

structure

ELIXIR

Training

de.NBI-

Cloud

Service

Partner

Projects

de.NBI Quarterly Newsletter

EDITION NOVEMBER 2016

1) EDITORIAL

This Quarterly Newsletter Edition November 2016 will be the fourth and last newsletter of the year 2016. Therefore, the main achievements of the de.NBI network of the current year are summed up. As

presented in the accompanying figure the de.NBI network started several new activities which enlarged the scope of the network significantly.

Originally the network consisted of eight service centers based on 23 individual projects which were responsible for service and training tasks of the network. On 1 November 2016 this scheme was significantly modified since 17 new partner projects joined de.NBI and nearly doubled the number of projects involved.

A further modification of the de.NBI structure was the decision to establish a de.NBI cloud which is planned to solve the compute problem with-

in de.NBI. The Central Coordination Unit of de.NBI recognized that the establishment and operation of such a cloud needs a lot of guidance. Therefore, a further Special Interest Group designated "de.NBI cloud" has been established.

The most important achievement in 2016 was without doubt the German membership in ELIXIR. The ratification of the ELIXIR Collaboration Agreement by the BMBF took place in August 2016. In order to celebrate this event, a special session on the de.NBI-ELIXIR collaboration was incorporated into the de.NBI Symposium on "Bioinformatics in Human Health and Disease" in Heidelberg.

This de.NBI newsletter also informs on the de.NBI activities of the last three months. There is a report on the CCU decision to install a so-called "associated de.NBI membership". In addition, two service centers have been renamed as "Center for Biological Data" and "de.NBI Systems Biology Service Center". Further on, the de.NBI Midterm Review has been announced by the Project Management in Jülich (PtJ) to take place in September 2017. The actual de.NBI newsletter reports again on recent scientific events organized by the network. There are reports on the de.NBI Summer School at Schloss Dagstuhl, a Data Management Workshop in Kassel and the first training courses organized by partner projects in Dresden and in Halle, respectively. In the section "Upcoming Events", finally, all the future training courses scheduled so far, are listed, demonstrating that the de.NBI training activities will be extended significantly in the coming year.



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A. Pühler (de.NBI coordinator)

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2) INTERNATIONAL de.NBI SYMPOSIUM HEIDELBERG

The 1st International de.NBI Symposium was hosted by the Service Center HD-HuB at the Communication Center of the German Cancer Research Center (Deutsches Krebsforschungszentrum, DKFZ). About 130 members of the scientific community attended the three-day event which focused on "Bioinformatics for Human Health and Disease". Ten scientific sessions

BIOINFORMATICS FOR HUMAN HEALTH AND DISEASE

featured a total of 38 talks. Among these, some were given by international invited speakers such as Lodewyk Wessels (NL), Noah Palm (US), Anna Heintz-Buschart (LUX), Peter Horvath (FL), Ernest Fraenkel (US), Prisca Liberali (CH), Juan Antonio Vizcaino and Magnus Rattray (UK).

A special dedicated de.NBI/ELIXIR session celebrated the full membership of Germany in the European life sciences infrastructure initiative ELIXIR with presentations by Yvonne Pfeiffenschneider (Project Management Jülich, on behalf of the Federal Ministry of Education and Research), the de.NBI network coordinator Alfred Pühler, Niklas Blomberg (Director of ELIXIR), Andreas Tauch (Head of de.NBI Administration Office) and Roland Eils (Coordinator of the de.NBI Service Center HD-HuB and ELIXIR Board member). In his presentation Alfred Pühler stressed the exceptional quality of all session speakers.



many's membership of ELIXIR

At a **poster session** on the first day and a conference dinner on the second evening attendants could exchange ideas and intensify discussions in a relaxed atmosphere. The de.NBI Office would like to thank all speakers of the 1st International de.NBI Symposium as well as the HD-HuB staff involved in the organization of the event, in particular Dr. Julia Ritzerfeld.



Poster session at the de.NBI symposium in Heidelberg

3) SAVE THE DATE: 18-19 SEPTEMBER 2017, de.NBI MIDTERM REVIEW

The Project Management Jülich (PtJ) has announced the date of the de.NBI Midterm Review. The review of the de.NBI consortium will take place in Berlin on 18-19 September 2017 (Monday/Tuesday). Detailed information on the venue and the agenda of this meeting will be announced at a later time. All de.NBI partners will be invited to present posters of their achievements in the de.NBI program and in the recently started de.NBI Cloud initiative. All de.NBI partner projects are also invited to present posters, although this funding program is not subject to midterm evaluation. Upon positive evaluation of the de.NBI partners, funding by the BMBF is extended to 29 February 2020 as already indicated in the approval letter.

4) DATABASE NODE RENAMED AS CENTER FOR BIOLOGICAL DATA (BioData)

The partners of the Database Node have announced the renaming of this de.NBI unit as **Center for Biological Data (BioData)**. The Center for Biological Data is hosting the four databases SILVA, PANGAEA, Bac*Dive* and BRENDA and it was recently expanded by the partner project 'EnzymeStructures: supporting structure-driven molecular life science research in BRENDA'. The new project partner is Matthias Rarey from the Research Group for Computational Molecular Design at the Center for Bioinformatics of Hamburg University. The core mission of the Center for Biological Data is to offer high-quality datasets and



The latest BacDive training course in Braunschweig

related services for users in academia and industry. All databases provide a set of highly curated reference datasets and three of these databases have been maintained for more than 25 years, indicating the importance of quality controlled reference datasets for the advancement in science.

5) DATAMANAGEMENT NODE RENAMED AS de.NBI SYSTEMS BIOLOGY SERVICE CENTER

The partners of the Data Management Node have announced the renaming of this unit as **de.NBI** Systems Biology Service Center (de.NBI-SysBio). The mission of de.NBI-SysBio is to provide data and models management support and modelling for systems biology projects. The de.NBI Systems Biology Service Center is coordinated by Wolfgang Müller (HITS, Heidelberg) and includes research groups from Rostock University (Dagmar Waltemath), Heidelberg University (Ursula Kummer) and the Max Planck Institute for Dynamics of Complex Technical Systems Magdeburg (Steffen Klamt). The latter two partners were recently integrated into the de.NBI unit with the new partner project NBI-ModSim covering the topics 'Services and developments for dynamic and quantitative modeling of biological systems' and 'Services and developments for stoichiometric and qualitative modeling of cellular networks'.

6) THE CCU ESTABLISHED THE STATUS 'ASSOCIATED PARTNER'

According to recommendations by the Scientific Advisory Board the Central Coordination Unit (CCU) of de.NBI has cleared the way for **associating scientific partners with the network**. Scientists who are interested to contribute to the service and training program of de.NBI are invited to present an application to the de.NBI coordinator. The application should provide information on the expertise of the associated partner and on the planned service and training activities. Services and training have to comply with the high quality standards of the de.NBI units. Although associated partners will collaborate closely with the de.NBI Service Centers in terms of provision of services or user training, they will be supervised and administered by the de.NBI Administration Office. Each application has to be approved by the CCU and associated partners are engaged to report annually to this supervisory committee. It is important to note that the de.NBI consortium has no financial resources to support the status 'Associated Partner'. Service and training activities are therefore subject to self-financing by the associated partners.

7) THE CCU ESTABLISHED THE SPECIAL INTEREST GROUP 6 'de.NBI CLOUD'

According to a decision by the Central Coordination Unit (CCU) of de.NBI, the de.NBI cloud funded by the BMBF will be established at the Service Centers HD-HuB (Heidelberg), BiGi (Bielefeld and

Gießen), CIBI (Tübingen) and RBC (Freiburg). Additional scientific staff will be appointed to these four Service Centers, to BioInfra.Prot (Bochum) and to the Administration Office. During the last meeting in Gatersleben, the CCU formally established the Special Interest Group 6 'de.NBI Cloud'. SIG 6 will continue the work of the task force 'AG de.NBI Cloud' that was founded on 1 July 2016 during the first special meeting of the CCU in Braunschweig. The CCU appointed Chris Lawerenz (HD-HuB) as provisional head of this new discussion group. A head and a deputy chairman of SIG 6 should be nominated by the SIG 6 members to be appointed by the CCU during the meeting in Bremen in January 2017. Most of the de.NBI scientists who worked already in the task force 'AG de.NBI Cloud' will also participate under the new label of this discussion group. A first objective of SIG 6 is to develop a working program to establish the de.NBI Cloud at five academic locations in Germany.

8) de.NBI SUMMER SCHOOL 2016 "FROM BIG DATA TO BIG INSIGHTS"



de.NBI Summer School particpants at Schloß Dagstuhl

This year's summer school "From Big Data to Big Insights – Computational Methods for the Analysis and Interpretation of Mass-Spectrometric High-Throughput Data" took place at Castle Dagstuhl from the 26th to 30th September. In one of the world's premier meeting centers for informatics research, topics concerning the data analysis of mass spectrometry based proteomics and metabolomics were presented by renowned invited speakers of the field and discussed by advanced PhD students and postdoctoral fellows.

The group of 20 participants was selected from more than 50 applicants and consisted to one half of scientists mainly working on the generation of data in the wet-lab, and the other half mainly creating bioinformatics tools and workflows. While most participants were working in Germany, we also had scientists working in Poland, Ukraine, the United Kingdom, the Netherlands, Denmark and Finland. This mix of backgrounds contributed to lively discussions and a very motivated atmosphere during the various sessions and workshops, which were held not only by the members of the organising de.NBI units, but also by a group of excellent keynote speakers: Samuel Payne (Pacific Northwest National Laboratory, USA), Oliver Serang (FU Berlin, DE), Juan Antonio Vizcaino (European Bioinformatics Institute, UK), Jürgen Cox (Max Planck Institute of Biochemistry, DE), Viktoria Dorfer (FH Hagenberg, AU), Lennart Martens (University Gent, BE) and Sebastian Böcker (Friedrich-Schiller-Universität Jena, DE) talked about their current advances in computational mass spectrometry and gave hands-on training in analysing big data. Even more important for the success of the summer school was the fact, that many speakers managed to stay several days and had time for discussions during the coffee breaks and the evenings.

The afternoon and evening of the Wednesday was used for a social event in Trier. All participants, organizers and speakers took part in a guided tour highlighting the medieval past of the Roman city. After getting this wrap-up in history and having time to admire historic sights, we tasted original Roman cuisine in a local restaurant.

The summer school was jointly organized by the three de.NBI units Bioinformatics for Proteomics (Bio-Infra.Prot), Center for Integrative Bioinformatics (CIBI) and the Bielefeld-Gießen Resource Center for Microbial Bioinformatics (BiGi). It was sponsored not only by the BMBF (de.NBI), but also supported by the Medizinisches Proteom-Center (MPC) and one female speaker was funded by the German-Canadian DFG International Research Training Group "Computational Methods for the Analysis of the Diversity and Dynamics of Genomes" (DiDy). The overwhelmingly positive feedback of participants

and speakers concerning the program, organization, implementation, and also the venue emphasizes the ongoing excellent cooperation between the service centers inside de.NBI. More information on the program and photos of the summer school can be found at http://www.dagstuhl.de/16393.

9) DATA MANAGEMENT POLICY WORKSHOP (BY WOLFGANG MÜLLER & UWE SCHOLZ)

On 27th of October, members of SIG4 and SIG2 held a workshop in Kassel on **research data management in the de.NBI service projects**. Organized by the de.NBI-SysBio and GCBN centers, more than 20 participants (including Alfred Pühler, the de.NBI coordinator) from all de.NBI consortia discussed how data that is generated in the de.NBI service centers should be enriched, shared, and published, a challenging and worthwhile problem.

It was a common ground of the participants that de.NBI sends a strong message towards FAIR data management of de.NBI data. FAIR (<a href="https://www.force11.org/group/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgroup/fairgrou

In the workshop, the participants heard talks about data management in the projects, data management systems, different levels of curation. Then the participants discussed scope and steps to a de.NBI research data management guidelines document. Already on-site the participants collected the most important points of this document and drew an outline. After one day of friendly, vivid, and productive discussion, the participants took the way back to their centers.

10) FIRST TRAINING COURSES OF PARTNER PROJECTS

Just one month after the official project start two new de.NBI partners offer their first training courses. Both partner projects are new members of the de.NBI service center CIBI.

- FIJI, IMAGEJ, AND KNIME IMAGE PROCESSING HACKATHON

In December 2016 (06.12.2016 – 16.12.2016), the DAIS (Dresden Analysis-of-Images Suite) team around Florian Jug and Tobias Pietzsch is holding a 11-day hackathon in Dresden at the Max Planck Institute for Molecular Cell Biology and Genetics. The purpose of this hackathon is to bring together people working with image processing packages Fiji, ImageJ, and KNIME. Especially Fiji is a "batteries-included" distribution of ImageJ bundling a lot of plugins which facilitate scientific image analysis. Attendees will have the chance to consult with experienced core contributors from all three open source projects. All attendees should already have a solid background in Java and a strong interest in contributing to Fiji, ImageJ, and/or KNIME Image Processing. Goals are the integration of existing projects into Fiji and/or KNIME and extending existing plugins and frameworks by new and useful features. http://www.denbi.de/22-training-cat/training-courses/207-hackathon-fiji-imagej-and-knime-development

- IPB Metabolomics workshop 2016 - Christmas Edition

The new partner project MASH (Metabolite Annotation Sharing Halle) of Steffen Neumann offers a metabolomics workshop at the Leibniz Institute of Plant Biochemistry, Halle (Saale) on 8-9.12.2016. Participants will get a comprehensive overview of the metabolomics data processing pipeline from data to publication. The second day will feature a bring-you-own-data session. http://www.denbi.de/22-training-cat/training-courses/222-ipb1

11) de.NBI TWITTER CHANNEL



#denbi is now active via @twitter. The de.NBI profile name is @denbiOffice. We will use the channel to announce and document training courses, to announce #denbi events, and for all news related to #denbi, e.g. @ELIXIREurope news and news tweeted by #denbi partners or tools like @HITStudies or @OpenMSTeam. So if you are interested in latest #denbi news follow us on @twitter and use our tags #denbi @denbiOffice.

12) UPCOMING EVENTS

The calendar of upcoming events lists a number of events scheduled for the next three months. All offers are accessible via the de.NBI homepage http://www.denbi.de. The de.NBI training program is continuously updated on our homepage. Currently 40 courses are in the pipeline for 2017

MAJOR DE.NBI EVENTS - SAVE THE DATES

2nd SAB meeting including Workshop and Plenary Meeting, (28-29 November 2016), Berlin. This internal de.NBI Meeting for all de.NBI members will take place at the Seminaris Campus Hotel, Berlin. The invitation has been spread within the consortium.



OVERVIEW OF UPCOMING de.NBI EVENTS

	Date	Event	City	Organizer
>	21 Nov 2016	Differential analysis of proteomic data using R	Bochum	BioInfra.Prot1
>	22-25 Nov 2016	From Primer to Paper: Training in Biodiversity Analysis using NGS Amplicon Data	Bremen	BioData
>	28-29 Nov 2016	2nd de.NBI SAB meeting including workshop and plenary meeting	Berlin	CAU
>	01 -02 Dec 2016	3rd Systems Biology Developers Foundry by FAIRDOM & de.NBI	Frankfurt	de.NBI-SysBio
>	05-06 Dec 2016	2nd de.NBI Bioimage Analysis Workshop	Heidelberg	HD-HuB
>	06-16 Dec 2016	Hackathon – Fiji, ImageJ, and KNIME development	Dresden	CIBI (DAIS)
	08-09 Dec 2016	IPB Metabolomics workshop 2016 - Christmas Edition	Halle	CIBI (MASH)
>	15-16 Dec 2016	Galaxy RNA-sequencing data analysis workshop	Freiburg	RBC
>	16-19 Jan 2017	European Galaxy Developer Workshop	Ilkirch/ Strasbourg	RBC, div. ELIXIR partners
>	17 Jan 2017	9. CCU Meeting	Bremen	CAU, BioData
>	13-18 Feb 2017	3rd Galaxy High-Throughput-Sequencing (HTS) data analysis workshop	Freiburg	RBC

IMPRESSUM:

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