

de.NBI Quarterly Newsletter

This de.NBI Quarterly Newsletter in February 2020 informs about recent developments and current events in the project **German Network for Bioinformatics Infrastructure – de.NBI.**

Further information at: https://www.denbi.de/

SYMPOSIUM CELEBRATING THE 5TH ANNIVERSARY OF THE de.NBI

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In March 2015, the German

Ministry of Education and Research (BMBF) launched the de.NBI project with the aim of establishing a Germany-wide bioinformatics infrastructure offering bioinformatics service, training and international cooperation. Now, five years later, the network is operating very successfully and celebrated its 5th anniversary with a symposium on 13

February 2020 at the Seminars CampusHotel in Berlin.

More than 150 scientists took part in the symposium, most of them members of the network, but also the Scientific Advisory Board, members of the reviewer team, members of the de.NBI Industrial Forum, and representatives of the Ministry and project management.

The symposium was opened by the BMBF representative Matthias Kölbel who focused on the successful establishment of the bioinformatics infrastructure which now needs a sustainable continuation. In the first session, the de.NBI coordinator Alf Pühler started with an overview on the de.NBI highlights, followed by three de.NBI presentations focusing on bioinformatics for humans, plants and microbes. In the second session external experts presented their views on specific aspects of the de.NBI network. The ELIXIR director Niklas Blomberg informed on the ELIXIR organization and its cooperation with de.NBI. Rolf Apweiler, director of EMBL-EBI, used his talk to report on digital medicine in Germany and Europe. Finally, Dietrich Rebholz-Schuhmann, director of ZB MED Information Center for Life Sciences, presented his institute engaged in handling of research data in the life science.

Find more information at: https://www.denbi.de/events/661-sab-meeting-2020

Further reading on the web pages of PtJ and BMBF:

- 1) https://www.ptj.de/ueber-uns/aktuelles?backRef=83&news=Fuenf Jahre Deutsches Netzwerk fuer Bioinformatik Infrastruktur deNBI
- 2) https://www.bmbf.de/de/bioinformatik-detektivarbeit-im-erbgut-10896.html

THE 4TH SAB MEETING OF THE de.NBI

In the frame of the 5^{th} anniversary meeting of the de.NBI network, the de.NBI Scientific Advisory Board (SAB) assembled for its annual meeting on 13-14 February 2020 at the Seminaris CampusHotel in Berlin.

The current SAB consists of 8 internationally renowned bioinformaticians from Austria, France, Germany, Luxembourg, Spain, Sweden and the Netherlands and is chaired by Reinhard Schneider from Luxembourg. The task of the SAB is to collect information on the de.NBI development and to advise the de.NBI network on its future development. For this meeting the de.NBI Status Report was presented which contains the reports of the coordinators of the service centers and

the chair persons of the Special Interest groups. The de.NBI coordinator and the Head of the administration office contributed a chapter on structure, organization and tasks of the network.

The collaboration with ELIXIR was elaborated in the ELIXIR-DE report as a separate document. A poster session was held in the evening of the first day to inform about the developments and achievements in the individual de.NBI projects.

The second day of the SAB meeting was then used by the board to develop a recommendation document. In a feedback session the main statements of this document were presented to the de.NBI audience. In summary, the overall development of the de.NBI network was highly appreciated, but it was clearly stated that the sustainable continuation of the network as a whole should be the goal for the future.



Find more information on the SAB at: https://www.denbi.de/organisation/scientific-advisory-board-sab

6TH de.NBI PLENARY MEETING

The de.NBI and ELIXIR-DE plenary meeting took place on 14 February 2020. 125 de.NBI members participated in the two sessions focusing on the report of the de.NBI coordinator and the plans of the Service Centers and SIGS for the next project phase (bridge phase) that starts in March 2020. In the second session A. Tauch summarized the development of ELIXIR Germany with focus on the now completed legal framework consisting of the collaboration agreement and the German consortium treaty. B. Grüning and A. Goesmann gave insights into the tasks of the technical coordinator and the ELIXIR board, respectively. The new group photo of the de.NBI consortium shows a still growing community.



de.NBI HIGHLIGHTS BROCHURE

To mark the occasion of the 5th anniversary of the de.NBI network in 2020, the de.NBI Administration Office presented the brochure entitled "Von de Dael nanalyse zum Verstehen komplexer biologischer Systeme" which features contributions from de.NBI Service Centers and projects partners and provides information on the diverse activities of the de.NBI network. The brochure showcases the contribution of de.NBI as a national bioinformatics infrastructure in the field of life sciences and provides solid information about the advancement of research conducted in the field of big data on a national level. In order to target a large amount of readers, the brochure is presented in the German language. The document is divided into four chapters, namely the plant, microbial and medical bioinformatics followed by the description of the de.NBI network and its activities in the fields service, training, cloud computing, and industrial partnership. The interplay of research activities between biotechnology, molecular biology, genome research, systems biology, medicine and bioinformatics is presented from different perspectives. The brochure also includes an interview with the de.NBI coordinator and the head of the administration office and discusses the structure and organization of



the network as well as the many activities that have been carried out since de.NBI establishment. An English version is intended.

For further details, please refer to the full version at: https://www.denbi.de/images/Downloads/deNBI highlight brochure German.pdf

For the printed version please contact the de.NBI office at: contact@denbi.de

ELIXIR GERMANY COLLABORATION AGREEMENT SIGNED



On 9 January 2020, the National Collaboration Agreement to establish the German ELIXIR Node (ELIXIR-DE) became effective. This contract was signed by 21 German universities and research institutes, including Bielefeld University that will take over the legal role as 'Representing Entity' of ELIXIR Germany. The National Collaboration Agreement is the legal document that specifies the organization of ELIXIR-DE and the role of the Central Coordination Unit (CCU). This committee is the decision-making body of ELIXIR-DE and responsible for the effec-

tive operation of the national ELIXIR node. The CCU consists of nine members, including the Head of Node and representatives of the eight service units of ELIXIR-DE.

In addition, the ELIXIR Collaboration Agreement was signed by the Representing Entity and the ELIXIR Director, Niklas Blomberg. This contract became effective on 10 February 2020, thereby fully establishing the German ELIXIR Node. The ELIXIR Collaboration Agreement is the legal document that ties together the ELIXIR Hub with the national node and it forms the legal basis of Commissioned Services. These technical projects that guide future service developments are funded through the budget of the ELIXIR Hub and are implemented by ELIXIR members in the national nodes.

BJÖRN GRÜNING (RBC) APPOINTED AS LEAD OF THE ELIXIR TOOLS PLATFORM

In December 2019 ELIXIR announced new Platform Leads for the Tools, Data and Training Platforms. Björn Grüning (RBC Freiburg/ELIXIR Germany) was appointed as Platform Lead of the ELIXIR Tools Platforms together with Salvador Capella (ELIXIR Spain) and Hervé Menager (ELIXIR France). The Platform Leads will serve a two-year term starting from the 1 January 2020. They are collectively responsible for the operations and activities of the Platform, and help to drive new developments in the respective task areas. The main objective of the ELIXIR Tools Platform is to improve the discovery, quality and sustainability of software resources. Björn Grüning is also Co-Leader of the Galaxy Working Group of the Tools Platform, together with Frederik Coppens (ELIXIR Belgium). The goal of this working group is to contribute to the development of the Galaxy platform and to provide specific training for users, developers and system administrators.

More information: https://elixir-europe.org/news/elixir-welcomes-six-new-platform-leads

JOHANNES WERNER (IOW) ASSOCIATED as de.NBI TRAINING PARTNER

The Central Coordination Unit of de.NBI approved the application by Johannes Werner to become associated to the network as an external training partner. Since 2018, Johannes Werner is bioinformatics scientist in marine microbial bioinformatics at the Department of Biological Oceanography of the Leibniz Institute for Baltic Sea Research (IOW) in Rostock-Warnemünde. His research focus deals mainly with the meta-omics



(IOW) in Rostock-Warnemünde. His research focus deals mainly with the meta-omics analyses of microbial communities in contact with anthropogenous substances. Johannes Werner also conducts training in bioinformatics on a regular basis. He will contribute to the de.NBI training program by offering advanced training courses on 16S rRNA amplicon analysis with the R packages DADA2 (https://ben-jineb.github.io/dada2/index.html) and phyloseq (https://joey711.github.io/phyloseq/

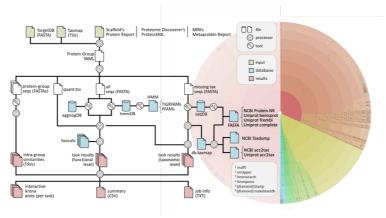


STEPHAN FUCHS (RKI) AFFILIATED AS ASSOCIATED de.NBI PARTNER

In January 2020, the Central Coordination Unit (CCU) of de.NBI unanimously approved the application of Dr. Stephan Fuchs to become an Associated Partner of the de.NBI consortium. Stephan Fuchs is researcher at the Robert Koch Institute (RKI Wernigerode). The RKI is the government's central scientific institution in the field of biomedicine and one of the most important bodies for the safeguarding of public health in Germany.



Stephan Fuchs gained scientific experience in the fields of multi- and meta-Omics analyses with a strong focus on nosocomial infections and antibiotic resistances. In the field of Metaproteomics, he already collaborated with the de.NBI partner project ,MetaProtServ' of Dirk Benndorf and Gunter Saake from Otto von Guericke University Magdeburg. Together with the Magdeburg team Stephan Fuchs will contribute to de.NBI services and training courses in metaproteome analysis with the MetaProteomeAnalyzer (MPA) Software (http://www.mpa.ovgu.de) and a de.NBI Cloud-based version of the Prophane analysis software (http://www.prophane.de).



Workflow and visualization of results in Prophane

THE de.NBI IN THE CONTEXT OF ARTIFICIAL INTELLIGENCE

During the last session of the Central Coordination Unit (CCU) on 21 January 2020 in Bielefeld, a paper with the title "de.NBI im Kontext von Methoden der Künstlichen Intelligenz", written by the Special Interest Group on de.NBI development, was discussed and finally accepted.

The key information of this document is:

- Deep learning and artificial intelligence require large amounts of data, bioinformatics tools and application domain experts to achieve breakthroughs in the life sciences.
- The de.NBI network, as an infrastructure where data from many sources are processed and subject-specific expertise is gathered, can make decisive contributions to enable artificial intelligence in the life sciences in Germany at an internationally competitive level.

Further, it should be mentioned that three PI from the de.NBI network were selected by the Federal Ministry for Education and Research (BMBF) to carry out research projects in the frame of the initiative "Computational Life Sciences (CompLS) - Deep Learning in der Biomedizin". The titles of these research projects deal with (a) Deep learning for the detection of protein variants, (b) Development of a tool to support the curation of text and bio data and (c) Identification of new antimicrobial resistance targets.

The German text of this white paper is available via: https://www.denbi.de/images/Downloads/deNBI KI.pdf.

GUIDELINES FOR de.NBI SERVICES ADOPTED

The de.NBI network has successfully established guidelines for Node service selection and quality assurance for services offered to the life science research community within Germany and Europe.

The Guidelines describe a list of required implementations for the continuation of a certain service within the de.NBI service portfolio. The procedure is set to facilitate the monitoring and constant evaluation of the existing services, as well as help in the process of endorsing new ones offered by external service providers. With such a procedure in place, the de.NBI network can guarantee the relevance and maximum performance of its services according to the highest scientific standards.

The quality assurance criteria for de.NBI services are inclusive and ensure that the offered services should fulfill high scientific and technical standards and comply with ethical and privacy legalities regarding data protection as well as the open science and FAIR data principle.

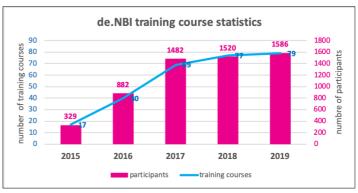
The document was unanimously approved by the de.NBI Central Coordination Unit (CCU) on their meeting on the 22^{nd} of October, 2019 in Bielefeld. The de.NBI administration office staff will run periodic checks on the existing de.NBI services

based on the approved quality assurance criteria in order to maintain their performance at the highest capacity.

For more details please refer to the full text under https://www.denbi.de/images/Service/deNBI_ELIXIR-DE_Gudielines_Services.pdf

NEW RECORD: 1,586 TRAINING COURSE PARTICIPANTS IN 2019

The fifth de.NBI year was very successful in the field 'training'. In 2015, de.NBI started with 17 training courses and 329 participants, with increasing numbers in 2016 (40 courses with 882 participants), 2017 (69 courses with 1,489 participants) and 2018 (77 courses with 1,520). In the last year, de.NBI further increased the number of courses and participants: 79 training courses with 1,586 participants. The largest course was attended by 72, the smallest one by four scientists. Approx. 75% of the participants were PhD students or Postdocs. The remaining



25% were PIs, undergraduates, and participants from industry. The gender ratio of the students was 56% male and 44% female. About 30% of the participants came from outside Germany. In general, the user survey shows satisfaction values around 90%. More than 60 training courses with a large variety of scientific topics are already announced for 2020.

UseGalaxy.eu PROVIDES HUMAN MULTI-OMICS DATA FROM UK PERSONAL GENOME PROJECT



The Freiburg Galaxy Team headed by Björn Grüning (RBC Freiburg) announced that socalled multi-omics reference panel data from the Personal Genome Project UK (PGP-UK) is now accessible directly on Galaxy Europe. This includes unprocessed data,

but also pregenerated results, from the 10 participants with complete multi-omics data (whole-genome, methylome and transcriptome). Interested users of Galaxy Europe are encouraged to use the data for establishing new workflows, for own training courses and to hone their own data analysis skills. The Galaxy Training Network provides hands-on tutorials to get you started with the analysis of this kind of data.

More Information: https://galaxyproject.eu/posts/2020/01/16/pgp/

INITIAL ANALYSIS OF COVID-19 DATA USING GALAXY, BIO-CONDA AND PUBLIC RESEARCH INFRASTRUCTURE (XSEDE, de.NBI-CLOUD, ARDC CLOUD)

The Galaxy development teams from galaxy.org, galaxy.eu, galaxy.be, and galaxyorg.au have provided the public repositories with descriptions of all workflows and software versions used for the initial analysis of COVID-19 data using Galaxy, BioConda and public research infrastructure (XSEDE, de.NBI-cloud, ARDC cloud). This work was accomplished with considerable involvement of staff from RBC Freiburg.

Abstract of the publication:

The current state of much of the Wuhan pneumonia virus (COVID-19) research shows a regrettable lack of data sharing and considerable analytical obfuscation. This impedes global research cooperation, which is essential for tackling public health emergencies, and requires unimpeded access to data, analysis tools, and computational infrastructure. Here we show that community efforts in developing open analytical software tools over the past ten years, combined with national investments into scientific computational infrastructure, can overcome these deficiencies and provide an accessible platform for tackling global health emergencies in an open and transparent manner. Specifically, we use all COVID-19 genomic data available in the public domain so far to (1) underscore the importance of access to raw data and to (2) demonstrate

that existing community efforts in curation and deployment of biomedical software can reliably support rapid, reproducible research during global health crises.

All analyses are fully documented at: https://github.com/galaxyproject/SARS-CoV-2.

Link to the original publication: https://doi.org/10.1101/2020.02.21.959973

NEWS FROM THE de.NBI OFFICE

Rabeaa Alkhateeb will leave the de.NBI Administration Office by end of February 2020 after almost two years of working as the de.NBI Service Coordinator and ELIXIR Germany Node Coordinator. Rabeaa will move on with her career working as a postdoctoral researcher in the field of single cell transcriptomics and genomics. We have enjoyed having Rabeaa as a member of our team and would like to wish her all the best for the next steps!



RECENT UPDATES OF de.NBI SERVICES

New versions of various de.NBI services and tools have been released in the last months accompanied by respective publications:

- SILVAngs Frontend updated to version 1.9.5. New features include: updated Fingerprint Tool, updated information and the de.NBI cloud and improved stability and performance. https://www.denbi.de/services/344-silvangs-a-data-analysis-service-for-ribosomal-rna-gene-rdna-amplicon-reads-from-high-throughput-sequencing-next-gene-ration-sequencing-ngs-approaches
- OpenMS: The new algorithms FLASHDecon, available through OpenMS provides 2-3 orders of magnitude faster deconvolution of top-down protein spectra Publication: FLASHDeconv: Ultrafast, High-Quality Feature Deconvolution for Top-Down Proteomics. https://doi.org/10.1016/j.cels.2020.01.003 Find OpenMS at: https://www.denbi.de/services/369-openms-a-c-library-for-lc-ms-data-management-and-analyses
- Mercator: The annotation tool for plat proteins offers now integrated FASTA functional annotation for plant proteins. https://www.denbi.de/services/507-mercator-annotate-and-classify-plant-protein-and-dna-sequences
- SeqAN 3.0.1: A new release has been published. See the new features at: http://www.seqan.de/seqan-3-0-1-released/
- Freiburg RNA Tools Webserver: New integration of MutaRNA tool to evaluate mutation effects on RNA structure and an updated IntaRNA 3.1.3 for RNA-RNA interaction prediction.https://www.denbi.de/services/356-freiburg-rna-tools-webserver
- **▶ UseGalaxy.eu** published a factsheet available at: https://github.com/usegalaxy-eu/branding/tree/master/factsheet. Exciting progress in the ELIXIR Galaxy community is described in the news post https://elixireurope.org/news/galaxy-europe-2020
- Location of repetitive sequences and thus facilitates the analysis of plant genomes. Find CATS at https://www.denbi.de/services/503-crop-analyis-tools-suite

de.NBI @ CONFERENCES

de.NBI supported conferences in the near future

6th joint conference of DGHM and VAAM, 8-11 Mar 2020, Leipzig de.NBI will exhibit a booth at the largest German conference in the sector microbiology and hygiene. An expected audience of >1000 scientists will provide the opportunity to introduce de.NBI services, training portfolio, and cloud to a large community.

General information and registration at: https://vaam.de/aktivitaeten/jahrestagung/



UPCOMING EVENTS

The calendar lists the de.NBI training courses and events scheduled in the next months. All courses are accessible via the de.NBI web page. A number of training events are in the pipeline but not yet scheduled. Please consult the de.NBI training program for updates.

Overview of upcoming de.NBI events



	Date	Event	City	Organizer
, <u>å</u> .	26 Feb 2020	<u>BioC++ - solving daily bioinformatic tasks with C++ efficiently - BIOSTEC 2020</u>	Valletta	CIBI
,	02-06 Mar 2020	Galaxy Admin workshop 2020	Barcelona	RBC
, <u>å</u> .	05 Mar 2020	Introduction to Data Management	Plön	de.NBI-SysBio
,	15-21 Mar 2020	OpenMS Developer Meeting	Corinth	CIBI
,	18 Mar 2020	Introduction to Regular Expressions	Heidelberg	HD-HuB
,4.	23-27 Mar 2020	Galaxy single cell RNA-seq data analysis workshop	Freiburg	RBC
, <u>å.</u>	30-31 Mar 2020	Software Carpentry 1.2020	Köln	Ass. Partner ZB MED
, å. ,	30 Mar - 01 Apr 2020	Introduction to Machine Learning using Galaxy	Freiburg	RBC
, <u>å</u> .	03 Apr 2020	KNIME Workshop at Spring Summit	Berlin	CIBI
, <u>å</u> .	21 April 2020	22. CCU Meeting	Berlin	CAU/HD-HuB
, <u>å</u> .	27-29 Apr 2020	Tools for Systems biology modeling and data exchange: CO-PASI, CellNetAnalyzer, SABIO-RK, FAIRDOMHub/SEEK 2020	Magdeburg	de.NBI-SysBio
, <u>å</u> .	04-06 May 2020	6th de.NBI Genomics training course	Gießen	BiGi et al.
, <u>å</u> .	18-19 May 2020	DNA Methylation: Design to Discovery 2020	Saarbrücken	HD-HuB/ de.NBI-epi
,	20 May 2020	Phylogenetic reconstruction course 2020	Kiel	Ass. Partner Kiel
,	15-17 Jun 2020	Computational genomics course for hands-on data analysis 2020 - Modules: Data visualization & machine learning. RNA Seq, Single Cell Seq	Berlin	RBC/de.NBI- epi
, å .	21-26 Jun 2020	CSAMA 2020: Statistical Data Analysis for Genome-Scale Biology	Bressanone- Brixen	HD-HuB
, <u>å</u> .	30 Jun 2020	23. CCU Meeting	Bochum	CAU/BioIn- fra.Prot
,4.	24-28 Aug 2020	CIC Summer School on Cheminformatics	Halle (Saale)	BioData
, <u>å</u> .	14 Sep 2020	OpenMS at the German Conference for Bioinformatics (GCB)	Frankfurt	CIBI
, <u>å</u> .	14 Sep 2020	SeqAn at the German Conference for Bioinformatics (GCB)	Frankfurt	CIBI
, <u>å</u> .	14 Sep 2020	ProteinsPlus at the German Conference for Bioinformatics [GCB]	Frankfurt	BioData
, <u>å</u> .	21-25 Sep 2020	de.NBI Summer School 2020 - Metagenomics	Gießen	BiGi,
,	11 Oct 2020	COMBINE & de.NBI Tutorial: Modelling and Simulation Tools in Systems Biology – ICSB 2020	Farmington	de.NBI-SysBio

Further information at: http://www.denbi.de/training

IMPRESSUM

RESPONSIBLE FOR CONTENTS

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