# Deliverable D12.1

<table>
<thead>
<tr>
<th>Project Title:</th>
<th>Building data bridges between biological and medical infrastructures in Europe</th>
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<tbody>
<tr>
<td>Project Acronym:</td>
<td>BioMedBridges</td>
</tr>
<tr>
<td>Grant agreement no.:</td>
<td>284209</td>
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<tr>
<td>Research Infrastructures, FP7 Capacities Specific Programme; [INFRA-2011-2.3.2.] &quot;Implementation of common solutions for a cluster of ESFRI infrastructures in the field of &quot;Life sciences&quot;</td>
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<tr>
<td>Deliverable title:</td>
<td>Documentation from workshops 1 and 2</td>
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<tr>
<td>WP No.</td>
<td>12</td>
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<td>Lead Beneficiary:</td>
<td>1: EMBL</td>
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<tr>
<td>WP Title</td>
<td>Training</td>
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<tr>
<td>Contractual delivery date:</td>
<td>31 December 2013</td>
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<tr>
<td>Actual delivery date:</td>
<td>23 December 2013</td>
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<tr>
<td>WP leader:</td>
<td>Cath Brooksbank</td>
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<td>Contributing partner(s):</td>
<td>1: EMBL</td>
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Authors: Tom Hancocks and Cath Brooksbank
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1 Executive summary

— This deliverable summarises the first two workshops run by WP12 Training as part of the BioMedBridges project.

— Practical solutions with ontologies, our first knowledge-exchange workshop for project partners, brought together ontology experts with domain experts who had little or no previous experience of using ontologies.

— Computational aspects of high-throughput screening; planning and analysis enabled us to disseminate one of the BioMedBridges’ early deliverables, the UniChem resource, to EU-OPENSSCREEN and others working on chemical screening.

— During both workshops we used ‘living documents’, which could be simultaneously edited by all the participants, to capture information on the delegates’ needs and expectations, and to address these.

— Subsequent work on these living documents is converting them into openly available documentation on the BioMedBridges website.

2 Project objectives

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

<table>
<thead>
<tr>
<th>No.</th>
<th>Objective</th>
<th>Yes</th>
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<tr>
<td>1</td>
<td>Deliver short courses to train project participants in relevant areas of bioinformatics that are outside of their current experience and necessary to build crosslinks between the data resources of the BMS RIs</td>
<td>x</td>
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<td>2</td>
<td>Produce documentation on the resources developed, for use initially within the project but ultimately by the end-users of the integrated services developed by BioMedBridges</td>
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<tr>
<td>3</td>
<td>Deliver short courses enabling end-users of the biomedical research infrastructures to benefit from the developments of work packages 3–11</td>
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3 Detailed report on the deliverable

3.1 Background

This report describes the first two workshops run by WP12 – Training – within the BioMedBridges project as part of deliverable 12.1 due for completion at the end of month 24 (December 2013). Task 1 focuses on internal training – through knowledge exchange workshops. These workshops are intended to disseminate key knowledge and skills among the project partners, providing access to state-of-the-art knowledge on technologies required to deliver the project. Task 2 focuses on delivering workshops aimed at end-users of BMB's products and services.

3.2 Workshop 1: Practical solutions with ontologies

3.2.1 Workshop overview

This knowledge-exchange workshop ran on 4-5 March 2013 at the EMBL-EBI, Hinxton, UK. The programme and course materials are available at www.biomedbridges.eu/trainings/knowledge-exchange-workshop-practical-solutions-ontologies. The purpose of the workshop was to raise awareness of ontologies, show how they can be used within the project and to spread basic skills in working with them.

The workshop combined presentations, discussions and hands-on practicals. This encouraged participants to consider how to resolve common data-sharing and integration problems within the project. Those new to the field were provided with a basic introduction to ontologies and how they are used in the molecular life sciences by Robert Stevens, a globally acknowledged leader in the bio-ontologies field; they were also introduced to freely available online ‘catalogues’ of ontologies and to other resources that would help them to gain confidence in using ontologies. Participants were requested to give a flash presentation summarising what they needed to describe using ontologies. Ontology experts from within the project gave presentations on how they are
using ontologies to develop BioMedBridges services, including the combination of parts of existing reference ontologies to build application ontologies. The participants worked together to map potentially useful ontologies onto specific use cases. The experienced ontologists were able to advise the novices on issues such as deciding whether it’s necessary to use an ontology, re-use of existing ontologies, and simple methods for getting input from domain experts who are not confident ontologists. The workshop also covered the role of ontologies in the wider framework of interoperability, touching on topics such as the semantic web and the use of RDF to describe data.

3.2.2 Workshop participants

A total of 26 people participated in the workshop, including representatives from 6 ESFRI-BMS RIs. Participants ranged in their previous experience of using and creating ontologies from complete novices to experts in the field.

![ESFRI BMS workshop participants](image)
3.2.3 Documentation from the workshop

During the workshop, participants contributed to a shared ‘living document’. This Google Doc allowed real-time note taking and documentation of the
training as it occurred, drawing out frequently asked questions and providing answers to them as the workshop progressed.

WP12 members used the document to record important points of interest as well as provide links to referenced papers and to websites that contained tools, resources or information. Questions asked by participants were also transcribed, along with the answers given by trainers. Additionally participants could ask their own questions using the document. These were followed up and answered by trainers after their session had been completed. It was also used to facilitate networking and exchange of contact information.

Outcomes of the workshop include the following:

- Raised understanding of ontologies amongst project members, and how they are currently being used
- Linked up the less confident ontologists with experts.
- Dissemination of practical knowledge in constructing, combining and utilising ontologies
- Creation of a list of ontologies that are used by, or of benefit to BMB partners
- Identification of BMB partner needs for ontologies by experts working in the field

These outcomes will help the BMB partners, especially those who are less experienced in using or developing ontologies, to develop products and services for the project. Some partners will make direct use of ontologies in their deliverables (standard development in WP6; phenotype mapping in WP7), while it will help others to make use of BioMedBridges WP3 Service Registry.

Documentation derived from the living document is available on the BioMedBridges webpage for the training event:


Additional materials from the workshop can also be found there.
3.2.4 Workshop feedback

Feedback was gathered at the end of the workshop to understand what participants thought of the event, and to identify where improvements could be made to future workshops. 6 participants completed the feedback survey following the course. 2 rated the course excellent and 4 rated the course as good. The feedback response rate was disappointing and we took steps to ensure a higher feedback rate for workshop 2.

One common theme in the feedback we received was a request for more practical sessions on creating ontologies. This is an area that a future workshop could address although we would have to set careful prerequisites to ensure that all participants would benefit from the practicals.

Positive comments were made about the living document created during the workshop. This led to further work on how best this method could be used in future training events.

3.3 Workshop 2: Computational aspects of high-throughput screening, planning and analysis

This workshop, aimed at end-users of ESFRI-BMS RIs, ran on the 14-16 October 2013 at EMBL Heidelberg, Germany. It was planned in collaboration with EU-OPENSSCREEN (represented by Umeå University) and ELIXIR (represented by EMBL). The purpose of the course was to explore the available approaches for computational work prior to conducting high-throughput screens of chemical libraries.

3.3.1 Workshop overview

This workshop ran on 14-16 October 2013 at the EMBL Advanced Training Centre, Heidelberg, Germany. The programme and course materials are available at:

The course introduced the basic concepts of chemical screening to researchers working in a wide range of life-science backgrounds. The trainers outlined each step in the chemical screening process, provided useful resource links, and ran short practical demonstrations. There was a focus on open-access resources and software (such as ChEMBL, PubChem, ZINC and KNIME). Sessions delivered by industry representatives provided explanations of the challenges faced by ‘big pharma’, important criteria to consider in assay validation and solutions to finding suitable targets in a cost-effective manner.

### 3.3.2 Workshop participants

A total of 23 participants attended the workshop. 4 participants attended from Umeå University, which is a partner in the EU-OPENSCREEN RI. 2 participants working on the EU-OPENSCREEN project in Germany were also in attendance.

In addition, 12 trainers were involved in course delivery, and the majority stayed throughout the event. They included: Tom Hancocks and Jon Chambers from EMBL-EBI (both involved in BioMedBridges); Per-Anders Enquist and Anna Linusson from Umeå University (Umeå University is responsible for EU-OPENSCREEN’s training work package); Anne Hersey and George Papadatos from ChEMBL at EMBL-EBI (EMBL-EBI leads EU-OPENSCREEN’s chem & bioinformatics/e-Infrastructure work package); John Irwin from the University of Toronto; Jeremy Everett from University of Greenwich; David Murray from AstraZeneca; Steffen Renner and Peter Ertl from Novartis; Joe Lewis from EMBL Heidelberg’s chemical screening lab. The workshop took place in Heidelberg so that the EU-OPENSCREEN delegates could benefit from a tour of the chemical biology facilities at EMBL.

During the course Per-Anders Enquist introduced the participants to EU-OPENSCREEN and the aims of the infrastructure. Several participants made enquiries about participation in the project and how to be involved further in future. Tom Hancocks introduced BioMedBridges to participants and explained the problems the project is attempting to solve. Jon Chambers presented the UniChem tool developed as part of WP4 and WP5 to provide cross-references between chemical structure identifiers from different
databases. This demonstrated the work BMB is involved in to solve integration and data sharing problems in the chemical screening community.

**Figure 4** ESFRI BMS Bridges

**Figure 5** Participants’ country of origin
3.3.3 Documentation from the workshop

Following on from the successful introduction of ‘living documents’ in the ontologies workshop, we used the same technique to document ‘Computational aspects of high-throughput screening, planning and analysis’.

Outcomes from the workshop include:

- Raised understanding of chemical screening strategies
- Dissemination of practical knowledge on how to use open-access resources and software, including the BioMedBridges UniChem tool
- Increased awareness of ESFRI-BMS research infrastructures

Documentation derived from the living document is available on the BioMedBridges webpage for the training event:


Additional materials from the workshop, including trainers’ presentations, can also be found there.
3.3.4 Workshop feedback

23 participants and 5 trainers completed the feedback survey following the course. 10 rated the workshop excellent, 13 rated it very good and 5 rated it good.

The ratio of trainers to participants provided a highly conducive atmosphere for discussion, scientific debate and problem solving. Participants were able to spend time speaking with trainers following their talks, gain additional insights and to ask questions in relation to their own work. Exposure to both academic and industry scientists was a positive outcome of the event for many participants.

4 Delivery and schedule

The delivery is delayed: ☑ Yes ☐ No

5 Adjustments made

None

6 Background information

This deliverable relates to WP 12; background information on this WP as originally indicated in the description of work (DoW) is included below.

WP 12 Title: Training  
Lead: Cath Brooksbank (EMBL)  
Participants: EMBL

This work package will provide training on the tools and services developed within the BioMedBridges project.

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<th>Work package number</th>
<th>WP12</th>
<th>Start date or starting event:</th>
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<tr>
<td>Activity Type</td>
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Participant number | 1:EMBL
Person-months per participant | 42

Objectives

1. Deliver short courses to train project participants in relevant areas of bioinformatics that are outside of their current experience and necessary to build crosslinks between the data resources of the BMS RIs.
2. Produce documentation on the resources developed, for use initially within the project but ultimately by the end-users of the integrated services developed by BioMedBridges.
3. Deliver short courses enabling end-users of the biomedical research infrastructures to benefit from the developments of work packages 3–11.

Task 1: Workshops for project participants and documentation of resources developed

This task will deliver four workshops aimed at the BioMedBridges project participants during the first three years of the project, beginning towards the end of year 1. The topics of these workshops will be defined by the personnel working on each of the technical work packages, and coordinated by a full-time scientific training and outreach officer whose duties will be divided between this work package and WP2 (outreach). This individual will maintain an overview of the entire programme, work with the representatives from the technical work packages to develop the programmes for each workshop, ensure that the workshops are promoted effectively to relevant people within the project, and chair each workshop. The personnel working on the technical work packages will therefore need to dedicate a small but significant part of their time (estimated at two person months per work package throughout the project) to developing their workshop programmes and delivering training.

Workshop topics

Suggested topics include (but are not limited to) the following. This is likely to evolve, and workshop topics may merge or become further specialised as the project progresses.

- Practical solutions to interoperability standards development. This workshop will be led by WP3 (standards) and the main target audience will be WP4 (technical integration). The goal will be to enable those integrating the different BMS RI data sets to do so using an agreed set of standards and molecular identifiers defined by WP3. Input from the use cases will ensure that discussions and actions remain rooted in practical solutions to real data integration problems. The technology watch group will select trainers who can educate the delegates about any new...
developments beyond BioMedBridges that might provide solutions to ongoing interoperability problems within the project.

- Practical solutions to secure data access. This workshop will be led by WP5 (Secure access) and the main target audience will be WP4 (technical integration). The goal of the workshop will be to enable those constructing the links between the BMS RIs’ data sets to do so in a way that respects the rights of patients and healthy volunteers without impeding legitimate research. This workshop will include sessions led by experts on ethical and legal aspects of personal data sharing, and may involve representatives from patient groups.

- Practical solutions to development of web services. This will be led by WP4 (technical integration) and the main target audience will be the use cases (WPs 6–10). The goal will be to inform the development of programmatic access to integrated data sets spanning several BMS RIs and to develop workflows that reflect the needs of researchers using the BMS RIs. Input from the use cases will ensure that discussions and actions remain rooted in practical solutions to real data integration problems. The technology watch group will select trainers who can educate the delegates about any new web service or search technologies beyond BioMedBridges.

- Practical solutions to database development and interoperability. This will be led by WP4 (technical integration) and the target audience will be the use cases. The goal of the workshop will be to stimulate the development of integrated search tools spanning multiple BMS-RIs. This workshop will also include opportunities for the different use cases to learn from each other.

Workshops will be short and intensive (2–3 days), based on a combination of presentations, discussions, practical computer-based problem solving, and documentation writing. Each workshop will be hosted by a different BMS RI.

As these workshops are intended to define, and begin to action, a set of practical solutions, numbers of delegates will be kept small and that the ratio of trainers to delegates high – typically 5 trainers and 20 delegates in each workshop making 25 in total. Logistics and administrative support (registrations, inviting trainers, travel arrangements, answering delegates’ queries, etc.) will be provided by the BioMedBridges Project manager with support from the EMBL-EBI’s Outreach and Training Team. We will use events management systems and standard operating procedures that are already successfully running at the EMBL-EBI. The fact that we have considerable experience of running courses and workshops, and tried and tested systems for doing so, represents excellent added value for BioMedBridges.

Documentation

An outcome of each workshop will be the production of documentation to support the target audience of each workshop in implementing what they have learned. The trainers and trainees will take joint responsibility for writing clear guidelines for a specific topic. On the last day of each workshop, the delegates will define a set of frequently asked questions, and will work with the speakers/trainers to produce a clear set of answers. The BioMedBridges Scientific Training Officer will compile, edit and make this documentation available, initially to project members, and ultimately to end-users of the services developed by BioMedBridges. Members of personnel from the technical work packages will take responsibility
Task 2: Training for end-users of the BMS RIs.

In the fourth year of the project we will deliver training to end users of the integrated services developed by BioMedBridges. We will deliver two courses, which will be a combination of lectures, demos, discussions and hands-on computer-based tutorials. Personnel from the use cases will deliver these courses, and each course will be aimed at a different target audience – one focused on fundamental research, the other on translational and clinical research. By the end of year 3 of BioMedBridges, we anticipate that the individual BMS research infrastructures will be funded and are likely to be running training programmes for their own stakeholders. Using materials developed for the abovementioned courses, and our extensive network of training contacts developed through other initiatives such as the IMI Education and Training projects, we will also make the most of any opportunities to support these training programmes. We will also identify appropriate conferences at which we can offer training workshops.

7 Attachments

1. Workshop 1 – documentation:

2. Workshop 2 – documentation: