ISBE Infrastructure for Systems Biology Europe

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Definition of ISBE overlap and synergies-

How can ISBE operate in the landscape of accessible European infrastructures

Workpackage 5

Synergies and Community Building

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1. Background information

A. Objectives of WP5

The ISBE Work package 5 (WP5), Synergies and Community Building, aims to identify and engage with relevant European stakeholders, including

- researchers who already see themselves as systems biologists
- those who do not, but would benefit from the ISBE infrastructure
- broader groups of stakeholders like clinical researchers, industry, the media, policy makers, funding organisations and the general public at large
- existing and emerging ESFRI projects in the field of Biological and Medical Sciences.

One of the general goals is therefore to identify and address the various needs of these different categories of stakeholder, including additional technology applications especially in the fields of Bioinformatics, Bioimaging, Chemical Biology and Synthetic Biology.
This document outlines the "Synergies-objectives" of WP5, focusing on the coordination and communication of the ISBE preparatory phase with ongoing and emerging projects of ESFRI initiations in the area of Biological and Medical Sciences (BMS).

B. This document

Many ESFRI Infrastructures are cross-cutting and serve complementary fields of technology and research. In this document we aim to define the ISBE overlap, complementarities as well as the added value of active ESFRI initiatives. More specifically, we will highlight the scientific interfacing with bioinformatics, screening and imaging as well as data resources, and biobanks of European infrastructures. After compiling the overlap and synergies with other infrastructures, ISBE will elucidate the perspective of collaboration agreements between ISBE and potential partners for the exchange of knowledge, the provision of capacities and, if applicable, harmonisation of experimental and computational approaches. Since most RIs are developing during their pilot phases, the mode of collaborative options and agreements is also developing during this time. Characteristics for potential multi-ESFRI- nodes will be defined based on aspects of data generation, analysis and analytical approaches.
Thus, this document aims to set the basis for developing collaboration agreements with existing ESFRI initiatives and objectives for multi-ESFRI nodes (Deliverable 5.8). We describe here the work in progress, development and activities of WP5 during the first 15 months of the ISBE preparatory phase and show in particular:

- WP5 actions and meetings related to the "synergies-objectives" of the WP
- description of overlap and synergies with other BMS-ESFRIs as developed from the ongoing work and activities of WP5
- planned follow-up actions and next steps

2. General developments, progress and actions of WP5 in respect to Synergies with other European infrastructures and networks

Inter-ESFRI-RI exchange requires scientific and strategic concepts. Therefore the participation, contribution and presentation of ISBE at Systems Biology Conferences, European and national infrastructure and network meetings, as well as the establishment of working groups on novel technologies and applications are highly important. They provide the necessary information to reveal the overlap of expertise and demands for European infrastructures.
Along this line, ISBE WP5 developed and actively engaged in the following activities:

- **Project Management**
  A project manager has been recruited at the MDC to coordinate WP5 activities and integrate with other ISBE WPs and relevant ESFRI-BMSRIs to develop this document and the upcoming deliverables.

- **European Network Integration**
  WP5 representatives attended and presented at the EC-BMS-ESFRI meeting in Brussels on June 9th and at the EC-JPI-BMS-ESFRI meeting on October 18th 2013. This enabled strengthening liaisons with existing European BMS-RIs as well as obtaining a better overview of existing Joint Program Initiatives (JPIs). Relevant contacts were established for elaborating potential future collaborations, as described further in Section 3 of this document.

- **International Outreach**
  ISBE was presented by the coordinator, a large number of Steering Committee members, work package leaders as well as project managers at the International Conference of Systems Biology (ICSB) in Copenhagen, Aug. 29th –Sept. 3rd 2013. Aim and status of ISBE was introduced to the Systems Biology community during a lunch-break presentation, a poster session as well as by the distribution of flyers. In addition, the launch of the ISBE community website and ISBE survey was promoted, both serving to receive feedback from the Systems Biology Community and a diverse range of stakeholders, including other European infrastructures and networks, to involve them in the ongoing construction of ISBE.

- **Inter-ESFRI Synergies Workshop**
  A Synergies workshop was organized by WP5 on Sept. 23, 2013 in London to engage all BMS-ESFRIs in the construction of ISBE to avoid duplication and use synergies and to elaborate on collaboration potential. 11 out of 13 BMS-ESFRIs participated; ISBE was represented by the coordinator, steering committee members and relevant workpackage leaders. Overlaps between infrastructures were specified and future actions substantiated. Moreover, potential collaborations and thematic interfaces were discussed and specified (details and results in Section 3 and 4 of this document).

- **Bilateral conversations with other BMS-ESFRIs**
  In preparation for the workshop, WP5 carried out bilateral telephone calls with all participating ESFRI representatives to maximize the outcome of the meeting. The following topics were discussed:

- Who are/will be the users of your infrastructure? (other ESFRIs, external users, industry, others)
- What is the scientific background of (potential) users of your infrastructure? What scientific questions/topics do they address?
- What are the Horizon 2020 topics that your infrastructure is aiming to support? Would it be beneficial to collaborate with ISBE in those?
- Which technologies, analysis tools, data etc. offered by ISBE are of interest for your infrastructure? In which scientific questions would it be of bi-lateral interest to use synergies/to collaborate?

Details on the outcome of the actions are described in the next section and summarized in the Synergy Matrix.

3. Description of Synergies and Overlap between ISBE and other BMS-ESFRIs

The strategic and scientific meetings, in particular the Synergies workshop, served to specify actions for harmonising data generation, data management and integration approaches. It was agreed to further define how ELIXIR, EuroBioImaging, and BioMedBridges will feed into the ISBE concept to avoid duplication and use synergies. Moreover, thematic interfaces and areas of potential collaborations between ISBE and other initiatives were identified and developed.

Interface between ISBE and ELIXIR: <u>Management of biological data</u>

ISBE Stewardship Centres (Scs) provide a unified view of the whole systems biology project, including data, models, tools, maps and literature. ISBE's SCs have the task to organise the gathering of relevant information from literature, databases and from unpublished sources. SCs define, develop and adjust criteria and standards that must be met by data, maps, tools and models. Based on such standards, SCs will check on the accuracy, reliability and quality of data, models, tools and maps. Together, these activities will make the re-use of data sets etc. in future systems biology projects possible.
As ELIXIR is also providing access to computing and data resources, data storage and data mining, overlaps exist between ISBE's stewardship centres and ELIXIR per definition.
However, as the data generated by systems biology approaches is quite unique and differs in its specific requirements from most other data in life sciences, ELIXIR is not covering this aspect of data storage and data integration. To confine the boundaries of types of data and tasks between ELIXIR and ISBE, discussions of a working group consisting of ISBE WP3 and relevant ELIXIR representatives will start in December 2013. The overlaps will be defined and the unique aspects of ISBE will specify the interface of capacities and collaborations.

Interface between ISBE and BioMedBridges: <u>Data integration between RIs</u>

BioMedBridges is planning to provide seamless access to high-capacity computing and data resources, combining all BMS-RIs for IT/data harmonization and data standardization. ISBE is currently associated partner. In order to analyse how to make best use of BioMedBridges as a bridge between data and RIs it is aimed to develop a case study of ISBE with BioMedBridges on data standardization and cataloguing to define types of data that ISBE can use for modelling.

Interface between ISBE and EuroBioImaging: <u>High-throughput imaging for Systems Biology approaches</u>

Through EuroBioImaging, ISBE users will get access to novel imaging and image analysis technologies. Overlaps exist in technologies (eg. automatic imaging facilities) as well as data analysis (eg. analysis and integration of high-throughput imaging data). Collaborations to make use of these synergies are foreseen, e.g. for efficiently streamlining data generation – data integration processes (i.e. to couple imaging to modelling). In this respect, the establishment of dual nodes is being analysed.
To further define all synergy aspects and overlaps as well as the possibility of dual centres, conversations between relevant workpackages of both RIs (including representatives involved

in ISBE as well as EuroBioImaging) will take place and suggestions will be made to both steering committees by Spring 2014.

Interface between ISBE and BBMRI: Integration of biological resources and technologies

The Biobanking and Biomolecular Resources Research Infrastructure (BBMRI) manages biological specimen and data for biomedical research. Collaboration potential with ISBE lies in the use of ISBE centres as expert centres for *in situ* work because biological material cannot travel long distances. For example, ISBE's data generation centres are of interest for BBMRI for molecular characterization of biological samples. Moreover, options for integrating data and repositories with ISBE's modelling expertise into one process pipeline are being discussed as well as the option of dual nodes.

Interface between ISBE and EATRIS, ECRIN and ERHINA: Translational research: Systems- and personalized medicine

For the translational research infrastructures EATRIS, ECRIN and ERHINA there is potential for collaborating with ISBE's planned Data Modelling and Integration Centres. More specifically, **ECRIN** would see value in utilising ISBE's modelling expertise for the prediction of compound (drug) selection, to model the safety/ toxicity of drugs, as well as to predict the efficacy of treatment.
Areas of common interface with **EATRIS** are rare diseases, personalized medicine, as well as biomarker development. There is potential for collaborations between EATRIS and ISBE in the translation of compounds into drugs. It is being considered to integrate into existing collaboration agreements between EATRIS, ECRIN, BBMRI and EUOpenscreen to establish a pipeline for the development of drugs for rare diseases.
ERINHA could use ISBE's modelling expertise to identify compounds against high-risk pathogens. Also, collaborating with ISBE's data generation centres in –omics analysis of patient data, and host-pathogens is an option. Together with INSTRUCT, a streamlined process from compound structure to drug testing could be elaborated.

Interface between ISBE and INSTRUCT: Integration of 3D structural data for systems biology modelling

For the structural biology infrastructure INSTRUCT there are options for use of ISBE centres as expert centres for data analysis and modeling.
As potential collaborative activities it is being discussed to establish streamlined processes on diverse platforms, i.e. a software for integrating structural data into systems wide modelling analysis, e.g. for the prediction of protein-protein (drug-target) interactions from the 3D structure of the individual molecular components.
Collaborations with INSTRUCT together with EuOpenScreen for an integrated compound analysis research pipeline could be further elaborated. To collaborate most efficiently, possibilities for dual centres (data generation-data integration centres) will be taken into account.

Interface between ISBE and EUOpenscreen: Integration of screening data for systems biology approaches including drug development

EU-OPENSCREEN, the European Infrastructure of Open Screening Platforms for Chemical Biology, integrates high-throughput screening platforms and chemical resources for hit discovery and optimization. As mentioned above, collaborations with ISBE in systems-wide compound analysis as well as for small molecule projects and biomarker development are foreseen, also together with other RIs. The establishment of a pharmacological use case for the translation of a compound into a drug is being discussed.

Interface between ISBE and Infrafrontier: Systems analysis of mouse phenotypes

Infrafrontier is providing tools for the systemic phenotyping, archiving and distribution of mouse models. Potential areas for collaboration with ISBE are the full level systems analysis of the mouse including the modelling of pathways and molecular effects. Thus, ISBE's Modelling and Integration centres could be used for the systems-wide phenotypic analysis, data integration, medical modelling.

Interface between ISBE and EMBRC: Systems approaches in marine research

The European Marine Biology Research Infrastructure EMBRC allows access to marine ecosystems, providing collaboration potential for the systems wide analysis of uncharacterized organisms, natural products, biodiversity and ecosystems. In particular, using ISBE's expertise in -omics strategies could allow for the understanding of microbial-dominated pelagic ecosystems and biogeochemical drivers. Collaborations in the coupling of physical, chemical and biological metadata to systems biology analyses of communities, ecosystems, and processes would offer great opportunities for novel approaches in marine science research. Deep sea and polar biodiversity could be examined to exploit for biotechnological potential.
Thus, areas of potential collaborations with EMBRC cover data generation, integration, analysis and modelling, as well as data storage.

Interface between ISBE and MIRRI: Systems biology approaches for microbial research

The microbial resource infrastructure MIRRI provides access to novel natural products and organisms. MIRRI aims to use ISBE's expertise for the characterization of Microorganisms and systems wide analysis.
There are options for collaborations with ISBE's Data Generation Centres to carry out -omics analysis and/or sequencing of new strains, organisms and biological material. Moreover, MIRRI is interested in collaborations with ISBE's stewardship centres to facilitate access to microbiological data, for data mining, the integration of data from publications, patents, to introduce the use of SOPs, as well as in all other aspects of all e-infrastructures.
Collaboration potential with ISBE's Modelling and Integration centres exists for the integrated analysis of uncharacterized organisms/ biological material.

4. Synergies Matrix

A quick overview of the collaboration potential and interfaces of ISBE with other European BMS research infrastructures can be obtained from the Synergies Matrix below:

+ overlaps
+ ISBE offers
+ expertise provided by other RI

	Data Generation/ Technologies	Data Access/ Management	Data Integration/ Analysis/ Modelling
BioMedBridges		+	+
BBMRI	+	+/+	+
EuroBioImaging	+/+	+	+
EATRIS	+	+	+
ELIXIR		+/+/+	
ECRIN	+	+	+
EU Open Screen	+/+/+	+	+
EMBRC	+	+	+
ERINHA	+	+	+
Infrafrontier	+	+	+
Instruct	+/+	+	+/+/+
MIRRI	+	+	+

	Data Generation/ Technologies	Data Access/ Management	Data Integration/ Analysis/ Modelling
BioMedBridges		Data access, standardization and harmonization between RIs	Data integration between RIs
BBMRI	Systems biology technologies	Management of biological data and resources	Data integration and modelling
EuroBioImaging	High-throughput imaging for systems approaches	Data storage and integration	Streamlining data generation-integration processes for SB modelling purposes
EATRIS	systems approaches for translational research	storage of data and models	Modelling for compound/drug selection
ELIXIR		data storage, mining and management, high-capacity computing facilities	
ECRIN	-omics approaches for translational research	Management of data and models	Prediction of drug safety/toxicity and efficiency of treatment
EU Open Screen	Combining high-throughput compound screening facilities with Systems biology technologies	Access, storage and integration of screening-, -omics-, and modelling data/ models	Integration of screening data for systems biology modelling
EMBRC	-omics and high-throughput sequencing of uncharacterized organisms, natural products ect.	Data access, storage and integration	Coupling of physical, chemical and biological metadata to SB analysis of communities, ecosystems, and processes
ERINHA	-omics analysis of patient data and host pathogens	Data access, storage and integration	Modelling for ID of compounds against high-risk pathogens
Infrafrontier	High-throughput systems analysis of mouse phenotypes	Storage and integration of phenotypic data (together with BioMedBridges)	Systems-wide analysis of the mouse, phenotypic data integration and modelling
Instruct	Combining 3D structure technologies and Systems biology facilities	Management and integration of structural data and models	Streamlining the integration of structural data into systems wide modelling analysis, e.g. for the prediction of compound-target interactions
MIRRI	-omics, high-throughput sequencing of microorganisms	Data mining, data access, and integration, SOPs,	Integrated analysis of uncharacterized organisms/bio. material

5. Outlook and next steps

Systems biology research needs all technologies, data and resources arising from the increasing number of (potential) European research infrastructures and other scientific initiatives in order to build high-quality models of complex systems. However, a lot of expertise is not properly promoted and visible. ISBE aims to exploit and combine expertise and resources from different RIs and to facilitate their access to the life science community. This places ISBE in the centre of the European Research infrastructure network. Coordinating the activities of European RIs is essential to avoid double-funding as well as to ultimately get a more global understanding of the functioning complex systems, pathways and diseases. Moreover, it will enhance the role of Europe in high level research and facilitate the dissemination of knowledge.

To expand the integration and coordination of ISBE with other RIs, the WP5 actions illustrated in this document were undertaken and the following next steps are planned:

1. ISBE aims to set up case studies to define, explain and show the added value of collaboration between ISBE and other RIs.
   - Between ISBE and EuOpenScreen it is aimed to establish a pharmacology use case.
   - For MIRRI, the use of systems approaches for the characterisation of microorganisms should be developed further.
   - For EMBRC, the use of ISBE expertise for the analysis of novel organisms, ecosystems and biological processes is aimed to elucidate further.
   - A use case with INSTRUCT for the establishment of a pipeline from 3D structure to drug-target interactions is being discussed.
   - Together with BioMedBridges, ISBE aims to work on standardization and cataloguing tools, to explore how all RIs can produce data that is useable for ISBE modelling.

2. To define the interface between ISBE and ELIXIR, discussions started in December 2013. Here, the ISBE WP2 has the lead and act together with WP3 and WP1.

3. To distribute tasks of Data Generation Centres in the field of imaging, discussions with EuroBioImaging and ISBE's WP3 and WP4 have started in December 2013.

4. It is aimed to elaborate the integration into established collaboration agreements on a translational research pipeline for rare diseases between BBMRI, EUOpenscreen, EATRIS, and ECRIN.

5. To extend the established contacts and to further promote collaborations, ISBE is planning to be represented at the BioMedBridges Annual General Meeting on 10-11 March 2014 in Florence, Italy.

6. The next ISBE synergies workshop organized by WP5 is planned to be in autumn 2014, when the first RIs are already implemented and ISBE has further defined its infrastructure.

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