

de.NBI Quarterly Newsletter

EDITION OCTOBER 2015

1) EDITORIAL

Dear de.NBI members, dear de.NBI followers,

The second edition of the de.NBI Quarterly Newsletter provides you the essentials in brief on the recent and future development of the German Network for Bioinformatics Infrastructure – de.NBI. This edition is focused on the **activities of de.NBI's Special Interest Groups (SIGs)** that are small discussion panels of de.NBI experts. Five such subcommittees have been established by the Central Coordination Unit (CCU) to discuss bioinformatics infrastructures topics relevant for operational and strategic decisions by the de.NBI management and to put forward recommendations to the CCU. The SIGs, named Web presence (SIG 1), Service and service monitoring (SIG 2), Training and education (SIG 3), Infrastructure and data management (SIG 4), and de.NBI development (SIG 5) present in this newsletter their tasks and initial results of intensive discussions. As shown in the right panel, each SIG is headed by a member of the CCU. The articles presented in this Quarterly Newsletter were prepared by the chairpersons of the different SIGs.

The five Special Interest Groups and their chairpersons

SIG	Title	Chairperson	Co-chairperson
SIG 1	Web presence	J. Stoye	A. Tauch
SIG 2	Service and service monitoring	F. O. Glöckner	U. Scholz
SIG 3	Training and education	O. Kohlbacher	R. Backofen
SIG 4	Infrastructure and data management	M. Eisenacher	W. Müller
SIG 5	de.NBI development	A. Pühler	R. Eils

This newsletter also addresses recent and future training activities of the de.NBI consortium. In the past quarter, the **1st de.NBI Late Summer School** on Microbial Bioinformatics was held as a one-week course at Gießen University. The **8th OpenMS User Meeting** at the Ruhr University Bochum is another example of recent de.NBI user training. The organizers provide short retrospectives of these very successful training events. A tabular list of planned training courses and workshops is composed at the end of this newsletter. An upcoming major event of de.NBI is the **1st SAB Meeting** including a de.NBI Workshop and the **2nd de.NBI Plenary Meeting** in Berlin (26–27 November 2015) that brings together in a two-day meeting the members of the international Scientific Advisory Board (SAB) and the de.NBI community.

To conclude, the de.NBI Administration Office hopes you enjoy reading the second edition of the de.NBI Quarterly Newsletter and that we touch upon some interesting topics for you.



Andreas Tauch
(Head of de.NBI Administration Office)

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2) WEB PRESENCE – REPORT OF SIG 1

The Special Interest Group 1 (SIG 1) "Web presence" has been appointed by the Central Coordination Unit of de.NBI to develop a **concept for one central website** at www.denbi.de. This common website will include background information on the de.NBI consortium and detailed information for users on the wealth and diversity of de.NBI services and the de.NBI training program. Professional design agencies have been assigned to create a modern web presence, including logo and corporate design. The preliminary logo of the de.NBI initiative is available for download in jpg and eps format from the de.NBI ownCloud. Please contact the de.NBI Administration Office or your SIG 1 representative.



3) SERVICE AND SERVICE MONITORING – REPORT OF SIG 2

The SIG Service and service monitoring (SIG 2) works on the following tasks

- **Service presentation:**

The SIG 2 will generate an overview of the software tools, databases, web servers, computing facilities, and other services offered by de.NBI. SIG 2 will take care that all services are intuitively presented and documented on the website.

- **Service monitoring:**

Considering the various user profiles and the variety of services provided by the de.NBI centers, numbers of requests and user acceptance of the services are only measurable with a set of different parameters. SIG 2 will tackle this complexity by the definition of a set of services and corresponding parameters for monitoring from which each de.NBI unit selects the best fitting parameters for each of the provided services. The SIG 2 will take care that the baseline as well as a continuous monitoring of the usage of de.NBI services as well as user numbers are established.

- **Customer satisfaction:**

The SIG 2 will take care that appropriate measures are taken to investigate customer satisfaction. This will be tackled by user meetings, training units as well as short questionnaires to explore potential discrepancies and gaps between user expectations and the services provided. Additionally, an effective workflow and guidelines for handling user requests will be established. Finally the SIG will provide detailed usage statistics and end-user statements for the mid-term review.

The **present achievements** can be summarized as follows:

In a collaborative effort of all service centers 80 services have been identified that are currently offered to the users. Furthermore, the SIG 2 has defined a list containing 30 parameters for monitoring the acceptance/usage of the services.

4) TRAINING AND EDUCATION – REPORT OF SIG 3

The Special Interest Group 3 (SIG 3) "Training and Education" was appointed by the Central Coordination Unit of de.NBI to handle the coordination of **training activities** in the network. SIG 3 members of all de.NBI units have jointly defined the general requirements of de.NBI training courses to ensure high quality standards. To increase the visibility of de.NBI training events, courses will be uniformly advertised based on a standardized form developed by the SIG 3 and distributed to the user community by applying a number of different channels (e.g., websites, mailing lists). To assess and further improve the quality of de.NBI training, a standardized procedure to document the courses was developed, including the preparation of templates for feedback questionnaires. This feedback is crucial for organizers to improve the de.NBI training courses offered in the future.

The de.NBI consortium has planned 15 de.NBI training events in the first year of funding. About 200 participants were already trained in the use of different de.NBI tools in recent training events. The number of applicants generally exceeded the maximum number of places offered. The variety and thematic breadth of planned events (seven additional events already planned in 2015/2016; see also the table at the end of the newsletter) shows that the de.NBI partners are exceptionally active in and highly committed to user training.

5) INFRASTRUCTURE AND DATA MANAGEMENT – REPORT OF SIG 4

The de.NBI consortium's remit includes the development and implementation of standard procedures to maximize compatibility, interoperability, safety, reproducibility, and quality of the provided services. With regard to this the de.NBI Special Interest Group (SIG) 4 "Infrastructure and Data Management" is collecting which hardware is currently used and is discussing which hardware should be used in the future to provide services. As a corollary the SIG 4 is discussing suitable pricing structures for using hardware and services. SIG 4 will also define a **catalogue of harmonized standards** (e.g. standard data formats) and guidelines for the de.NBI units for working with data while performing services. Furthermore, the SIG will define a set of rules for the hand-out of data sets to open and closed research data repositories. It is self-evident that the members of the de.NBI consortium are following the applicable national and international regulations, in particular laws governing data protection and data security when handling clinical and person-related data. So far, SIG 4 had three meetings (in May, July, October 2015) with lively, yet very friendly and productive discussions. Obviously, a diverse consortium as de.NBI poses an interesting challenge when trying to provide unified information across all services.

The SIG4 already drafted the following lists after extensive discussions which will be frequently updated during project runtime:

- **Service-oriented hardware usage list:** For all services offered by the different de.NBI service centers the contacts and available hardware resources (e.g. number of cores, available RAM) are listed.
- **List of (standard) formats:** All the (standard) formats and minimum information documents used by de.NBI services are listed. For each format or document the list contains the latest version, URL of specification documents, standard organizations and the EDAM ("EMBRACE Data and Methods") ID's are listed. The EDAM ontology describes bioinformatics concepts such as types of data, data identifiers, data formats and operations and is also used by ELIXIR to describe their services.
- **Service and hardware pricing structure list:** Here the cost factors (i.e. without taking into account new developments or costs caused by growth effects) and assumptions about cost-influencing parameters will be recorded and thus an estimation of the service and hardware-usage costs can be derived. To be able to do this for each offered service of the de.NBI service centers a specific "service provision" unit will be defined and the costs for these units are estimated.

6) de.NBI DEVELOPMENT – REPORT OF SIG 5

The tasks of SIG 5 comprise the development of the de.NBI network, the cooperation with national and international organizations as well as cooperations with industrial partners.

The SIG 5 focused on the development of **cooperation with the European bioinformatics infrastructure network ELIXIR**. The de.NBI coordinator A. Pühler met the ELIXIR director N. Blomberg and the ELIXIR external relations manager A. Smith at the beginning of this year at the ELIXIR Hub in Hinxton, UK to discuss a collaboration strategy. As a result of this discussion, a strategy paper entitled "Towards a German membership of ELIXIR" has been developed. Three phases of cooperation are proposed in this strategy paper. Phase 1 deals with knowledge exchange based on awareness raising of activities within both organizations and linking of key groups and individuals. In phase 2 a strategic

collaboration on specific and mutually agreed areas such as tools and service registry, ontologies and training is developed. Finally phase 3 aims at the full membership of Germany allowing de.NBI to act as national node in ELIXIR.

In the course of the last two SIG 5 meetings, in Heidelberg (19 May 2015) and Bielefeld (21 July 2015), the cooperation strategy was discussed. In the meantime there are already good examples for cooperation designated to phases 1 and 2. Also within phase 3 some progress can be reported, as the BMBF started to analyze conditions for joining ELIXIR. The members of SIG 5 follow this development with great interest and hope very much, that based on a full membership de.NBI can expand its cooperation with ELIXIR.

7) de.NBI LATE SUMMER SCHOOL 2015

The 1st **de.NBI Late Summer School (LSS) on Microbial Bioinformatics** was held from 20-26 September 2015 at Gießen University. The course focused on the workflow from genome assembly to the analysis of genome sequences and transcription data and included lectures and hands-on sessions by de.NBI and renowned experts in the fields. The target group comprised Ph.D. students, postdoctoral fellows and other scientists with a solid background in bioinformatics and molecular biology.



Participants in the 1st de.NBI Late Summer School 2015

A group of **twenty participants** was selected from almost 40 applicants, the majority of whom came from Germany, however participants from Poland, Austria, United States and South Africa also attended. This created an interesting mix of Ph.D. students, postdocs and scientists from very different backgrounds and guaranteed lively discussions during the course of the week. In addition, in poster session many participants

informed on their research topics. A notable feature of the de.NBI Summer School was the involvement of **high-profile speakers**. We were fortunate in being able to bring together an excellent group of keynote speakers; Gene Myers (Dresden, DE), Tatiana Tatusova (Bethesda, US), Paul Kersey (Cambridge, UK), Jan Gorodkin (Copenhagen, DK) and Ursula Kummer (Heidelberg, DE).

During the afternoon sessions, intensive analysis and practical exercises were carried out. The offer to work with own data sets was much appreciated by the participants and a high percentage took advantage of this opportunity. In addition, during a company presentation by CLC bio / QIAGEN the CLC Genomics Workbench was introduced.

Social events were also offered and the participants enjoyed an experimental lecture at the Justus-Liebig-Museum and a tour to the nearby Gleiberg castle. The week's training ended with a farewell dinner in the Dachcafé which gave participants and instructors alike the chance to share experiences and discuss possible improvements.

Three of the eight de.NBI service centers were involved in the LSS program, namely the Bielefeld-Gießen Center for Microbial Bioinformatics (BiGi), the RNA Bioinformatics Center (RBC) and the Data Management Node (NBI-SysBio). This reflects the intensive collaboration between the individual de.NBI service centers that already exists on the sector of bioinformatics training in Germany.

More details about the program and some photos taken during the course can be found online at www.denbilss.computational.bio

<http://www.uni-giessen.de/fbz/fb08/Inst/bioinformatik/Education/denbilss>

8) IMPRESSIONS FROM THE OpenMS USER MEETING

From 16-18 September 2015, the **8th OpenMS User Meeting** took place at the Ruhr University Bochum. OpenMS is an **open-source software for LC/MS data management and analysis**. It consists of a vast variety of pre-built and ready-to-use tools for proteomics and metabolomics data analysis (TOPPTools) and powerful 2D and 3D visualization (TOPPView). The OpenMS User Meeting was conducted by the de.NBI units BioInfra.Prot and CIBI. In total, 20 participants from Europe and the United States as well as an equal number of OpenMS developers got together to discuss the latest developments in software libraries and tools for mass spectrometry.

On the first day, new users were introduced to OpenMS and KNIME followed by tutorials on “small molecule quantification and identification” and advanced topics. On the second day, **two international guest speakers**, Lukas Käll (Royal Institute of Technology, Solna, Sweden) and Fredrik Levander (Lund University, Sweden), presented their research in two keynote talks on computational proteomics and metabolomics. On the second and third day, OpenMS developers and a number of users presented their respective research projects. The successful event was complemented by a visit to the German Mining Museum Bochum (<http://www.bergbaumuseum.de>) followed by a conference dinner.



OpenMS trainees visiting the Bergbaumuseum

9) 1ST SAB MEETING INCLUDING WORKSHOP AND PLENARY MEETING

The first **meeting of the Scientific Advisory Board (SAB)** will take place at the Seminaris Campus Hotel Berlin (www.seminaris.de/berlin) from 26–27 November 2015. This major event includes a **de.NBI Workshop** and the 2nd **de.NBI Plenary Meeting**. It brings together the members of the international SAB and the de.NBI community and provides an opportunity to learn about the totality of activities and recent achievements in de.NBI. The programme is structured around **two distinguished lectures** by Niklas Blomberg (Director of ELIXIR) and Ron Appel (Executive Director of the Swiss Institute of Bioinformatics) and a poster session with presentations by all de.NBI partners. The poster session will allow the meeting participants to get a shared understanding on the de.NBI services and training activities. The SAB meeting will kick-off with a welcome address by a representative of the Federal Ministry of Education and Research (BMBF) and presentations on the five Special Interest Groups (SIGs) followed by talks about the eight de.NBI Service Centers on the second day. The event will end with the 2nd de.NBI Plenary Meeting in the early afternoon.

[Draft Agenda of the 1. SAB Meeting including Workshop and Plenary Meeting, 26-27 November in Berlin](#)

Thursday, 26 November 2015		
12:00	Registration	Internal SAB meeting
13:00	Session I: Opening session	
14:20	Session II: SIG presentations	
16:30	Session III: Distinguished Lectures	
	– ELIXIR	
	– SIB - Swiss Institute of Bioinformatics	
20:00	Session IV: Poster session on individual de.NBI projects	
Friday, 27 November 2015		
9:00-12:10	Session V: Presentations on achievements of the eight service centers	
13:15	Plenary Meeting	Internal SAB meeting
14:30	End of conference	

10) UPCOMING EVENTS

The calendar of upcoming events lists quite a number of events scheduled for the next four months.

➤ **Bioinformatics – Data Interpretation for Next Generation Sequencing Data in Cancer Research (07-08 October 2015), Heidelberg.** The DTK School of Oncology and the Heidelberg Center for Human Bioinformatics (HD-HuB) invite researchers working with larger datasets of next-generation sequencing (NGS) data arising from patient tumor samples. The course will teach background knowledge on technologies used for data generation and for data analysis. Commonly used tools for data interpretation will be presented and can be applied in hands-on sessions on provided

data sets. The flyer of this training course is available at <http://www.dkfz.de/de/dktk/download/FlyerDKTK-BioinformaticsWorkshop.pdf>.

- **Introduction to BRENDA enzyme database and BacDive bacterial diversity metadata-base (13-14 October 2015), Braunschweig** is organized by the Database Node. Participants will learn history, scope and content of the two databases, use of the web interface queries, functionalities and interpretation of results.
- **CLC bio Workshop (03-04 November 2015), Gießen.** This course hosted by BiGi will teach participants how to use the CLC Genomics Workbench for genome analysis. The CLC Genomics Workbench is a commercial software for the analysis and visualization of next generation sequencing data. Professional trainers from CLC bio will present the Genomics Workbench with a focus on de novo genome assembly, short-read mapping, and RNA-Seq experiments. For information see: <https://www.uni-giessen.de/fbz/fb08/Inst/bioinformatik/News/Notes/clc-workshop-vom-03-11-04-11.2015>
- **High throughput genome analysis & comparative genomics (16-17 November 2015), Gießen.** Topic of this two-day workshop organized by BiGi will be microbial genome annotation and comparative genomics with focus on the usage of the BiGi software tools GenDB and EDGAR. The course ranges from introduction of basic principles of annotation, tools and algorithms for the different annotation steps using GenDB and a new stand-alone high-throughput annotation pipeline to hands-on training in manual genome. The second part features comparative genomics with focus on differential gene content analysis and core-genome-based phylogenetic analyses including hands-on training using public EDGAR projects. Registration is here: http://www.bioinformatics-platform.dzif.de/?page_id=1342
- **Introduction into targeted and untargeted metagenome analysis (23-25 November 2015), Bielefeld.** This BiGi course will broach the issues of targeted (16S rDNA operon gene amplicons) and untargeted (whole-genome shotgun, WGS) metagenome analysis based on high throughput next-generation sequencing (NGS) data. The first part covers different aspects of general NGS data handling and presents different techniques and tools for quality measurement, filtering, and sequence correction. The second part focuses on 16S amplicon data analysis utilizing the popular command line tools QIIME and mothur. In the third part, advantages and disadvantages of whole metagenome sequencing are illustrated.
- **ARB/Silva and BacDive: Training on microbial phylogeny and diversity analysis (01-04 December 2015), in Bremen** is hosted by the Database Node. The course will provide knowledge of and skills on primary and secondary databases, concepts of marker gene sequence analysis, details of phylogenetic reconstruction, workflows for analysis of rRNA gene amplicon reads from NGS projects. <http://www.ribocon.com/home/arb/training/course-details/>
- **de.NBI Bioimage Analysis Workshop (02-04 December 2015), Heidelberg.** HD-HuB will introduce basic concepts of the KNIME image and data analysis platform. During the course state-of-the-art applications in how to analyze bioimage data will be addressed.
- **From Genotypes to Phenotypes - Access & Manage Plant Data (07-08 December 2015), München/Neuherberg.** GCBN will introduce into the plant genomic resources at Helmholtz Center Munich. Participants will learn to set-up and configure a Data Publication Repository; JAVA Programming for the e!DAL API; using ISA-TAB for Managing Plant Phenotyping Data. Each day offers tutorials, hands-on training and reflective roundtable discussions.
- **CIBI - KNIME Bioinformatics Hackathon (12-22 January 2016), Konstanz.** A hackathon is an event at which software developers and researchers collaborate intensively on software projects. The purpose of this hackathon is to bring together people from the de.NBI community to create new or enhance existing extensions of the KNIME open-source platform, which then can be used by life-science researchers. This comprises the integration of other well-established software packages or algorithms. The focus is on three projects: Improving SeqAn and OpenMS KNIME integrations, KNIME

Image Processing and ImageJ2 and the KNIME Cluster extension to process huge amounts of bio-data in parallel. Attendees will have the chance to consult with KNIME experts at the University of Konstanz, University of Tübingen and FU Berlin.

➤ **de.NBI – ELIXIR Workshop on EDAM ontologies (19-20 January 2016), Freiburg.** This hackathon for de.NBI members will introduce into the ELIXIR Service Registry and is intended to register all de.NBI services and tools offered within the consortium in a standardized mode.



Overview of upcoming de.NBI events

Date	Event	City	Organizer
➤ 07.-08.10.2015	Data Interpretation for Next Generation Sequencing Data in Cancer Research	Heidelberg	HD-HuB
➤ 13.-14.10.2015	Introduction to BRENDA enzyme database and BacDive bacterial diversity metadatabase	Braunschweig	Database Node
➤ 21.10.2015	4 th CCU meeting	Bochum	BioInfra.Prot, CAU
➤ 03.-04.11. 2015	CLC-Workshop	Gießen	BiGi
➤ 16.-17.11.2015	High-throughput genome analysis & comparative genomics	Gießen	BiGi
➤ 23.-25.11.2015	Introduction into targeted and untargeted metagenome analysis	Bielefeld	BiGi
➤ 26.-27.11.2015	1st SAB Meeting including de.NBI Workshop and Plenary Meeting	Berlin	CAU
➤ 01.-04.12.2015	ARB/Silva and BacDive: Training on phylogeny and diversity analysis	Bremen	Database Node
➤ 02.-04.12.2015	de.NBI Bioimage Analysis Workshop	Heidelberg	HD-HuB
➤ 07.-08.12.2015	From Genotypes to Phenotypes - Access & Manage Plant Data	München	GCBN
➤ 19.01.2016	5 th CCU Meeting in Freiburg	Freiburg	CAU
➤ 19.-20.01.2016	de.NBI – ELIXIR Workshop on EDAM ontologies	Freiburg	RBC, SIG 2
➤ 12. – 22.01.2016	CIBI – KNIME Bioinformatics Hackathon	Konstanz	CIBI

IMPRESSUM:

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de.NBI Quarterly Newsletter is an exclusive service of de.NBI – German Network for Bioinformatics Infrastructure for members, partners and interested public.
For questions and remarks please address to contact@denbi.de
The de.NBI is supported by BMBF grants FKZ 031A532-031A540

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