http://www.cerm.unifi.it/about-cerm/eu-projects

3.3. Report on COSMOS application development

The outcome of several COSMOS coordination activities such as the kick-off meeting in Barcelona, annual meeting in Leiden and regular monthly Google hangout communication has establishing three standards working groups; MS, NMR and ontology-metadata subgroups.

MS standards working group – The aim of this working group, in coordination with the PSI and MSI community, is to extend existing exchange standards to technologies used in metabolomics, e.g. gas chromatography. This working group is lead by WP2 with the help of WP3 and WP partners aiming to add the required terms and concepts, required for mzML that can capture all information contained in netCDF or other MS based file formats. The initial step for GC-MS has been completed and our aim is to pave the way for further adoption of the PSI-MS data standards in the GC-MS community. The next step would be a similar initiative for adaptation of MS based technologies such as LC-MS and MS based imaging (MALDI, DESI, SIMS). Coordination between other initiatives and stakeholders is crucial for the success and enabling integration of metabolomics data into large e-science infrastructures

NMR standards working group - Compare to the well established mass spectrometry open source file format (mzML) that is commonly in use, a substantial work is required to achieve similar levels for the NMR based open source file formats (nmrML). Therefore an active focus group was setup and coordinated for the wide participation of the NMR community and stakeholders interested in development of such NMR file format. The working groups aim to focus on the following task:

- Development of nmrML, nmrQunatML, nmrIdentML and nmrTab file format standards and Schema
- nmrML development and Schema, are distributed to public via monthly release from the Github dedicated web space devoted to this https://github.com/nmrML/nmrML/ and to also to collect feedback.
- nmrML Google forum was setup by WP1 to coordinate meetings and communications between interested metabolomics groups, this is public and can be access via https://groups.google.com/forum/#!forum/nmrml
- Facilitate MetaboLights, BML-NMR & HMDB metabolomics databases to represent their raw experimental and reference NMR data in nmrML format.
    - Ability to visualize raw FID and processed 1D nmrML spectral data
- Develop Website plugins and parsers and converters for
    - Bruker & Varian file formats to nmrML
    - nmrML to MAF (MetaboLights)
    - nmrML to JCAMP-DX
    - nmrML to others – output based format e.g. nmrTab
- Create and setup ISA-Creator configuration files for MetaboLights data acquisition & submission implementing the COSMOS requirement of metabolomics standards in NMR data acquisition resulting in ability to:

- Search experiments in DB by metadata descriptors
- Verify experimental data by means of rules and ontologies
- Check file structure, cardinalities & correct usage of CV

General nmrML wiki with all the relevant links and connections are kept at http://cosmos-fp7.eu/nmrML/ with a brief overview of the project. The existing namespaces for modules developed earlier by Prof Wishart group, would be kept but renamed to reflect current agreement:

xmlns:nmr-ml=http://nmr-ml.org/nmr-ml

xmlns:nmr-quant-ml=http://nmr-ml.org/nmr-quant-ml

xmlns:nmr-meta-ml=http://nmr-ml.org/nmr-meta-ml

The later links to be renamed to: nmrQuantML and nmrTab respectively.

Metadata standards working group (CV and ontology terms) - The aim of this working group is primarily focused on developing controlled terminology and vocabulary (CV) for supporting underdeveloped nmrML/mzML file formats. This includes collecting community agreed metabolomics application and specific terminology for mass spectrometry, to be submitted later to the PSI-MS vocabulary ontology resource, as well as collecting NMR based CV and terminologies for NMR based experiments. Improving initial works on metabolomics standards started initially within the MSI community and this group will re-engage with the MSI working groups. Finally the working group will refine MetaboLights configurations and templates based on community input for improving data collection and completeness. The user group would be lead by WP1 parent Leiden, eventually engaging with the MSI community working groups and metabolomics stakeholders. We have setup a Google user group (https://groups.google.com/forum/?fromgroups#!forum/metadata-cosmos-fp7) used for coordinates and discussion.

3.4 Next steps

1. Preparation and submission of COSMOS related publications, with all COSMOS partners is in progress. Submission of a communication letter and a more detailed technical manuscript on the new nmrML open standard file format.

2. Expand COSMOS in social media, though further use of the EMBL-EBI Twitter and Facebook account.

3. Workshop plan for the Metabolomics 2013 meeting in Glasgow, EMBL-EBI Hackathon, Birmingham meeting and others

4. Schedule Stakeholders meeting at Metabolomics 2013 in Glasgow

5. Carrying out several COSMOS workshops nationally and internationally promoting standards in metabolomics

6. Pooling resource PSI & MSI

7. Coordination of development and dissemination of MS XML formats; mzML, mzIdentML, mzQuantML and mzTab

8. Coordination of development and dissemination of NMR XML formats; nmrML, nmrIdentML, nmrQuantML and nmrTab

9. Coordination on developments of tools, convertors and API for nmrML and mzML file formats

10. Coordination and dissemination of ontology and CV development

11. Interaction with vendors, software developers, Journals and databases to make COSMOS more inclusive and economically viable for them to participate in the development of the file formats, essential for the success of the initiative.

4 Publications

The MetaboLights repository: curation challenges in metabolomics. Database 2013, (doi:10.1093/database/bat029) Salek RM,

Haug K, Conesa P, Hastings J, Williams M Mahendraker T, Maguire E, González-Beltrán A, Rocca-Serra P Sansone SA and Steinbeck C.

Editorial Publication Drafted: A roadmap to an open metabolomics standard for NMR data exchange and visualization by nmrML subgroup including stakeholders involved in the effort.

Draft Main COSMOS publication

5 Delivery and schedule

The delivery is delayed: ☐Yes ☑No

6 Adjustments made

N/A

7 Efforts for this deliverable

Institute	Person-months (PM)		Period
	actual	estimated	
1:EMBL-EBI	2		6
2:LU/NMC	0		6
Total	2	4	

Appendices

1. N/A

Background information

This deliverable relates to WP1; background information on this WP as originally indicated in the description of work (DoW) is included below.

WP1 Title: Management
Lead: Christoph Steinbeck, EMBL-EBI
Participants: Christoph Steinbeck

This work package will provide the management infrastructure for the proposed work. It will make use of the existing electronic communication platforms of the Metabolomics Standards Initiative and the Metabolomics Society, and further develop them, in order to be used by the COSMOS consortium. We will also organize the annual COSMOS consortium and stakeholder meetings, as well as regular staff exchanges between the COSMOS partners.

We will systematically document the decision-making process and decisions made in teleconferences, meetings and by mail exchange. This will be compiled regularly into COSMOS consortium documentation.

Work package number	WP1	**Start date or starting event:**			Month 1			
Work package title	Management							
Activity Type	COORD							
Participant number	1: EMBL-EBI	2: LU/NC						
Person-months per participant	12	6						

Objectives
The consortium management activities will include

1. Coordination at consortium level of the 'technical' activities of the project.
2. The overall legal, contractual, ethical, financial and administrative

management of the consortium.
3. Co-ordination of knowledge management, IPS and other innovation-related activities.
4. Preparing, updating and managing the consortium agreement between participants.
5. Maintaining communications with the Commission.
6. Overseeing the promotion of gender equality in the project.
7. Overseeing science and society issues related to the activities conducted within the project.

Description of work and role of participants

It is in the very nature of a coordination action to focus on communication between the participants for the sake of policy making, to document the outcome and spread the word to promote widespread community adoption.
We therefore wish to highlight the following:

Personal Communication
As part of this work package, we will organize monthly tele-meetings (Skype, phone, webex) of the COSMOS steering committee. Discussions and decisions will be minuted. We will invite international collaborating PI's to participate if needed.
Technical teleconferences of the work package participants will be held more frequently and likewise carefully documented.

Formal Communication
The policies, standards and workflows developed in this endeavour will be formally documented and published in the form of manuals, white papers and recommendations. Any document created under this umbrella will be released under Creative Commons License to allow for barrier-free dissemination.
At the beginning of the project in month 2 we will deliver a project plan which will include a list of success indicators to monitor during the whole project, as well as the data we will gather that will help in assessing its impact. These indicators and metrics will be subject to change during the first review meeting and they will be reported at least in the annual reports.

Participants
The management work package will be coordinated by the EMBL-EBI, building on EMBL-EBI experience in the management of large consortia, for example in the BioSapiens, Embrace, and Felics projects. The Netherlands Metabolomics Center (LU/NMC) will be co-coordinator with their extensive experience in maintaining the largest national Metabolomics initiative in Europe and networking with an extensive set of international partners. In addition to EMBL-EBI and LU/NMC as the coordinators, all work package leaders are formal participants of this deliverable, due to the higher communication and reporting effort. EMBL-EBI have included the cost for an audit certificate under management subcontracting.

Deliverables

No.	Name	Due month
D 1.1	Project Plan	2
D1.2.1	COSMOS Project Report	6
D1.2.2	COSMOS Project Report	12
D1.2.3	COSMOS Project Report	18
D1.2.4	COSMOS Project Report	24
D1.2.5	COSMOS Project Report	30
D1.2.6	COSMOS Project Report	36