Deliverable D7.3.1

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	
Grant agreement no.:	312941	
Work Package 7 description	FP7-INFRASTRUCTURES-2012-1	
Deliverable title:	Updated Outreach activity plan (including publications)	
WP No.	7	
Lead Beneficiary:	13:UBHam	
WP Title	Report on annual stakeholder meetings	
Contractual delivery date:	30 Sep 2013	
Actual delivery date:	1 July 2013	
WP leader:	Ulrich Günther	UBHam
Contributing partner(s):	UBHAM, EMBL-EBI, UB	

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Contents

1 Executive summary

The aim of this deliverable is to summarize outreach activity by the partners:

1. Report on COSMOS stake holder meetings

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 the COSMOS stakeholder meetings	X	

3 Detailed report on the deliverable

3.1 Background

We will initially employ the usual channels for the disseminations of COSMOS standards, including scientific publications, workshops and presentations at metabolomics conferences to reach the wider metabolomics community. The project will plan activities adequately resourced devoted to dissemination for specialised constituencies and the general public, in particular for awareness and educational purposes. The dissemination plan deliverable will consider adequate messages about the objectives of the project and its societal and economic impact.

For this COSMOS builds on existing links with other EU and International initiatives, in particular the annual Metabolomics Society Meeting, where the majority of the metabolomics stakeholders is present, to build links with metabolomics groups across the world, including in Canada (HMDB, Wishart) and the US (BMRB; see letters of support), and Asia (Wang, China, Wuhan; Arita, Tokyo, Japan). These meetings will ensure that all stakeholders get the opportunity to

discuss the progress at a meeting once a year, in order to take an inclusive approach that gives the wider metabolomics area a chance of involvement.

3.2 Description of Work

The COSMOS stakeholder meeting was held on July 1st in Glasgow UK as planned, coinciding with the metabolomics 2013 meeting, held at the same location. By scheduling the stakeholder meeting during the Metabolomics Society meeting 2013 we have substantially saved on our costing, logistics and the time required to arrange the meeting. This was due to the fact that most of the stakeholders invited, were already present or planning to attend the society annual meeting. In total, we invited 52 (Including COSMOS) researchers with diverse backgrounds and relevant expertise to metabolomics standards, metabolomics databases, including members of the metabolomics standard initiative, the proteomics standards initiatives, metabolomics journals, directories and members of the metabolomics society. We also had representation from NIH USA, MassBank database Japan, HMDB database Canada, GOLM Germany, PRIDE UK, NMC Netherlands and Metabolomics workbench USA that were present at the meeting. The invited stakeholders were from diverse geographical locations all involved with standardization, databases and data repositories from across Europe, USA, Australia and Asia (Japan and China).

Attendee list:

Philippe Rocca-Serra	PRS	University of Oxford, UK
Kenneth Haug	KH	EMBL-EBI, UK
Padma Maruvada	PM	NIH, USA
Theo Reijmers	TR	NMC/LACDR, NL
Dan Bearden	DB	NIH, USA
Robert Mistrik	RM	HighChem, Slovakia
Roy Goodacre	RG	Univ Manchester, UK
Malcolm McConville	MM	Uni Melbourne/Metabolomics Australia, AUS
Yulan Wang	YW	Wuhan Institute of Physics Chinese academy of Science, CHINA
David Wishart	DaW	Univ Alberta, CANADA
Jean-Charles Martin	JCM	AIX-Marseille Universite, FR
Eloy Correa	EC	Univ Manchester, UK

Betsy Wilder		BW	NIH, USA
Philip Smith		PS	NIH, USA
Merlijn van Rijswijk		MvR	NMC, NL
Oliver Kohlbacher		OK	Univ Tübingen, DE
Thomas Hankemeier		TH	NMC/Leiden University, NL
Jan Hummel	JH		Max planck institut, plant phys, DE
Wolfram Weckwerth		WW	University of Vienna, Austria
Dirk Walter	DiW		Max planck institut, plant phys, DE
Leonardo Tenori	LT		CERM, Univ Florence, IT
Annick Moing		AM	INRA, bordeaux Univ, FR
Henning Hermjakob		HH	EMBL-EBI, UK
Masanori Arita		MA	Univ Tokyo, RIKEN CSRS, JAPAN
Charles Burant	CB		Univ Michigan, USA
Saravanan Dayalan		SD	Univ Melbourne, Metabolomics Australia
Ute Roessner		UR	Univ Melbourne, AUS
Arthur Castle	AC		NIH, USA
Shankar Subramaniam		ShS	UCSD, USA
Susan Sumner	SuS		RTI RCMRC, USA
Christoph Steinbeck	CS		EMBL-EBI, UK
Rima Kaddurah-Daouk		RK	Duke, Univ, USA
Marta Cascante	MC		Univ Barcelona, ES
Reza Salek	RS		EMBL-EBI, UK

Apologies and could not attend

Mark Viant, University of Birmingham, UK
Warwick Dunn, University of Birmingham, UK
Ulrich Gunther, University of Birmingham, UK
Lloyd Sumner, Noble foundation , USA
Steffen Neumann, IPB-Halle, Germany
Tim Ebbels, Imperial College, UK
John Shockcor, Waters Technologies Corp
Jules Griffin, MRC-HNR, UK
Oliver Fiehn, UC Davis, USA
Susanna-Assunta Sansone, University of Oxford, UK
Kurt Zatloukal, Medical University of Graz, Austria
Richard Beger, FDA, USA
Sunil Kochhar, Nestle, Switzerland
Sebastian Böcker, Friedrich-Schiller-Universität Jena, Germany
Kazuki Saito, RIKEN Plant Science Center, Japan
Neil Taylor, Chenom, Canada
Fadi Abdi, AB SCIEX.
Douglas Kell, Manchester University

- Matters discussed at the meeting

- Purpose and need for a stakeholder group
- How to re-launch existing repositories (MSI and PSI)
    - COSMOS reuses formats from PSI
    - Further needs discussed (Data STD, ontology and nomenclature, metadata STD, metabolomics STD for quantification and others)
    - Needs for data exchange were discussed
- Collaboration with the NIH common funds consortium
- Measures for quantification (isotopically labelled reference materials)
- Organisational requirements:
    - Who can host an independent umbrella? Ideally the Metabolomics Society
    - Smaller focussed groups in different places
    - Role of the NIH (USA) for standards
    - Can standards be imposed?
        - e.g. by setting standards for journals?
        - Issues of uptake in the community.
    - Role of instrument vendors for standardisation
        - Should be on board from an early stage
        - Several vendors have been approached:
            - Bruker won't change before community has accepted a common standard
            - Similar position for Varian, Agilent

- **Journals**
    - The *metabolomics journal* (Springer) is committed to implementation of metabolomics standards
    - Reviewers should ask for data availability via public repositories

- **Role of outreach for establishing standards**
    - COSMOS fundable activities
    - Back-communication to the community

- make people feel equal (community involvement in the initiative). Sort of feel good factor to bring as partners

- **Action plan:**
  - Importantly we need early discussion between NIH and EBI to flesh out the important question striving to make equally easy to submit metabolomics datasets to NIH or EBI.
  - Then we can start to have a global metabolomics organisation for implementation of standards and workflows (Similar to Genbank), we need input on how to do it?

- **Importance of reference compounds**
  - Standard conditions (NMR spectra in water based solvent is required)
  - MS data on modern instruments to replace the old reference spectra, via community effort
  - Community effort required considering the size of the effort, task and variety and availability of instruments
  - Involve companies (Sigma Aldrich, software and instrument manufacturers)
  - We have to show that the community and metabolomics society is happy to pay for such calibration reference compounds in an open letter (to make standardization main stream). Then capture this information within our databases in our community and reporting such concentration would be facilitated
  - Costing of reference compounds is an issue
  - Due to the heterogeneity nature of these tasks (issues and problems with MS) we need small groups within the metabolomics society to tackle it.
  - Currently under Metabolomics Society the ID group working toward standardizing such processes.
  - We have less problem for NMR as it is more quantifiable and Bruker BioSpin has a very good platform and has provided protocols from

samples preparation, samples acquisition and processing in use within universities and we should get them involved (concentration response library that can be used across field strength that can be queried).

- Chemonix have also developed a tool for NMR quantification platform for the number of instruments (different fields) and concentration response library so you only need to adjust pH for it, its limitation is that it has reference only for about 400 compounds.
- Links to ChEBI should be considered (has already 30k compounds)
- PubChem is working with NIH on tagging such functionality.
- Other existing databases: Japan DB for plants, HMDB, NIH NIST

Action items arising from the meeting:

- To set up next meeting and to invite partners from NIH common funds initiative, metabolomics society members and metabolomics standards initiative members. Also representatives from Japan, Australia, Canada and others.
- Have a better means of communicating with one another and those interested in standards effort.
- We need small working groups for the initial MSI initiative and to get it restarted and updated the requirements and working groups to reflect current trends and technologies
- We need small groups for suggesting and forming the recommendation and the entire community for consultation
- We have several initiatives that generate data and disseminate data; we need coordination amongst us backed up by substantial funding
- Closer collaboration between MSI and PSI initiatives

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	12
1:EMBL-EBI	1		
7:UB	1		
13:UBHAM	0		
Total	2	2	

Appendices

1. N/A

Background information

This deliverable relates to WP7; background information on this WP as originally indicated in the description of work (DoW) is included below.

WP7 Title: Outreach and Training
Lead: Ulrich Günther, UBHam
Participants: Ulrich Günther

This work package will provide a close link between the COSMOS consortium and the wider metabolomics and the biomedical community. We will raise community awareness for the services provided by the COSMOS consortium, from data submission support to different views on metabolomics data, but also for the increasingly stringent requirements for data availability as part of the metabolomics publication process. Through the existing framework of the Metabolomics Society, we will ensure broad community input into the services developed by the COSMOS consortium and the standards for Metabolomics data representation developed in this proposal. This deliverable relates to WP7; background information on this WP as originally indicated in the description of work (DoW) is included below.

Work package number	WP7	**Start date or starting event:**			Month 1			
Work package title	Outreach and Training							
Activity Type	COORD							
Participant number	1: EMBL-EBI	2: LU/NC	7: UB	13UBHam				
Person-months per participant	8	2	4	8				

Objectives

1. Provide link between the COSMOS consortium and the wider metabolomics and the biomedical community
2. Raise community awareness for the services provided by the COSMOS consortium
3. Collect broad community input into services developed by the COSMOS consortium

Description of work and role of participants

We will initially employ the usual channels for the disseminations of COSMOS standards, including scientific publications, and workshops and presentations at metabolomics conferences to reach the wider metabolomics community.

The project will plan activities adequately resourced devoted to dissemination for specialised constituencies and general public, in particular for awareness and educational purposes. The dissemination plan deliverable will consider adequate messages about the objectives of the project and its societal and economic impact. The tools we will use will include web-based communication, press releases, brochures, booklets, multimedia material,etc. The 'dissemination material' will be regularly updated to provide the latest version of the project status and objectives. Electronic and/or paper versions of this 'dissemination material' will be made available to the Project Officer beforehand for consultation and upon its final release. In all material produced in all dissemination activities we will properly acknowledge the source of funding by prominently placing the FP7 logo and the European Commission logo.

We will create and maintain the consortium website in an open source content management

system. The website will have an EU domain such as www.cosmos-fp7.eu. This website will have a specific COSMOS branding with a professionally designed COSMOS logo to reflect the collaborative and international nature of the consortium. The COSMOS website will allow for content management by the partners, additional component (intranet, calendar, web site search), advanced analytics, functional testing, and communication via mailing lists. COSMOS will also build close links between the COSMOS consortium and the European and International metabolomics community, and the wider biomedical community. For this COSMOS will build on existing links with other EU and International initiatives (e.g. EU projects including the ESFRI infrastructures ELIXIR, BioMedBridges, EU Openscreen, and the IRSES Word Wide NMR to build links international stakeholders in China, specifically the Wuhan metabolomics center, India, and South America). Moreover, COSMOS will build links metabolomics groups in Canada (HMDB, Wishart) and the US (BMRB; see letters of support), both running major metabolomics WEB portals. COSMOS will also build an intensive dialog between mass spectrometry and NMR instrument vendors, search engine providers, experimentalists, data resources, and journal offices. This will require travel funds for all COSMOS stakeholders. Stakeholders are key members and opinion makers of the wider metabolomics community worldwide, in particular the USA, Canada and Japan. These will be invited to workshops and the annual stakeholder meetings where COSMOS standards are disseminated. COSMOS will react dynamically to requests from participants and outside advisors. The stakeholder meetings will preferably be held attached to the annual Metabolomics society meeting or the MetaboMeeting, where the majority of the metabolomics community is present.

Two ELearning WEB tutorials on “Metabolomics Data Deposition” through COSMOS will be made available through partner websites, links from conferences, and announcements on the project web site. The tutorials will be step-by-step 20-30 minutes guides to “Metabolomics Data Deposition and Dissemination through COSMOS”.These tutorials need to be carefully scripted, rehearsed and produced in the Media Production room of the Wellcome Trust Genome Campus.We expect that COSMOS standards will be adapted quickly considering this wide-spread array of dissemination channels involved.

Task 1: Development of outreach material (Website, flyer, brochures, etc)

Task 2: Publication of results in scientific journals

Task 3: Presentation of work of the consortium at conferences, in particular the MetaboMeeting and the annual meeting of Metabolomics Society.

Task 4: Development and dissemination of a web tutorial about the workflows and standards developed in this consortium.

Task 5: Provide training workshops on Metabolomics data deposition, dissemination and access through the general EBI outreach department. (EMBL-EBI)

Deliverables

No.	Name	Due month
D7.1.1	Outreach activity plan (including publications)	2
D7.1.2	Updated Outreach activity plan (including publications)	12
D7.1.3	Updated Outreach activity plan (including publications)	24
D7.2	Report on the COSMOS consortium website	2

D7.3.1	Report on annual stakeholder meetings	12
D7.3.2	Report on annual stakeholder meetings	24
D7.4.1	Web-based tutorial	18
D7.4.2	Updated web-based tutorial	24
D7.5.1	Report about training workshops	24
D7.5.2	Report about training workshops	36