de.NBI – GERMAN NETWORK FOR BIOINFORMATICS INFRASTRUCTURE

de.NBI Quarterly Newsletter

EDITION FEBRUARY 2016

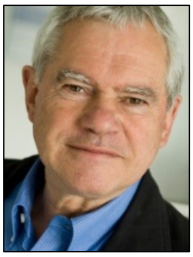
1) EDITORIAL

With this 3rd de.NBI Quarterly Newsletter (Edition February 2016) we are going to celebrate the 1st anniversary of the de.NBI network, which was officially started 1 March 2015. During the last 12 months de.NBI was very active and able to reach nearly all the goals on the agenda for the first year. In particular, the Central Coordination Unit (CCU) as well as five Special Interest Groups (SIGs) have immediately been established. They structured the work carried out by the eight service centers. As de.NBI coordinator I would like to thank all de.NBI members for supporting the different tasks of the network. I hope very much that in the current year the de.NBI development will be continued with the same enthusiasm.

This de.NBI newsletter contains a series of interesting contributions. I would like to point to the SAB meeting from 26-27 November 2015 in Berlin. Actually, the SAB meeting was a highlight for de.NBI, since an international group of bioinformatics experts stated that de.NBI developed extremely well during the first year. Based on the recommendations of the SAB, the coordinator together with the CCU prepared a de.NBI development plan for the year 2016. The plan consisting of six topics is presented in this newsletter.

Last but not least, it has to be pointed out that the decision of the BMBF to support a German membership in ELIXIR is the outstanding event within the last three months. This really means that in future de.NBI will have all opportunities to harmonize its activities on the European level. The de.NBI-ELIXIR collaboration is described in this newsletter.

The Quarterly Newsletter, of course, also informs again on upcoming events. In particular, de.NBI supports a workshop on the topic “Towards Cloud Solutions For Life Sciences And Translational Medicine” which will take place in Heidelberg on 21-22 April 2015. Furthermore, a minisymposium on “Bioinformatics for Metagenome Analysis” is planned at Bielefeld University on 6 July 2016. The de.NBI Summer School entitled “From Big Data to Big Insights” is scheduled for 26-30 September 2016 at Schloss Dagstuhl, Wadern.



A. Pühler

Alfred Pühler
(de.NBI coordinator)

CONTENT:

2) THE de.NBI SCIENTIFIC ADVISORY BOARD MEETING 2015 - RETROSPECTIVE

The de.NBI Scientific Advisory Board meeting 2015 took place on 26-27 November 2015 at the Seminaris Campus Hotel, Berlin. Four of the six SAB members attended the meeting. In order to inform the SAB members on the de.NBI achievements a status report was distributed beforehand. At the beginning of the meeting overviews of the de.NBI network were presented by the coordinator and the head of the Administration Office. The overviews were followed by presentations by the chairpersons of the Special Interest Groups and the coordinators of the Service Centers. In addition, a poster session illustrated the work of each individual project partner.


Four members of the Scientific Advisory Board with the de.NBI coordinator and the head of the Adminstration Office. (from left to right: R. Appel, I. Hofacker, R. Schneider, J. Thornton, A. Pühler, A. Tauch)

The report of the SAB panel was sent by the chairperson Janet Thornton to the de.NBI the coordinator on 15 December 2015. After discussing the report at the CCU meeting in Freiburg it was sent to the BMBF. The SAB report contains a number of valuable recommendations which will play an important role in the further development of de.NBI. The SAB report is preceded by a general statement demonstrating that the de.NBI network is on the right track to reach the aspired goals.

A general statement of the de.NBI SAB report on de.NBI network:

“The SAB congratulates the Coordinator and members of de.NBI on establishing the network and the significant progress made in the first 9 months. The network is well organised and coordinated with good communication between the members. The structure of the organisation is well designed to meet the challenges which de.NBI faces. The Central Administration Unit (CAU) and the Central Coordination Unit (CCU) appear to be working well. Although the CCU takes advice from the five Special Interest Groups (SIGs), the CCU is the decision making body for the whole infrastructure and has primary responsibility for de.NBI vision and strategy. If the infrastructure is to be successful, it is essential that this body works effectively. To date they have successfully organised many meetings of the SIGs and the Centres and helped to coordinate an extensive training program. The members of the network are also thoroughly engaged in delivering the infrastructure and enthusiastically participate in de.NBI.“

3) 2ND de.NBI PLENARY MEETING IN BERLIN

The 2nd plenary meeting of the German Network for Bioinformatics Infrastructure (de.NBI) was held on 27 November 2015 at the Seminaris Campus Hotel Berlin following the 1st meeting of the Scientific Advisory Board (SAB). The latter event already brought together the SAB group and the de.NBI community to discuss the recent achievements of the service centers. Two Distinguished Lectures enriched the workshop. R. Appel, director of SIB, presented key aspects of the Swiss Institute of Bioinformatics, the Swiss bioinformatics network. Subsequently N. Blomberg, director of ELIXIR gave a talk on “Enabling Europe-wide sharing of data in life sciences”, presenting the trans-European bioinformatics network ELIXIR. The subsequent de.NBI plenary meeting provided information on the internal work of the network by presentations given by the members of the Central Coordination and Administration Unit. The de.NBI coordinator, Alfred Pühler, briefly informed the plenum about the de.NBI status report, the Quarterly Newsletter, and the BMBF announcement of partner projects. The meeting was completed by reports of the head of the administration office, the web and service coordinator and the training coordinator. The 2nd plenary meeting in Berlin was attended by 75 de.NBI associates.

The de.NBI team at the 1st SAB meeting in Berlin

4) PARTNER PROJECTS OF de.NBI

The Federal Ministry of Education and Research (BMBF) announced the funding guidelines for partner projects of the German Network for Bioinformatics Infrastructure (de.NBI) on 18 November 2015. The deadline for application was 22 February 2016. Altogether, nearly 40 proposals have been submitted. The expansion of de.NBI by partner projects is intended to provide bioinformatics services in all areas of life science research. Therefore, partner projects will be funded that complement and enhance the expertise of the existing service centers and the database and data management nodes. The size of a partner project will be determined by the topic and the existing capacity in this field. After funding has been granted, the new project partners will be incorporated into the existing network structures as equal partners that make their bioinformatics services available during the entire funding period of three years.

5) THE de.NBI-ELIXIR COLLABORATION

During the last year a common statement has been developed which was entitled “ELIXIR and de.NBI collaboration strategy: Towards a German membership of ELIXIR”. This statement was finally signed at the beginning of this year by Niklas Blomberg, director of ELIXIR, and Alfred Pühler, de.NBI coordinator. The collaboration strategy comprises three phases, namely knowledge exchange (phase I), strategic collaboration (phase II) and full membership (phase III). See also http://www.denbi.de/index.php/news/92-elixir-and-de-nbi-agree-collaboration-strategy .

In 2015 the first two phases have already been started successfully, demonstrating that the collaboration is of advantage for both organizations. With the beginning of the current year also phase III took up speed. The Federal Ministry of Education and Research decided to officially start negotiations on a full membership of Germany in ELIXIR. The first official meeting with representatives from BMBF, ELIXIR and de.NBI is scheduled for 16 March 2016 in Berlin. It is expected that the negotiations are straight forward and that the contracts concerning a full German membership of ELIXIR can be signed in the near future. Subsequently, extensive preparations will be necessary to enable de.NBI to act as a national node within ELIXIR.

To summarize, the BMBF is now supporting a German membership of ELIXIR. de.NBI will act as the national node in the ELIXIR network.

6) de.NBI DEVELOPMENT PLAN 2016

As a response to the meeting of the Scientific Advisory Board on 26-27 November 2015 in Berlin the de.NBI coordinator prepared the de.NBI development plan 2016 which was discussed and finally approved on 19 January 2016 by the CCU at the meeting at Freiburg University. The de.NBI development plan 2016 consists of six points listed the adjacent box.

Content of the de.NBI development plan 2016

1. Integration of partner projects into the de.NBI network
2. Establishment of a de.NBI research program with doctoral students
3. Integration of the de.NBI as a national node of ELIXIR
4. Establishment of an industrial branch of the de.NBI network
5. Development of a de.NBI cloud to solve the de.NBI compute problem
6. Sustainability of the de.NBI network

The first topic deals with integration of partner projects into the de.NBI network. Details can be taken from chapter 4 of this newsletter.

A second topic is the establishment of a de.NBI research program with doctoral students. The program should cover the missing research component within the de.NBI network and simultaneously educate bioinformaticians in the field of bioinformatics infrastructure. The establishment of such a program should be financially supported by the BMBF.

The third topic focuses on the integration of the de.NBI network as a national node of ELIXIR. This subject is treated in chapter 5 of this newsletter.

Furthermore, the establishment of an industrial branch of de.NBI is on the agenda. Here it is planned to integrate small- and medium-sized enterprises as well as larger industrial companies by an industrial branch into the de.NBI network.

The next objective deals with the development of a de.NBI cloud which should help to solve the de.NBI compute problem. Here it is intended to work out how a de.NBI specific cloud can be used to analyze sets of big data generated in life sciences.

The last topic of the de.NBI development plan 2016 addresses the sustainability of the de.NBI network. This point is without doubt one of the most important tasks which have to be handled by de.NBI. The goal is to develop a procedure which will lead to a continuation of de.NBI beyond the funding period of five years.

7) REVIEW OF TRAINING COURSES 2015

The first de.NBI year was very successful in the field 'training'. In total, 15 training courses and one de.NBI late summer school took place. Altogether more than 550 applications were filed. Finally 329 participants took part in the training courses. The largest course was attended by 33 participants, the smallest one by nine scientists. About 98% of the participants were PhD students or Postdocs. The remaining 2% were PIs, undergraduates, and participants from industry. The courses were attended by 56% men and 44% women. About 10% of the participants came from outside Germany. The first feedback on the quality of the training courses showed a high degree of participants' satisfaction. In 2016, we intend to scale up the number of participants to more than 500. At the moment 34 training courses are announced for 2016 (http://www.denbi.de/index.php/training-courses).

8) REVIEW OF THE TRAINING COURSE: INTRODUCTION INTO TARGETED AND UNTARGETED METAGENOME ANALYSIS

From 23-25 November 2015, 15 participants from all over Europe and Germany took part in the targeted and untargeted metagenome training course in Bielefeld. The first part covered different aspects of general NGS data handling and presented different techniques and tools for quality measurement, filtering, and sequence correction. The second part of this course focused on 16S amplicon data analysis utilizing the command line tool QIIME. Problems and pitfalls as well as the correct usage of different specialized data bases were discussed with the attendants. In the third part, advantages and disadvantages of whole metagenome sequencing were illustrated. Two different techniques to analyze WGS metagenome data were part of this section. Firstly, for the read-based approach the software solution MGX, an integrated platform for metagenome analysis and data visualization, was demonstrated. Secondly, the assembly-based approach based on the reconstruction of genomes by assembling reads into contigs was shown.

9) DATA MANAGEMENT FOR PLANT GENOMICS & PHENOMICS STANDARDS, TOOLS AND INFRASTRUCTURES, A REVIEW

Organized by scientists of the German Crop BioGreenformatics Network (GCBN), which includes members of the German Plant Phenotyping Network (DPPN) nodes, a training workshop on “Data Management for Plant Genomics & Phenomics - Standards, Tools and Infrastructures”, held at the Helmholtz Zentrum München on 7-8 December 2015, was a big success.


Participants in the Plant Genomics workshop

More than 20 participants from international facilities used the opportunity for hands-on training and intense discussions on the future of data handling. The de.NBI-GCBN is specialized in the field of omics data analysis for crop plants and is well-known for its software platforms. In this context, the training modules focused on the workflow from genotypes to phenotypes. In particular, the participants gained insights into the use of web portals to access plant genome resources as well as into standards to exchange and annotate plant phenotypic data. Finally, infrastructures for publishing phenotypic data and APIs for embedding into own programs were presented.

10) ELIXIR TOOLS AND SERVICE REGISTRY HACKATHON

The BioTools Workshop, held on 19-20 January 2016 in Freiburg, was an example of what close collaboration in the bioinformatics community can achieve. The event was hosted by the RBC team, in particular Björn Grüning and Rolf Backofen. Twenty-seven scientists from de.NBI and ELIXIR attended the workshop that was entitled “ELIXIR Tools and Service Registry Hackathon”.

After an introduction by Björn Grüning, a talk on the BioTools registry was given by Jon Ison (CBS-DTU, DK). While Ison focused on the use of the EDAM Ontology to register services in BioTool, insight into the XML/JSON based structure behind the registry was given by his Danish colleague Emil Rydza. In this cooperative atmosphere all participants listed their respective services in BioTools with support from the experts. There was a vivid exchange of ideas on how to further enhance the functions and usability of the registry. Hervé Ménager (Institut Pasteur, FR) gave a talk on ReGaTE, a tool to directly convert Galaxy workflows to ready-to-insert descriptions for the BioTools registry which can easily be added afterwards. All in all, six ELIXIR instructors from Denmark, France, Norway and the USA participated in the event.

11) ANNOUNCEMENT OF THE de.NBI MINISYMPOSIUM “BIOINFORMATICS FOR METAGENOME ANALYSIS”

A minisymposium sponsored by de.NBI on “Bioinformatics for Metagenome Analysis” will take place in frame of the 11. CeBiTec Symposium entitled “Microbial Genomics and Metagenomics in Human Health and Disease” at Bielefeld University (4-6 July 2016). On 6 July, two sessions to be chaired by Peer Bork, HD-HuB and EMBL Heidelberg, and Alexander Sczyrba, BiGi and Bielefeld University, will focus on bioinformatics tools for analyzing metagenome sequences and human microbiomes in health and disease, respectively.

12) UPCOMING EVENTS

The calendar of upcoming events lists quite a number of events scheduled for the next four months. All offers are accessible via the de.NBI homepage http://www.denbi.de. The de.NBI training programme is continuously updated on our homepage.

- **Galaxy workshop on HTS data analysis (22-26 February 2016), Freiburg.** This course is hosted by RBC in cooperation with MPI-IE Freiburg. Participants will learn to use Galaxy as framework for an easy accessible, reproducible and transparent HTS data analysis. The workshop combines theoretical lessions with practical exercises. Preliminary topics are introduction into Galaxy, RNA-seq data analysis, ChIP-seq data analysis, Exome-seq data analysis, and Methyl-seq data analysis. http://www.denbi.de/index.php/11-training-cat/55-hts1

- **KNIME Spring Summit Workshop 2016, (22-26 February 2016), Berlin.** KNIME's annual conference for KNIME users and enthusiasts is taking place in Berlin. A CIBI workshop on 26 February will treat bioinformatics integrations in KNIME. The workshop will give a brief introduction to proteomic, metabolomics and genomic sequence analysis using OpenMS and SeqAn with KNIME.

- **Spezielle Aspekte von Bioinformatik - Methoden in der MS-basierten Proteomik (28 February 2016), Hamburg.** In the frame of the 49th annual meeting of the German Society for mass spectrometry (DGMS) BioInfra.Prot staff will give insights into protein sequence databases, the decoy approach in protein identification, protein interference and targeted proteomics. A special focus will be on every-day handling of data and optimization of parameters for better analysis of data.

- **Von Spektren zu Ergebnissen: Effiziente Analyse von massenspektrometrischen Daten mit Workflows (28 February 2016), Hamburg.** This DGMS workshop organized by CIBI provides an introduction to the powerful workflow system KNIME and the OpenMS pipeline tools. Hands-on material is provided for the construction of basic analysis workflows. For participants with advanced background in computational mass spectrometry or workflow systems, topics like, e.g. integration of R scripts for statistical analysis are interspersed.

- **OpenMS Developer Meeting (11-18 March 2016), Milford Hall, near Belford, Northumbria, UK.** The OpenMS developer’s meeting, instructed by CIBI staff, aims at coordinating the mid and long-term development of OpenMS. It is targeted at bioinformaticians with background in software development (ideally C++ and python, OpenMS).

- **SeqAn de.NBI User Meeting (30 March - 01 April 2016), Berlin** is offered by CIBI. For tool developers and programmers, the workshop will offer guided tutorials, which aim at getting programmers acquainted with the programming paradigms, the content and the structure of the SeqAn template library. For end users, the workshop offers courses in selected SeqAn applications (e.g. Yara or Lambda), talks by groups using SeqAn and tutorials of workflow integration into KNIME.

- **Towards Cloud Solutions For Life Sciences And Translational Medicine (21-22 April 2016), Heidelberg.** The workshop by DKFZ, EMBL and de.NBI is a platform for discussing the needs and demands for establishing a comprehensive cloud solution for computing and storage of various data types in life sciences. International experts from science and industry will present state-of-the-art solutions to meet these demands. Further information at:
http://www.applied-translational-genomics-cloud.de/joomla/index.php/en/workshop

- **Workflow based metabolomics - a de.NBI teaching event at the Metabolomics in Biomedical Research workshop (26 April 2016), Tübingen.** This CIBI event is targeted at experimentalists and data analysts interested in metabolomics workflow construction using KNIME and OpenMS. The workshop starts with an introduction to the powerful workflow system KNIME and the OpenMS pipeline tools. Hands-on training will focus on the construction of basic analysis workflows. In addition to highly customizable workflows in KNIME, a brief introduction to the commercial Thermo Compound

Discoverer application will be given and it will be shown how an OpenMS workflow can be integrated as community extension.

- **de.NBI Summer School 2016 - From Big Data to Big Insights (26-30 September 2016), Schloss Dagstuhl (Wadern).** This year's de.NBI Summer School featuring computational methods for the analysis and interpretation of mass-spectrometric high-throughput data is jointly organized by Bio-Infra.Prot, CIBI and BiGi. The de.NBI summer school aims at providing deeper insights into the details of existing algorithms or software systems in proteomics and metabolomics. Participants will use – instructed by international keynote and de.NBI speakers – existing tools to analyse and visualize real-world datasets (data specifically prepared for the tutorials as well as the participants' own data). Beyond that, the end users will be put into a position to be able to combine their own existing and future algorithms or tools with other solutions as well as to integrate them into a sustainable software system. To this end the summer school will also contain hackathons to quickly prototype novel tools. http://www.denbi.de/index.php/news/100-lss2016-2 or https://goo.gl/ZRgxuV

Overview of upcoming de.NBI events

	Date	Event	City	Organizer
➢	22-26 Feb 2016	**Galaxy workshop on HTS data analysis**	Freiburg	RBC
➢	22-26 Feb 2016	**KNIME Spring Summit Workshop 2016**	Berlin	CIBI
➢	28 Feb 2016	**Spezielle Aspekte von Bioinformatik - Methoden in der MS–basierten Proteomik**	Hamburg	BioInfra.Prot
➢	28 Feb 2016	**Von Spektren zu Ergebnissen: Effiziente Analyse von massenspektrometrischen Daten mit Workflows**	Hamburg	CIBI
➢	13-18 Mar	**OpenMS Developer Meeting**	Milford Hall, UK	CIBI
➢	30 Mar-01 Apr 2016	**SeqAn de.NBI User Meeting**	Berlin	CIBI
➢	19 Apr 2016	**6. CCU Meeting in Bielefeld**	Bielefeld	CAU
➢	21-22 Apr 2016	**"Towards Cloud Solutions For Life Sciences And Translational Medicine" workshop**	Heidelberg	HD-HuB, DKFZ, EMBL, CAU
➢	30-31 May 2016	**Kinetics on the move: practical workshop on data and tools for quantitative modelling**	Heidelberg	HD-HuB
➢	4-6 July 2016	**"Microbial Genomics and Metagenomics in Human Health and Disease" 11. CeBiTec-Symposium including de.NBI Minisymposium**	Bielefeld	BiGi, CAU
➢	21-23 Sep 2016	**9th OpenMS User Meeting**	Tübingen	CIBI
➢	26-30 Sep 2016	**de.NBI Summer School 2016**	Schloss Dagstuhl (Wadern)	BioInfra.Prot, CIBI, BiGi

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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