Deliverable D7.4.1

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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Lead Beneficiary:	1:EMBL-EBI	
WP Title	Outreach and Training	
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WP leader:	Ulrich Günther	UBHam
Contributing partner(s):	EBML-EBI, IPB	

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1 Executive summary

The aim of this deliverable is to created tutorials for:

1. A web-based tutorial about “Metabolomics Data Deposition and Dissemination” through out COSMOS.
    a. Using video clips
    b. Using Web based guide
2. A Web-base tutorial on introduction to metabolomics
3. A Web-base tutorial on data deposition to MetaboLights (metabolomics experimental repository)
4. A Web-base tutorial on usage of data exchange formats developed by COSMOS community

2 Project objectives

With this deliverable, the project has reached or the deliverable has contributed to 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 create e-learning, web tutorials and video clips on "Metabolomics Data Deposition and Dissemination", *i.e.* tutorials on the subject of metabolomics, on data deposition to MetaboLights repository and on the data format conversion workflows currently being developed by COSMOS such as nmrML and mzML.

3.2 Description of Work

3.2.1 e-learning web-based tutorial for introduction to metabolomics as a technology

This course provides a basic introduction into the rapidly emerging field of metabolomics and its importance and applications (Figure 1). The level of the course is basic and requires only an undergraduate-level understanding of biology (Figure 2).

Learning objectives:

- Comprehend the purpose and importance of the field of metabolomics
- Describe some principles of metabolomics study design
- Evaluate advantages and limitations of some analytical techniques used in metabolomics studies
- Discuss some of the modern-day applications of metabolomics

The metabolomics online course is free and hosted by the EMBL-EBI training website, one of the most widely used data resources within Europe. The course is designed in a way that no previous expertise in metabolomics or bioinformatics is required. The main idea is to encourage users to learn in their own time and at their own pace about metabolomics in general. The courses could be repeated as many times as required, or to just complete part of a course that is of interest.

Finally we provide links and means to access metabolomics resources at the EMBL-EBI (Figure 3). The e-learning courses makes the most of EMBL-EBI data resources and tools provided as well as links to other courses, workshops and conferences.

This course is linked to resources from EMBL-EBI on metabolomics data deposition and dissemination, such as MetaboLights (http://www.ebi.ac.uk/metabolights) for metabolomics experimental data deposition and ChEBI (http://www.ebi.ac.uk/chebi/) a resource on small molecules and metabolites and finally Reactome (http://www.reactome.org) for chemical reaction. ChEBI, EMBL-EBI's database of **Ch**emical **E**ntities of **B**iological **I**nterest, is a freely available, manually annotated database of small molecular entities (molecules not encoded by the genome). These could include any constitutionally or isotopically distinct atom, molecule, ion, ion pair, radical, radical ion, complex, conformer, or anything else that is a separately distinguishable entity. ChEBI focuses on chemical nomenclature and structures, and provides a wide range of related chemical data such as formulae, links to other databases and ontology for the chemical space. It aims to bridge the gap between small molecules and the macromolecules with which they interact in living systems. Reactome, aims to represent all human biological processes as interconnected molecular events or 'reactions'.

The link for this course can be found here:

http://www.ebi.ac.uk/training/online/course/introduction-metabolomics

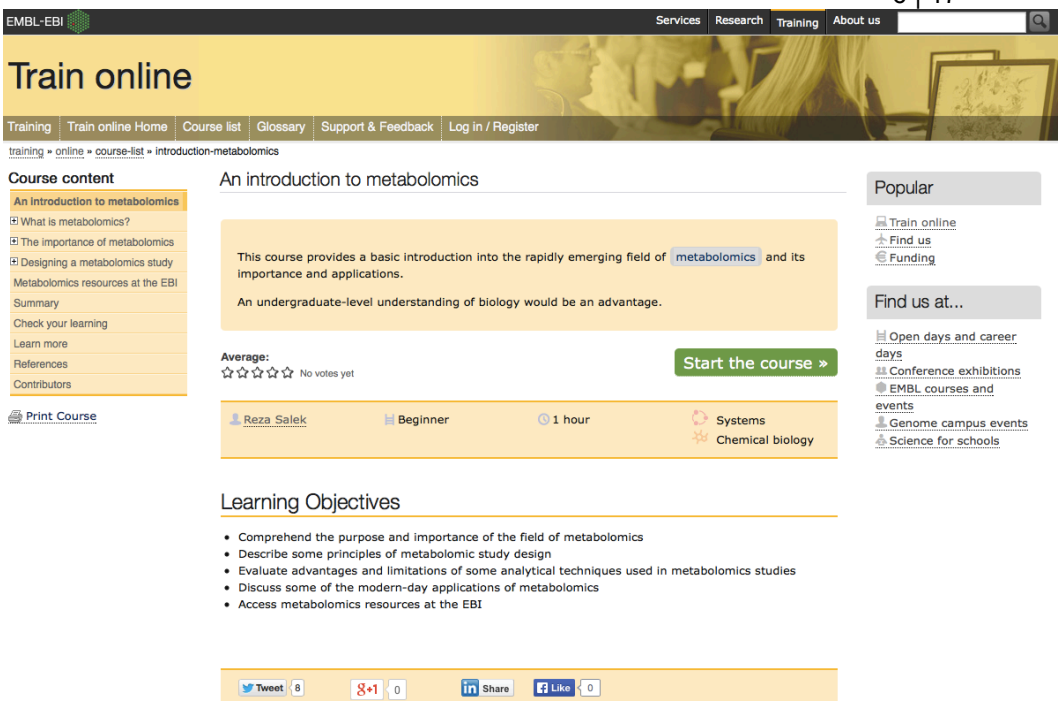


Figure 1 General layout and landing page of the e-learning website

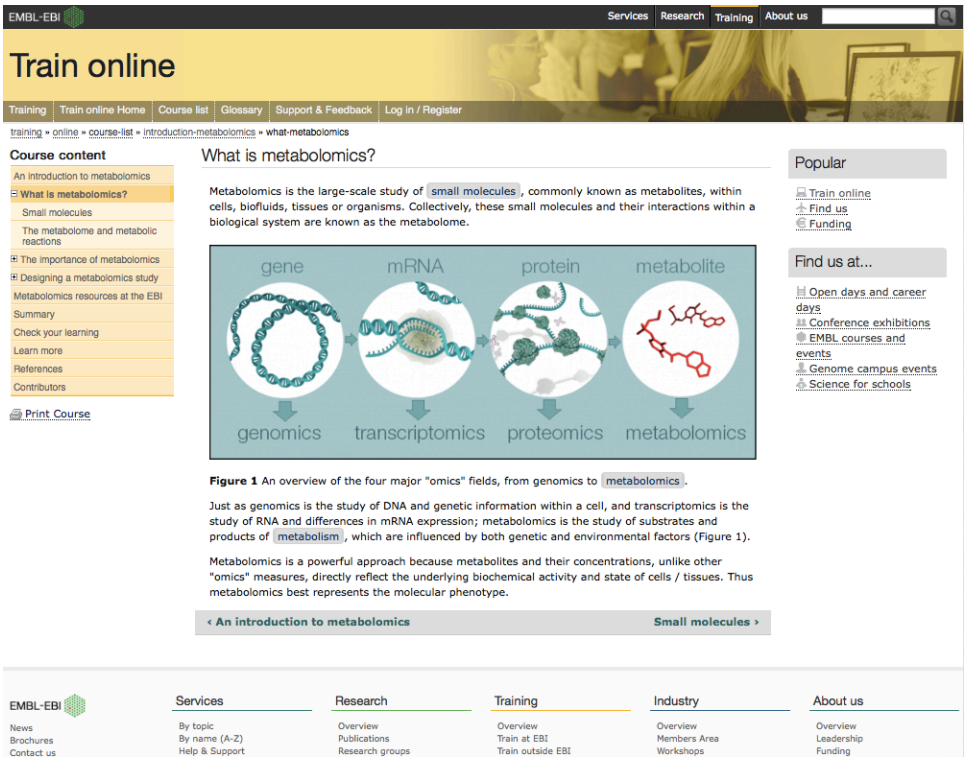


Figure 2 Course general layout page

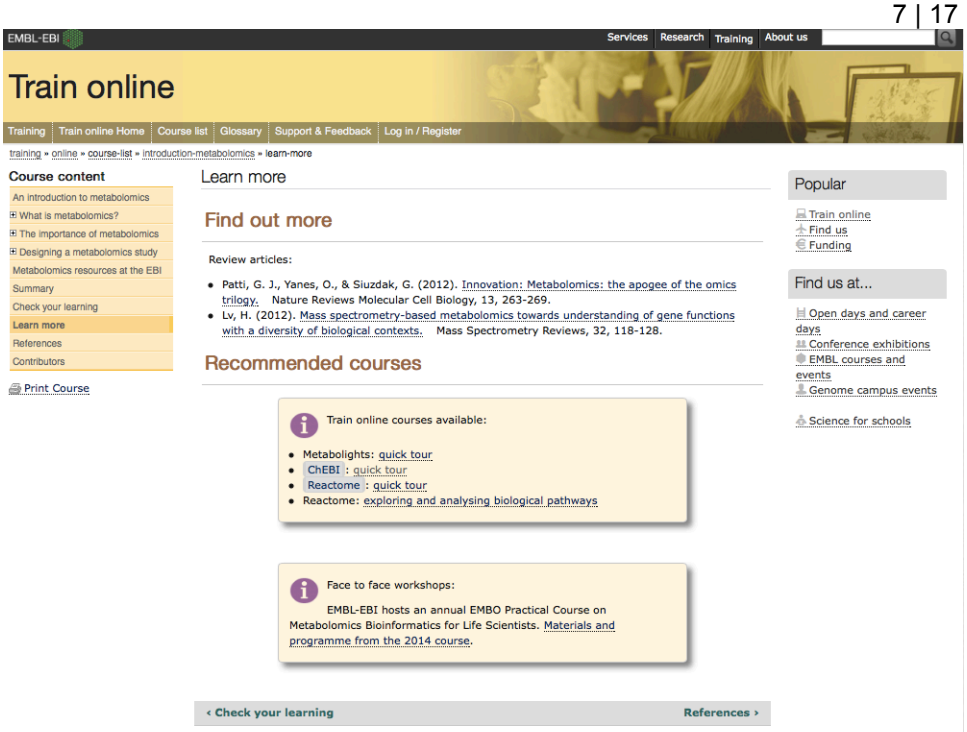


Figure 3 links to resources from EMBL-EBI on metabolomics data deposition and dissemination, such as MetaboLights for data deposition and ChEBI for resource on small molecules and metabolites and finally Reactome for chemical reaction

3.2.2 e-learning web-based tutorial on metabolomics deposition and dissemination

This course gives an overview as well as an introduction to MetaboLights, the first general purpose, open access repository for metabolomics studies, their raw experimental data and associated metadata, maintained by one of the major open access data providers in molecular biology (Figure 4).

MetaboLights consists of two distinct layers:

1) a **repository**, enabling the metabolomics community to share findings, data and protocols for any form of metabolomics study;

2) a **reference layer** of curated knowledge about metabolite structures and their reference spectra, as well as their biological roles, locations, concentrations, and raw data from metabolic experiments.

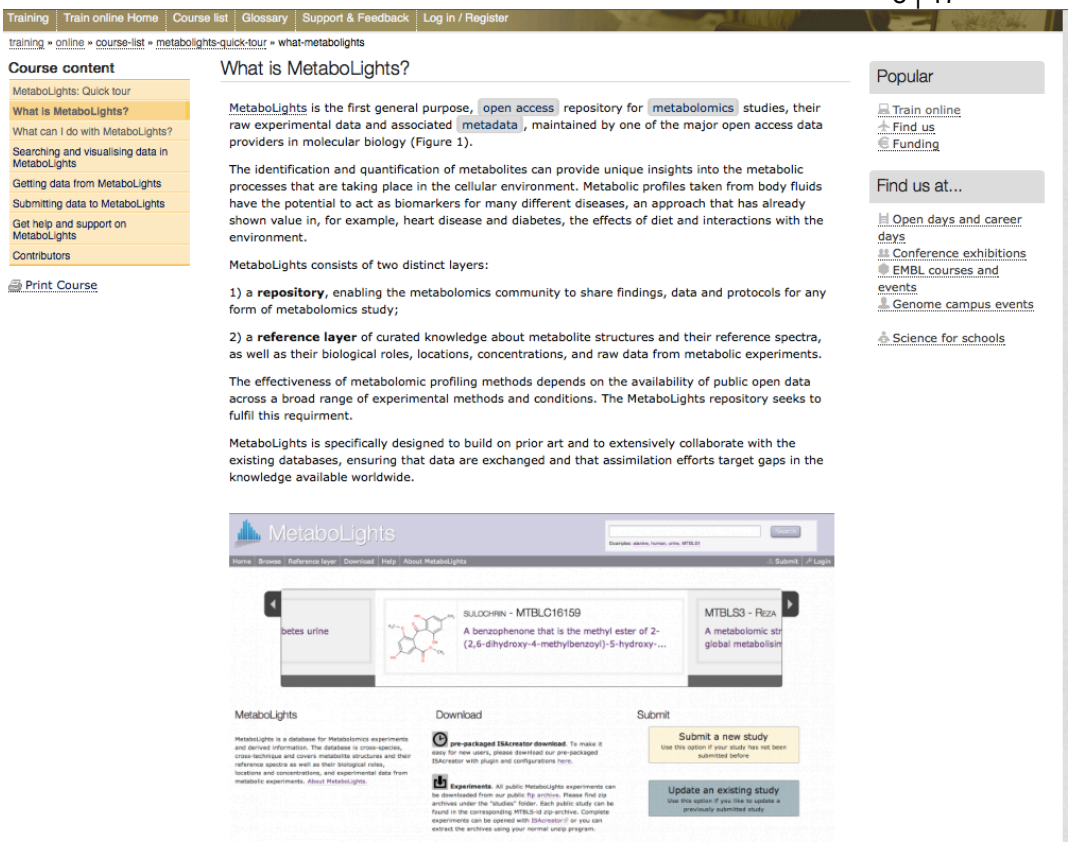


Figure 4 An e-learning course on overview and the usage of MetaboLights, metabolomics data deposition and dissemination resource

This course assists with using MetaboLights to:

- Find metabolites and related metabolomics studies by searching a wide range of associated metadata.
- Filter your search results on species, techniques and metabolites.
- Submit public or private studies.
- Steps required for receiving a stable and unique accession number that can be used as a publication reference.
- Share private studies with collaborators/peer reviewers.
- Download public metabolomics studies for further analysis.
- Retrieve molecular information from ChEBI or other linked compound databases.

Link to the resource:

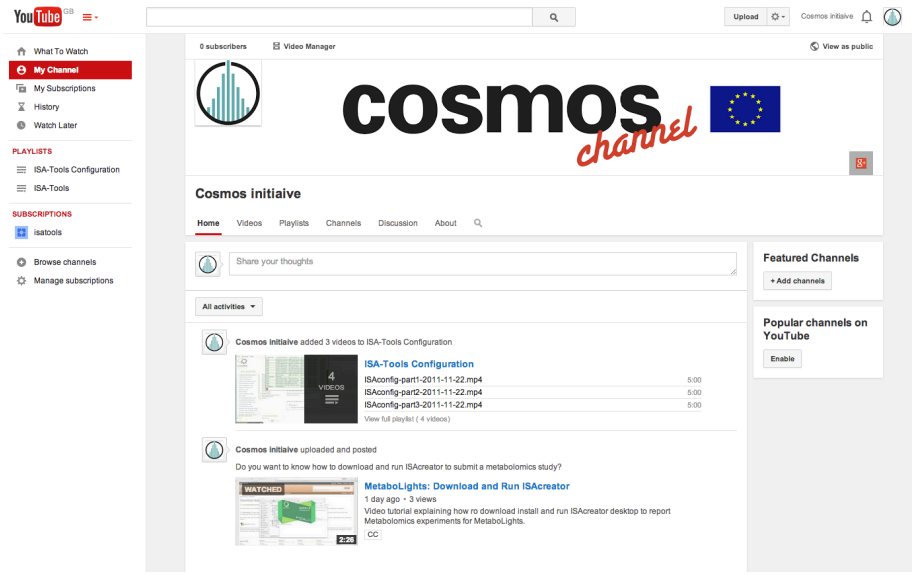
http://www.ebi.ac.uk/training/online/course/metabolights-quick-tour-0

3.2.3video clips (YouTube channel) on metabolomics deposition and dissemination

We have created and populated a Google plus account linked to a YouTube channel account dedicated for COSMOS related video based tutorials focused on metabolomics data deposition and dissemination. Using the facilities based on EMBL-EBI campus and the Wellcome Trust Genome media center, we have created video clips on how to collect metadata and the submission steps required for data deposition into MetaboLights using ISA-Creator tools. This channel will be successively expanded to include additional tutorial videos, e.g. on metabolomics data standard conversions.

The COSMOS channel can be found at:

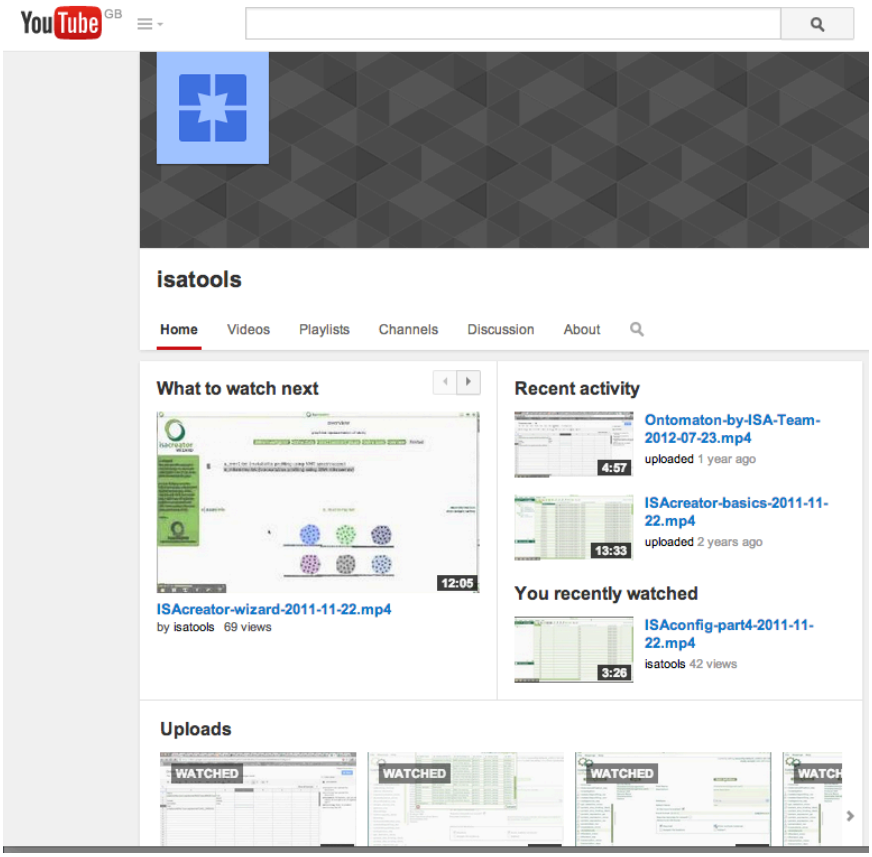
https://www.youtube.com/user/cosmosfp7



In addition we have linked our account with UOXF partner (University of Oxford) that develops ISA-Tools with their video based tutorial and hands on usage of the ISACreator and OntoMaton -- Ontology Search &Tagging for Google Spreadsheets. OntoMaton, a tool which allows users to search for ontology terms

and tag free text right in Google Spreadsheets. This video clip aims to introduce ISA-tools, and to provide instruction on how the tools work.

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



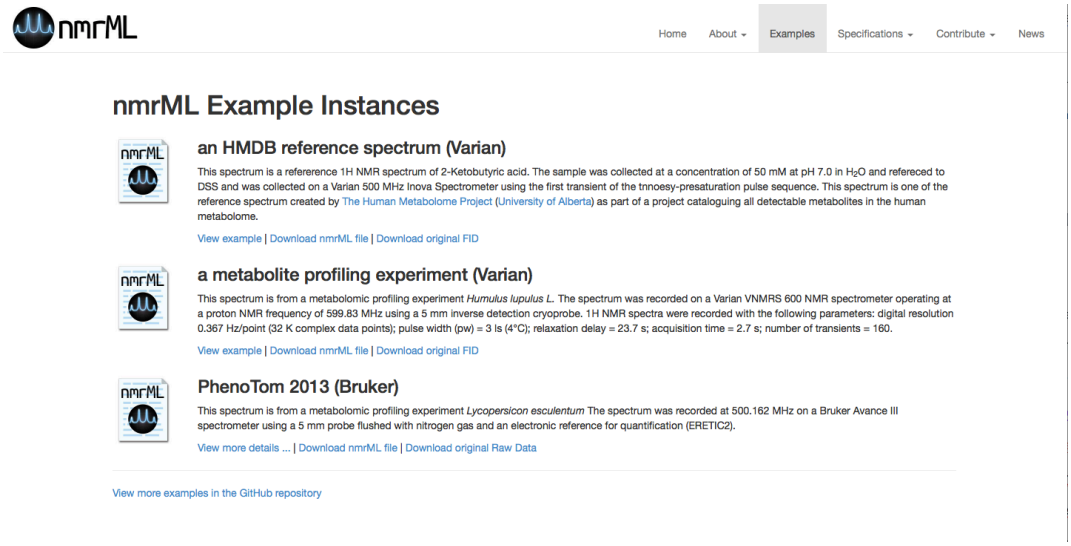
We also have created a comprehensive step-by-step guide on data deposition into MetaboLights using Google documents. This online document and tutorial would be continually updated and modified with new changes as required by MetaboLights repository. This document can be found at:

https://docs.google.com/document/d/1kvBdnleInVr1UMyV-sm91w2uK_IfkU11Rx-uxvILOFU/view

3.2.4Web-based tutorial data format exchange

nmrML is one of the new standards that are being developed within the COSMOS project and will hopefully adopted by a wide academic and commercial

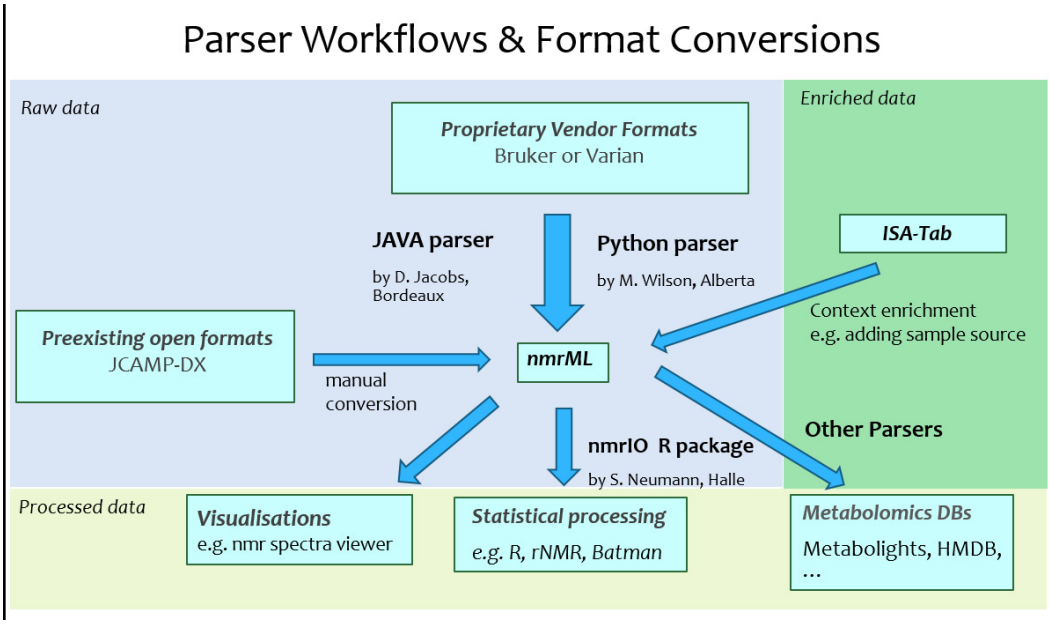
stakeholders. Its development requires collaboration with partners outside the consortium, including the wider NMR and metabolomics community. Our goal is to obtain an agreement on an open defacto standard NMR file format, which would be proprietary independent, and which can be implemented into any software used for NMR data exchange and processing. So far we have established a collaborative effort within the nmrML work-frame (multiple EU partners) with David Wishart's metabolomics groups in Canada. For the COSMOS nmrML subgroup, we have a separate website based on the MediaWiki platform to host and share information related to developments of the nmrML file format, please see: http://cosmos-fp7.eu/nmrML/. The user base would eventually be open to the public for anyone interested in the nmrML file format to participate and to contribute to the documentation. Implementing the Wikimedia service fulfills the requirements of making available the results of the collaborative nature of COSMOS with the wider metabolomics and NMR community.



Aside from the documentation in the nmrML wiki, a Github repository for the format exchange has been setup and it in use. We have created browser friendly HTML tutorial resources, which elaborate on typical reoccurring format conversion workflows and can amplify each step with initial examples of data in the respective formats. The particular data examples require constant updating to match the upcoming XSD changes, which are needed to allow re-use of the Open MS

semantic data validator software. A placeholder-landing page for the nmrML format tutorials can be found under http://nmrml.org/tutorials/

A PowerPoint presentation which contains the following conversion scheme can be found: https://github.com/nmrML/nmrML/blob/master/docs/SchemaDocumentation/nmrM_at_PSI.pptx



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 exchange tutorial for nmrML and mzML related to metabolomics.

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	1	6	18
13:UB			
12:IPB	1 (in kind)		
14:OXFU	1 (in kind)		
Total	3		

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