Deliverable D7.4.2

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	
	FP7-INFRASTRUCTURES-2012-1	
Deliverable title:	Updated Web-based tutorial	
WP No.	WP7	
Lead Beneficiary:	1:EMBL-EBI	
WP Title	Outreach and Training	
Contractual delivery date:	1 October 2014	
Actual delivery date:	1 October 2014	
WP leader:	Ulrich Günther	UBHam
Contributing partner(s):	EBML-EBI, IPB Halle	

Authors: Reza Salek, Michael van Vlite, Philippe Rocca-Serra and Daniel Schober

Contents

1 Executive summary

The aim of this deliverable is to report on our efforts to create tutorials for Cosmos developed resources, i.e.

1. Web-based tutorials about “Metabolomics Data Deposition and Dissemination” through out COSMOS.
    a. Using video clips
    b. Using Web based textual guides
    c. How to capture metadata
2. The usage of data exchange formats developed by COSMOS community
3. Tutorials explaining how to setup and use the new metaboloeXchange.org resource.

2 Project objectives

With this deliverable, the project has reached the following objectives:

No.	Objective	Yes	No
1	web-based tutorial about “Metabolomics Data Deposition and Dissemination” through out COSMOS	X	
2	Video clip format	X	
7	Web-based tutorials	X	

3 Detailed report on the deliverable

3.1 Background and abstract

This deliverables' main scope is to provide an update on generated didactic material for COSMOS resources, *i.e*. in the form of the web tutorials and video clips on "Metabolomics Data Deposition and Dissemination", data standards conversions and usage for metabolomics data. In addition we have new video clips added for usage and different functionalities of the metabolomxchange resource and Tutorials on the usage of Xeml Designer. This would be an update on the previous D7.4.1

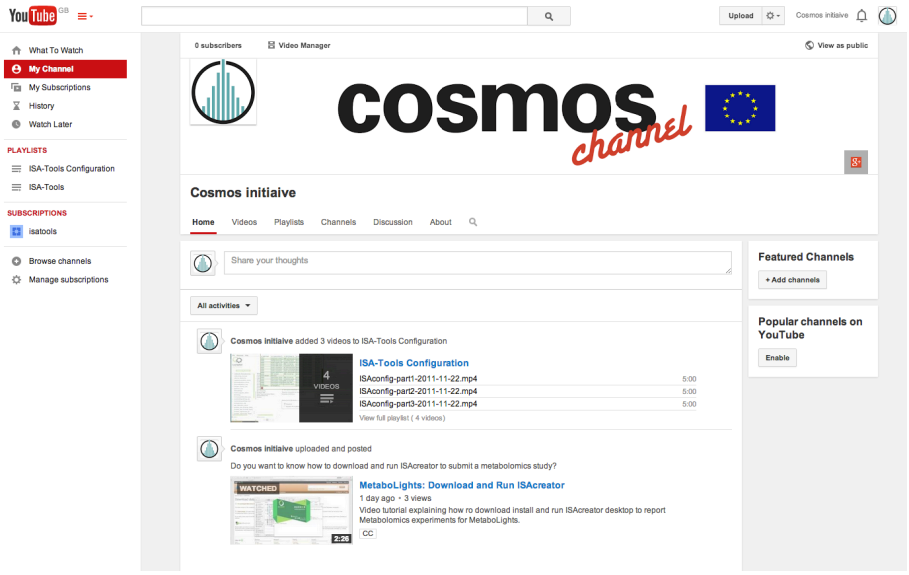
3.2 Description of Work

3.2.1 Updated video clips (YouTube channel) on metabolomics deposition and dissemination

We previously created and populated a Google plus account linked to a YouTube channel account dedicated for COSMOS related video based tutorials, This channel focused on metabolomics data deposition, dissemination, validataion and exploitation. This channel will be successively expanded to include additional tutorial videos, e.g. on metabolomics data standard conversions and content validation, e.g. according to CIMR minimal information checklists (http://biosharing.org/bsg-000175).

The COSMOS YouTube channel with the tutorial films can be found at:

https://www.youtube.com/user/cosmosfp7



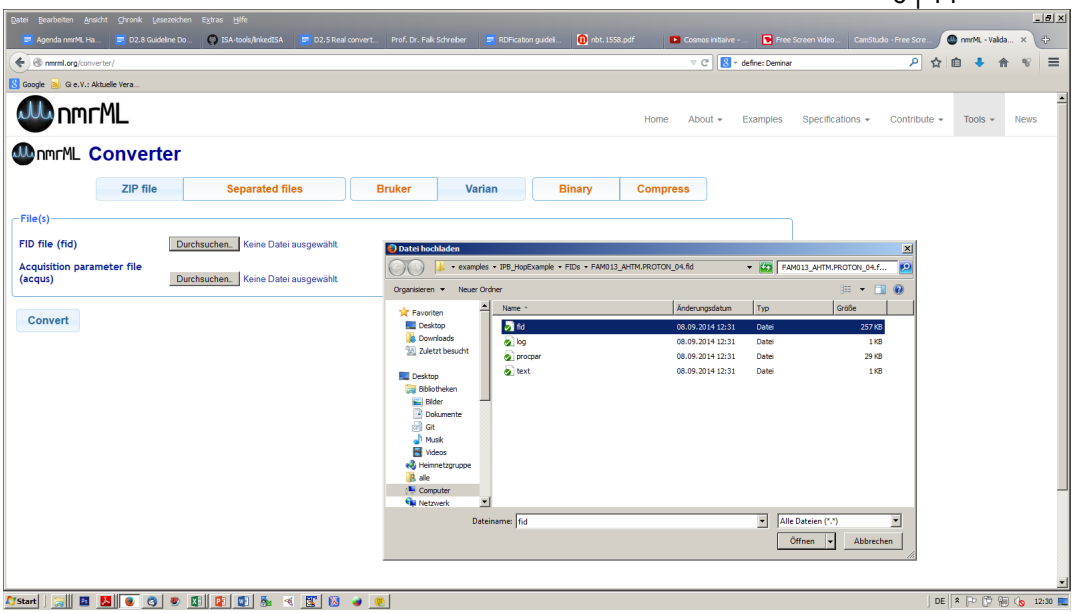
3.2.2 Web-based tutorial on data format exchange

Two new nmrML usage Tutorial Videos have been added to:

https://www.youtube.com/user/cosmosfp7

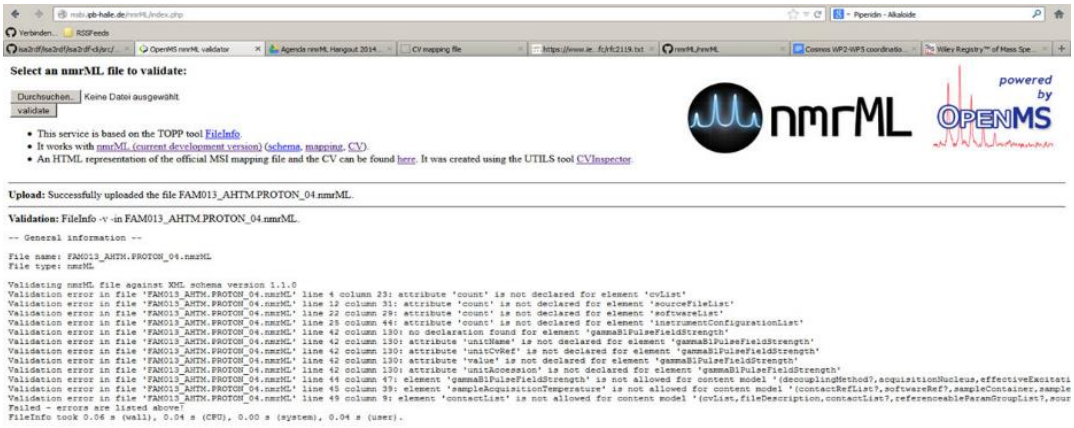
1. Vendor to nmrML Converter web-service:

This Tutorial video shows how a user can upload and convert a vendor specific NMR raw data file (Varian or Bruker) and how it is converted into the open access standard nmrML including automatic ontology term enrichment. The converter web-service with its required inputs and generated outputs is explained.



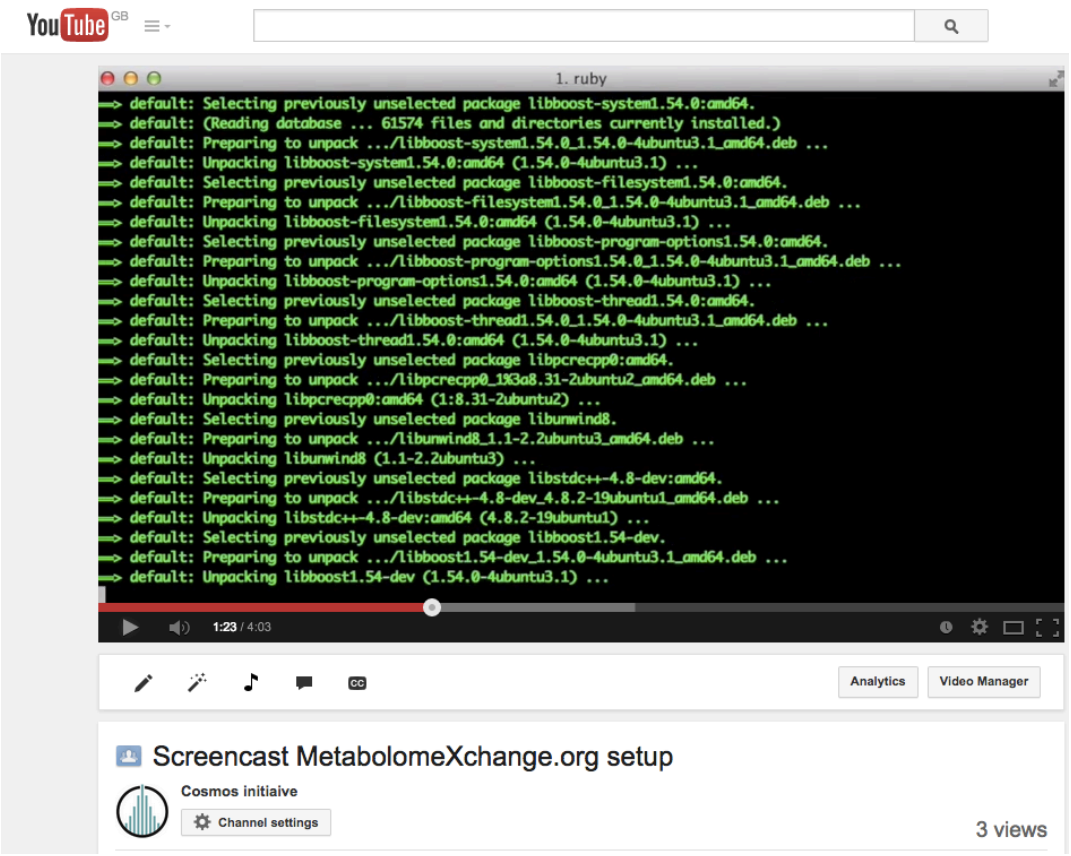
2. nmrML Data validation webs-service:

This tutorial video illustrates how a user can upload an nmrML data file to our semantic validator webservice and how the data is then checked and quality assured in multiple validation layers, i.e. how the XSD constraints the XML entities and how the semantic validator exploits mapping rules to verify that ontologies are used in the correct way at the correct positions in the nmrML data file. The provided error messages are explained and hints for correcting them are given.

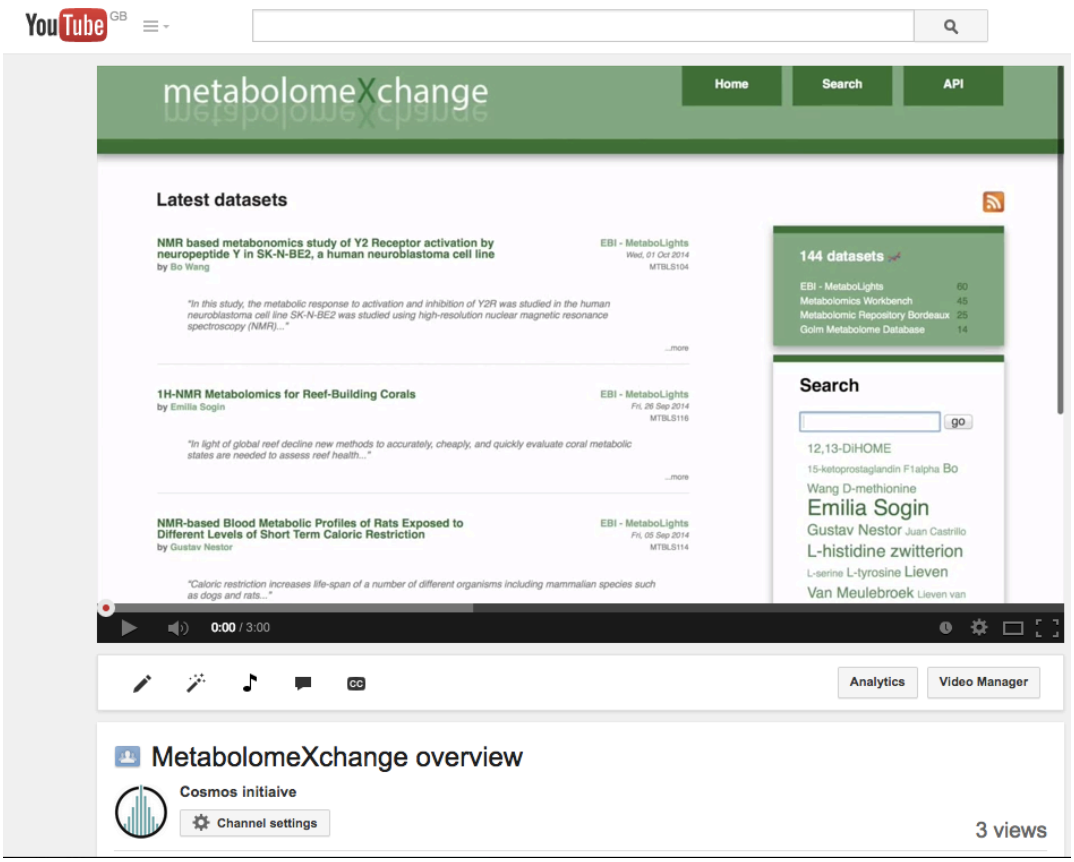


3.2.3 Web-based tutorial and screencast on metabolomexchange.org

MetabolomeXchange.org is a web application that aggregates information about Metabolomics data sets from various data repositories. A screencast was uploaded into the YouTube webpage to see how you can setup a local instance of MetabolomeXchange using Vagrant in combination with VirtualBox. Instructions are to install VirtualBox and Vagrant before downloading and running the Vagrant scripts from the Github of metabolomexchange-vagrant reposetory. The instruction are for people to contribute to the MetabolomeXchange codebase, and not a setup one in a production environment.



A second screen case explains general navigation and usage of the MetaboloeXchange portal.



3.2.4 A tutorial and screenshots on XEML usage

This tutorial and guideline explains all main functionalities of the Xeml Designer. This tutorial will cover topics such as: how to design your experiments using environmental ontology terms, how to build your experimental “story-line” with a timeline visualization and how to import data from tabular files and many others feature.

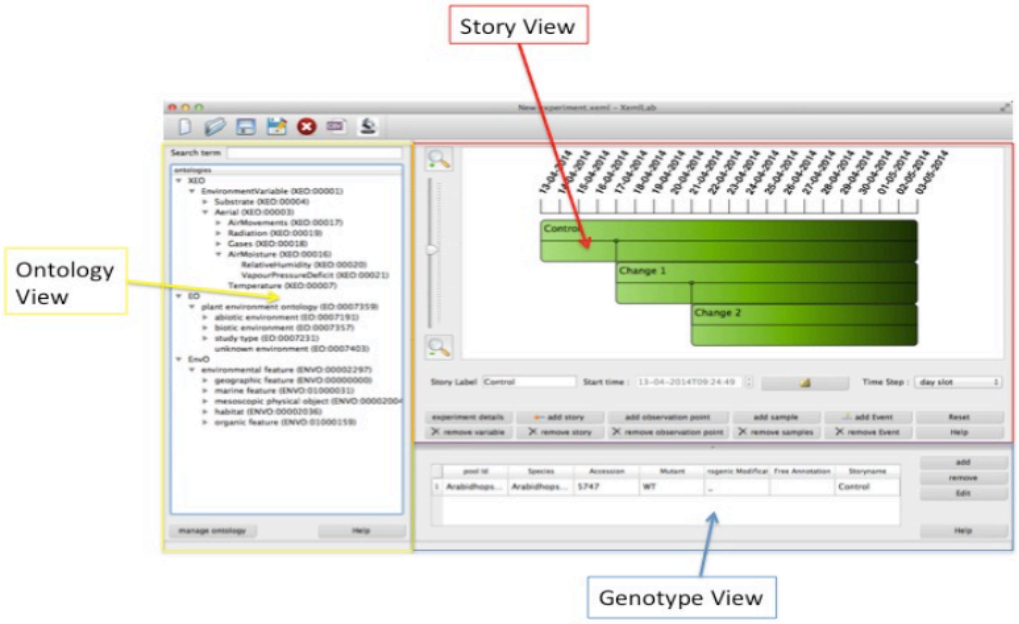
and the link where you can find the tutorial : https://github.com/cbib/XEML-Lab/blob/master/doc/XemlDesigner_Tutorial.pdf

In summary The Xeml Lab Designer:

- Describe Experiment in term of experiment Time (start date and end

date for the header story) experiment time will be further translate into numbers of days, hours, minutes and seconds in the xeml document.

- Add substories (split story) to the header story for different experimental conditions (you can set the time point by dragging the split story to the correct time position).
- Add Observation points to the given time point (you can set the time point by dragging the observation point icon to the correct time position).



Describe your Observation Point by adding observations (samples). A wizard helps users to document observation Point but you first need to describe a genotype related to your samples.(all genotypes are inherited by child stories).

3.3 Next steps

1. Adding more content to the COMSOS YouTube channel

2. Providing similar video clips or tutorials on usage of other resources with COSMOS partners

3. Extending the data format tutorials for nmrML and mzML.

4 Publications

N/A

5 Delivery and schedule

The delivery is delayed: Yes ☑No

6 Adjustments made

No adjustments done

7 Efforts for this deliverable

Institute	Person-months (PM)		Period
	actual	estimated	
1:EMBL-EBI	0.5		24
7:UB			
12:IPB	0.5 (in kind)		
2:LU	0.3 (in kind)		
12:UB2	0.2 (in kind)		
Total	1.5	2	

Appendices of websites

1. http://cosmos-fp7.eu
2. http://cosmos-fp7.eu/nmrML/
3. www.nmrml.org
4. https://github.com/nmrML/nmrML/tree/master/docs
5. http://sourceforge.net/projects/cosmos-fp7/
6. http://www.ebi.ac.uk/training/online/course/introduction-metabolomics
7. http://www.ebi.ac.uk/training/online/course/metabolights-quick-tour-0
8. https://www.youtube.com/user/cosmosfp7
9. https://www.youtube.com/user/isatools
10. http://nmrml.org/tutorials/

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:**			Month1			
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 WordWide 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 wil lbe 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