

de.NBI Quarterly Newsletter

This de.NBI Quarterly Newsletter in **November 2021** informs about current developments and recent events in the BMBF project

German Network for Bioinformatics Infrastructure – de.NBI.

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

Future of the de.NBI Quarterly Newsletter

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The de.NBI network has been established within the frame of a BMBF grant from 2015 to 2021. From 2022 onwards, the network will be continued within the Forschungszentrum Jülich, a member of the Helmholtz Association of German Research Centers. This will imply a restructuring of the network.

Nevertheless, we intend to continue our Quarterly Newsletters and look forward to providing information on our bioinformatics infrastructure in future. You will hear from us in the next year and we will use the existing subscription list.

A further SAB conference of the de.NBI network and ELIXIR-DE

The Scientific Advisory Board (SAB) of the de.NBI network and the ELIXIR-DE node was established to comment on relevant achievements and to provide recommendations for the network's future development. In order to inform SAB members of the actual progress, annual conferences were organized. Such a conference took place as an online event in the morning of 19 November 2021. The agenda of the conference informs on the presentations. The basic information on the de.NBI network was provided by the de.NBI coordinator **A. Pühler**. The major de.NBI activities concerning service, training and cloud computing were then contributed by de.NBI members. **U. Scholz**, chairperson of SIG 2 - Service & Service Monitoring, gave an overview on the broad range of services offered. **O. Kohlbacher**, chairperson of SIG 3 - Training & Education, reported on training activities, followed by **A. Sczyrba**, chairperson of SIG 6 - de.NBI Cloud, who presented the current status of the de.NBI cloud and its use for data analyses in the life sciences. The development of the ELIXIR-DE node was then summarized by **A. Tauch**, Head of Node. Of particular interest was the presentation of **F. Melchior**, member of the Board of Directors of the Forschungszentrum Jülich, since her presentation described a concept for the continuation of the de.NBI network and the ELIXIR-DE node under the umbrella of the Helmholtz Association.

The BMBF funding for the de.NBI project will come to an end in December 2021 and the German government appointed the Forschungszentrum Jülich to take care of the de.NBI continuation. Hence, it is of interest how the German Network for Bioinformatics Infrastructure can be continued from January 2022 on. The general discussion at the end of the SAB conference was therefore used to present all necessary information for the continuation of the network. The discussion showed that at the moment, there is no clear picture describing a successful continuation. Several de.NBI members, however, expressed their wish that the BMBF should help to bridge the de.NBI project for another year to gain time for finding a longer-lasting solution.

It should be mentioned that the SAB conference was open for all de.NBI members and that therefore, this SAB conference served as the plenary meeting 2021 of the de.NBI network and the ELIXIR-DE node.



5th SAB Meeting and Plenary Meeting
19 November 2021, 10:00 – 12:30, online

Agenda

Welcome and start of the SAB and Plenary Meeting	T. Dammann-Kalinowski, Beiefeld
Progress report of the German Network for Bioinformatics Infrastructure (de.NBI)	A. Pühler, Beiefeld
Service activities for life sciences in Germany	U. Scholz, Gatersleben
Training activities for life sciences in Germany	O. Kohlbacher, Tübingen
Development and operation of the federated de.NBI Cloud	A. Sczyrba, Beiefeld
Progress report of the ELIXIR Germany node (ELIXIR-DE)	A. Tauch, Beiefeld
The concept for the continuation of the de.NBI network and the ELIXIR-DE node at the Research Center Jülich	F. Melchior, Jülich
General discussion on de.NBI and ELIXIR-DE issues	all

2nd Annual Meeting of the de.NBI Industrial Forum, 25 Nov 2021



**Annual Meeting of the
de.NBI Industrial Forum**
Thursday, 25 November 2021
1 – 4:30 pm (CET)

This year's Annual Meeting of the de.NBI Industrial Forum will take place virtually on 25 Nov 2021. It will focus on the main topic **Artificial**

Intelligence (AI). Altogether, six forum members will contribute to this topic and report on AI projects carried out in their companies. In addition, a **frastructure (NFDI)**. The NFDI projects dealing with BioDiversity and with Microbiota were selected for presentations. Besides these two topics, the meeting will be used to inform on recent developments of the de.NBI network and the de.NBI Industrial Forum. The event will take place online and is open free-of-charge for all interested participants.

More information on the de.NBI IF: <https://www.denbi.de/industrial-forum>

Find program and registration at: <https://www.denbi.de/events/1309-2nd-annual-meeting-of-the-de-nbi-industrial-forum-virtual>

Program

01:00	Opening	A. Fühler / M. Wittchen, Uni Bielefeld
01:10	Future Developments of the de.NBI Network	
	- Expiring of BMBF funding	A. Fühler, Uni Bielefeld
	- Continuation in the frame of the Helmholtz Association	F. Meckler, FZ Jülich
01:30	Artificial Intelligence projects of the Industrial Forum members, Part 1	
	- Higher-order Machine Learning Models Act as an Approximation of Biological Regulatory Mechanisms	S. Schultheiss, Compomics GmbH, Tübingen
	- Open Ecosystem for Integrated Machine-Learning Workflows	S. Rhode, Carl Zeiss Microscopy GmbH, Jena
	- Promises and Progress in Applications of AI in R&D Sanofi-Aventis Deutschland	T. Klambunde, Sanofi-Aventis GmbH, Frankfurt
02:30	Virtual Coffee Break	
02:40	Artificial Intelligence projects of the Industrial Forum members, Part 2	
	- Adventitious Virus Testing - Exploring the Machine Learning's Potential	H. Tran, IDT Biologika GmbH, Dessau
	- AI or not AI - That is the Answer!	C. Stephan, Kalros GmbH, Bochum
	- Artificial Intelligence in a plant breeding company	J.-C. Sclater / A. Menze, KWS SAAT SE, Eintrach
03:40	NFDI projects supported by de.NBI	
	- The National Research Data Infrastructure (NFDI) and NFDI4Biodiversity	F.O. Glöckner, AWI Bremen
	- NFDI4Microbiota - FAIR data, analytical workflows and much more for the microbiology community	K. Förstner, ZB MED Cologne
04:20	Wrap-up and Closing	M. Wittchen







4th de.NBI Cloud User Meeting



**4th CLOUD
USER
MEETING** 21

The 4th de.NBI Cloud User Meeting is taking place as a virtual conference from **12-24 Nov 2021** with more than 60 participants in the various lectures and workshops on actual de.NBI Cloud projects and technical backgrounds. They will instruct users to develop or extend their services and tools to the cloud computing environment in de.NBI Cloud. Again the SIG 6 and de.NBI Cloud admin group are strongly engaged in this training and community event.

Oral presentations:

-  Introduction to the de.NBI Cloud
-  Virtual Research Environment
-  ESPACE-cloud - a data sharing and analysis platform for an international research project in the de.NBI Cloud
-  GHGA (German Human Genome-Phenome Archive) at the de.NBI Cloud
-  HuMAGs - Recovery of metagenome-assembled genomes from over 10 thousand human Microbiomes
-  The SARS-CoV-2 Genomics Data Portal - CoGDat

- Nils Hoffmann, Bielefeld University
- Petra Ritter, Charité Universitätsmedizin Berlin
- Sven Twardziok, Charité Berlin
- Kersten Breuer and Koray Kirli, DKFZ
- Ulisses Nunes da Rocha, UFZ, Leipzig
- Leon Kuchenbecker, University of Tübingen

Workshops:

- SimpleVM and Linux Command Line Introduction.
- OpenStack Introduction
- Bioconda and Biocontainers
- Deploying a compute cluster in OpenStack via Terraform
- Kubernetes Introduction I & II
- BiBIGrid Cluster Setup

Find program and further information at: <https://events.denbi.de/event/1/>

Women in Data Science – Perspectives in Industry and Academia II

After the successful inaugural event in June 2021 “Women in Data Science – Perspectives in Industry and Academia”, in which six female scientists gave insights into their careers in data science and related fields, Bayer AG & de.NBI / ELIXIR Germany will organize a second meeting virtually held on 2 December 2021. To show how attractive and diverse the job of a data scientist can be, regardless of whether it is industry or academia, we invited four outstanding female speakers, Janine

Joint Bayer AG and de.NBI/ELIXIR Germany Online Event

**Women in Data Science -
Perspectives in Industry and Academia**

**December 2nd, 2021
3:00 pm CET**

Anomida Zadissa
Senior Strategy Officer,
EMBL, EBI,
Hinxton, UK

Janine Fieldon
MARUM - Center for Marine
Environmental Sciences,
Alfred Wegener Institute -
Helmholtz Center for Polar-
and Marine Research
de.NBI / ELIXIR-DE
Bremen, DE

Jennifer Spindel
Plant Breeding,
Bayer Crop Science,
St. Louis, USA

Katharina Meier
Computational Molecular Design,
Bayer Pharmaceuticals,
Wuppertal, DE

Moderated and organized by:
Sami Cheong, Bayer AG, St. Louis, USA
Arwa Al-Dhalmi-Wendler, Bayer AG, Malsbenden, DE
Irena Maus, de.NBI/ELIXIR-DE, Bielefeld, DE

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Women in Data Science
BAYER
ELIXIR GERMANY
de.NBI

Felden (de.NBI/ELIXIR-DE), Amonida Zadissa (EMBL-EBI), Katharina Meier (Bayer Pharmaceuticals) and Jen Spindel (Bayer Crop Science), who will share their experiences, the challenges they face, and shed light on the opportunities for advancement.

Finally, a panel discussion with a special guest, Matt Dimmic (Bayer Crop Science) will focus on promoting women and recognizing their accomplishments in the data science world. Make an entry in your calendar and become part of it!

Please register at: <https://www.denbi.de/events/1321-women-in-data-science-part-ii-perspectives-in-industry-and-academia>

New ELIXIR Plant Sciences Community co-lead from ELIXIR-DE

Sebastian Beier (ELIXIR Germany, IPK Gatersleben) has been elected as the new co-lead of the Plant Sciences Community, joining Kristina Gruden (ELIXIR Slovenia) and Cyril Pommier (ELIXIR France). Sebastian Beier has contributed previously to the Plant Sciences Community as an interim co-lead. The objective of the Plant Sciences Community is to develop an infrastructure supporting the integration and linking of different plant data types from phenomics, genomics, transcriptomics, metabolomics, and of modeling and bibliographic data.



Find information at: <https://elixir-europe.org/communities/plant-sciences>

EOSC Task Force

The European Open Science Cloud (EOSC) opened a call for different task forces within its advisory groups to receive input on its future strategy and activities on 28 June 2021 (<https://www.eoscsecretariat.eu/eosc-liason-platform/post/call-members-eosc-association-task-forces>).

As a representative of ELIXIR-DE, Nils Hoffmann applied for membership in the Task Force Technical Interoperability of Data and Services, complementing his work in ELIXIR-DE as the platform coordinator for compute and interoperability. He was accepted as a member of the task force on 20 September 2021. In total, the 13 EOSC task forces received 545 applications from 41 countries (<https://eosc.eu/news/eosc-association-task-forces-community-agenda>).



ELIXIR-DE Brochure published

The ELIXIR Germany Administration Office has compiled its novel brochure, which outlines the main activities of the German Node and reports on the latest developments within ELIXIR-DE.

For more information please visit: https://www.denbi.de/images/Downloads/ELIXIR-DE_brochure_2021.pdf

AI Brochure entitled “Future-oriented Analysis of Life Sciences Data using Artificial Intelligence”

We are delighted to present our new de.NBI brochure entitled “Future-oriented analysis of Life Sciences Data using Artificial Intelligence”. The brochure provides an overview about de.NBI and ELIXIR Germany's activities in the field of Artificial Intelligence (AI), which were carried out by de.NBI members and/or with de.NBI resources. In total, we highlight 16 projects showing various aspects of integration and usage of de.NBI resources in AI projects, starting from prediction and modeling with the support of AI, improvement for research services and the acceleration of science through the application of AI. This booklet demonstrates that the existing diverse bioinformatics infrastructure of the de.NBI network and the German node of the European ELIXIR network is aware of the AI potential for the life sciences community.

The editorial team would like to thank the involved authors and hope that we can provide all interested readers with exciting insights into current research approaches in the field of AI. We wish you enjoy reading these articles.

For more information: <https://www.denbi.de/ai-projects> and https://www.denbi.de/images/Downloads/deNBI_KI_brochure.pdf



The de.NBI Summer Schools 2021 - Review

This year, de.NBI organized two online summer schools. These were summer schools no. 6 and 7 in our series:

- The de.NBI summer school **Analysis and integration of Mass Spectrometry based omics data in Proteomics, Metabolomics and Lipidomics**, 27-30 September 2021, was organized by the service centers BioInfra.Prot, CIBI and de.NBI-SysBio with a focus on the usage and understanding of tools and methods in mass spectrometry-based computational proteomics, metabolomics and lipidomics. 31 participants out of 73 applicants enjoyed great keynote lectures, interactive discussions, and hands-on workshops by leading researchers in these fields, e.g. Olga Vitek (Northeastern University) and Juan Antonio Vizcaino (EMBL-EBI).

Half of the group consisted of scientists working mainly on the generation of data in the wet-lab, and the other half consisted of scientists mainly creating bioinformatic tools and workflows. While most participants were working in Germany, we also had scientists from all over the world.

- de.NBI continued the successful summer school training program with the seventh summer school on **Microbial Community Analysis** one week later (4-9 October 2021). This training event was organized by the service centers BiGi and HD-HuB.

During the course week, 25 participants were instructed in sequence data preprocessing, amplicon data analysis (metabarcoding), read- and assembly-based metagenomics, and metaproteomics. A notable feature of this de.NBI summer school was the involvement of high-profile speakers. We were fortunate in bringing together an excellent group of keynote speakers: Maren Ziegler (JLU Gießen), Antonio Gonzalez (UC San Diego), Alice McHardy (TU Braunschweig) and Thilo Muth (BAM Berlin).

News from the de.NBI Office

Irena Maus will start her new position as **ELIXIR Germany Node Coordinator** in December 2021. She succeeds Vera Ortseifen in this function, who will switch to the biotech industry.

Irena finished her Ph.D. in the field of Industrial Biotechnology in 2017. Her main research focused on the composition and functional relationship of complex microbial communities in production-scale biogas plants. Applying genome-centered metagenomics and metatranscriptomics, she mainly looked for novel and abundant microbial species that feature important functional potential in the context of the anaerobic digestion process. Since 2017 Irena has been working as Communication & Outreach Officer at de.NBI Administration Office and took care of the network's public relations activities.

In her new role as Node Coordinator, Irena is responsible for coordinating all activities in the German ELIXIR Node. Furthermore, she supports the Head of Node and corresponds with the ELIXIR Hub.

We wish Irena every success in her new position in ELIXIR-DE and look forward to a fruitful cooperation and to Vera all the best for her professional and private future!



Recent Updates of de.NBI Services



New features or versions of various de.NBI services and tools have been released in the last months. [Check our services at: https://denbi.de/services](https://denbi.de/services).

- 🔗 **BIONDA**: a free biomarker database. New publication describing the features of this new database: Turewicz M, Frericks-Zipper A, Stepath M, Schork K, Ramesh S, Marcus K, Eisenacher M, **BIONDA: a free database for a fast information on published biomarkers**, Bioinformatics Advances, Volume 1, Issue 1, 2021, vbab015, <https://doi.org/10.1093/bioadv/vbab015> Find the service at: <https://www.denbi.de/services/920-bionda-database-for-biomarker-disease-relationships>









- 🔗 **EDGAR 3.0** introduces a completely new backend to the EDGAR webserver offering a better scalability and allowing the analysis of larger datasets than the previous platform. Corresponding publication: Dieckmann MA, Beyvers S, Nkouamedjo-Fankep RC, Hanel PHG, Jelonek L, Blom J, Goesmann A. **EDGAR 3.0: comparative genomics and phylogenomics on a scalable infrastructure**. Nucleic Acids Res. 2021, <https://doi.org/10.1093/nar/gkab341>.






- 🔗 **LipidCreator 1.2.1.787** is available from the Skyline tool store at <https://skyline.ms/skyts/home/software/Skyline/tools/details.view?name=LipidCreator> and from <https://github.com/lifs-tools/lipidcreator>. This release fixes issues with Skyline 21.1.





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MassBank: High quality mass spectral database MassBankEurope spectra annotations in PubChem are online now. Additionally, the massbank report 2021 has been uploaded on <https://zenodo.org/record/5504121>

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SeqAn 3.1.0. The New release of the modern C++ library for sequence analysis. Contains the first stable seqan module: *Alphabets*. Find out details about it at <https://www.seqan.de/release/2021/11/11/seqan-3-1-0-release>.
 
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BacDive: A new publication has been launched: Reimer LC, Sardà Carbasse J, Koblitz J, Ebeling C, Podstawka A, Overmann J. **BacDive in 2022: the knowledge base for standardized bacterial and archaeal data.** Nucleic Acids Res. 2021 Oct 29, <https://doi.org/10.1093/nar/gkab961>. Epub ahead of print.
 

Recent Publications by de.NBI partners:



- 
 Gatter T, von Löhneysen S, Fallmann, J, Drozdova P, Hartmann T, Stadler PF. **LazyB: fast and cheap genome assembly.** Algorithms Mol Biol 16, 8 (2021). <https://doi.org/10.1186/s13015-021-00186-5>
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 Jorge NAN, Ueberham U, Knobloch M, Stadler PF, Fallmann J, Arendt T. **Disturbance of phylogenetic layer-specific adaptation of human brain gene expression in Alzheimer's disease.** Sci Rep. 2021 Oct 12;11(1):20200. <http://doi.org/10.1038/s41598-021-99760-5>. Erratum in: Sci Rep. 2021 Nov 15;11(1)
- 
 Altuna Akalin, MDC Berlin summarized his experiences on **"How to organize an run remote data science internships"**, available at: <https://towardsdatascience.com/how-to-organize-and-run-remote-data-science-internships-fb51ce21715>

de.NBI @conferences

Recent de.NBI supported conferences

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GCB 2021 – German Conference on Bioinformatics, 06-08 September 2021 – virtual conference
 The GCB (German Conference on Bioinformatics and Precision Medicine) is an annual conference devoted to all areas of bioinformatics. This year, the GCB included two de.NBI supported industry talks by the industrial forum members Bernhard Fichtl (Carl Zeiss Microscopy) - APEER: A cloud-based digital microscopy platform to create image processing workflows and Jörg Peplies (Ribocoon) - JSpeciesWS: Calculating the extent of identity between microbial genomes on the total DNA level in microbial systematics. At the de.NBI online booth, questions concerning de.NBI, the de.NBI Cloud and the industrial forum were answered by training and web coordinator Daniel Wibberg. Furthermore, de.NBI partners taught various workshops:
 - Cell segmentation using KNIME Analytics Platform and its Tensorflow2 Integration
 - Bioinformatics tools for analyzing clinical metaproteomics samples of the human gut; Exploring target Structures with ProteinsPlus
 - Non-targeted label-free proteomics
 - BioC++ - solving daily bioinformatic tasks with C++ efficiently

General information and program at: <https://gcb2021.de>

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LipidomicsForum 2021, 5-8 October in Regensburg
 The annual Lipidomics Forum conference, co-organized by members of the LIFS consortium within the de.NBI network, was co-hosted with the 1st annual society conference of the International Lipidomics Society (ILS). More than 150 participants, eleven keynote lectures and a total of 30 selected short talks, and 41 posters made this hybrid event a great success and provided a unique opportunity to catch up on the latest research in lipidomics.
 

General Information and program at: <https://ils2021.org/>

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. The network is continuously developing alternative forms of training. Have also a look into our online training library, which is continuously expanded.

Please consult the [de.NBI training program](#) for updates.



Overview of upcoming de.NBI events

	Date	Event	City	Organizer
	12-24 Nov 2021	4th de.NBI Cloud User Meeting	Online	SIG 6, CAU, Cloud locations
	22-24 Nov 2021	3rd de.NBI/ELIXIR-DE metaRbolomics Hackathon	Wittenberg	CIBI/MASH
	22-26 Nov 2021	Applied Metaproteomics Workshop Magdeburg 2021	Magdeburg	BiGi
	25 Nov 2021	2nd Annual Meeting of the de.NBI Industrial Forum	Online	CAU
	25 Nov 2021	BacDive Community Meeting	Online	BioData
	29 Nov – 01 Dec 2021	Scientific Workflow Management Workshop	Online	HD-HuB
	02 Dec 2021	Women in Data Science – Perspectives in Industry and Academia	Online	CAU

Further information at: <http://www.denbi.de/training> and <http://www.denbi.de/events>

IMPRESSUM

RESPONSIBLE FOR CONTENTS

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SUBSCRIPTION

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