

de.NBI Quarterly Newsletter

This de.NBI Quarterly Newsletter in **August 2020** 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/>

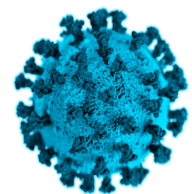
de.NBI Retreat on COVID-19 Research

de.NBI retreats are intended to discuss important developments of the network among project leaders. The recent de.NBI retreat took place on 29 June 2020 as an online event and focused on the topic *“Role of the de.NBI network in the processing of COVID-19 research questions”*. Fifty de.NBI members and guests participated in the meeting.

In the first part, selected de.NBI members reported on COVID-19 research projects carried out in Tübingen, Heidelberg and Berlin. In addition, further talks informed about the activities of the Galaxy platform as well as the involvement of the de.NBI cloud in the analysis of COVID-19 research data.

The second part of the retreat focused on the question, how the service and training infrastructure of the de.NBI network should be adopted to cover aspects of the ongoing COVID-19 research. As a result, it was concluded that the flexibility of the de.NBI service and training activities is high enough to adapt to the COVID-19 research area. In order to demonstrate the important contribution of the de.NBI network to COVID-19 issues, the participants of the retreat supported the idea to compile a new brochure with selected articles on COVID-19 research projects that are using the de.NBI infrastructure for the analysis of newly produced research data. It was proposed that the brochure should be written in English so that it could also be distributed in Europe among the national ELIXIR nodes.

The COVID-19-related de.NBI projects are presented at: <https://www.denbi.de/covid-19>.



Source: CDC/Alissa Eckert, MS; Dan Higgins, MAM, modified

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Constitutive Meeting of the Central Coordination Unit of ELIXIR-DE



On 10 February 2020, the ELIXIR Collaboration Agreement became effective, thereby fully establishing the German ELIXIR Node. This contract includes 20 German universities and research institutes and Bielefeld University that has taken over the legal role as “Representing Entity” of ELIXIR Germany (ELIXIR-DE).

The German ELIXIR Node is led by a Central Coordination Unit (CCU), which is the decision-making body of ELIXIR Germany and responsible for the effective operation of the scientific, technical and administrative structures. The CCU board consists of the Head of Node and delegates of the eight service units of ELIXIR-DE. Those delegates have been nominated by the members of ELIXIR Germany. During the first meeting, the CCU adopted its rules of procedure that provide amongst others guidelines for conducting CCU meetings and voting procedures. The CCU is supported by an international Scientific Advisory Board (SAB) that acts as a consultative body and provides recommendations on technical, organizational and strategic matters related to the mission of ELIXIR Germany.

The current delegates of the ELIXIR-DE CCU are listed on the de.NBI/ELIXIR Germany website at: <https://www.denbi.de/elixir-germany/central-coordination-unit-of-elixir-ccu>.

de.NBI/ELIXIR-DE Task Force for COVID-19 Human Omics Data established

Rapid and open sharing of data can greatly accelerate research and discovery, which is essential to respond to the current COVID-19 pandemic. The European Bioinformatics Institute (EMBL-EBI), together with research partners such as ELIXIR, operates a dedicated European COVID-19 Data Platform that enables the rapid collection and comprehensive data sharing of available COVID-19 research data (<https://www.covid19dataportal.org/>).

In this respect, de.NBI/ELIXIR Germany has very recently established the “de.NBI/ELIXIR-DE task force for COVID-19 human omics data”. This joint task force of de.NBI/ELIXIR service centers will address the challenge arising from managing human omics data in the COVID-19 context, together with the German Human Genome-Phenome Archive (GHGA) and the German COVID-19 OMICS Initiative (DeCOI). The goal of the task force is to engage the national communities generating COVID-19 data, to FAIR-ify the data, and to support the community in making this essential research data accessible for the international scientific community. The task force will act as the national point of contact for COVID-19 Omics data for ELIXIR. Head of this task force is Peer Bork of EMBL Heidelberg. He is supported by Oliver Kohlbacher (Tübingen University), Oliver Stegle (DKFZ Heidelberg) and Jan Korbel (EMBL Heidelberg). The named institutes bundle activities in German COVID-19 research and are also active in the national GHGA and DeCOI initiatives.

Find more information at: <https://www.denbi.de/covid-19/de-nbi-elixir-de-task-force-for-covid-19-human-omics-data>

6th ELIXIR All Hands Meeting

The sixth ELIXIR All Hands meeting took place virtually on 8 -10 June 2020. The meeting brought together around 500 members of the ELIXIR community from across all ELIXIR Nodes and collaborators from partner organizations.

In a series of plenary sessions, workshops and mini-symposia the participants reviewed ELIXIR's achievements and activities and discussed plans for the future. About 20 workshops focused on specific topics relevant for the ELIXIR community, complemented by a virtual poster session with almost 40 contributions from the ELIXIR Nodes.

Numerous de.NBI members participated in the various formats of the conference: BioData members introduced ProteinsPlus, BacDive and SILVA to the ELIXIR community. Björn Grüning (RBC Freiburg) talked about the Galaxy Community Project and GCBN presented three talks in the Plant Science Mini-Symposium. Posters were presented by several de.NBI members. The de.NBI SIG 3 – training poster “**The de.NBI/ELIXIR-DE Training Network**” won the **poster price** in the field “training & education”.

The seventh ELIXIR All Hands meeting 2021 is intended to take place in Prague.

Find the poster at: <https://doi.org/10.7490/f1000research.1117920.1>

Public videos, keynotes and posters are available via: <https://elixir-europe.org/events/elixir-all-hands-2020>

Find more information on ELIXIR-DE at: <https://www.denbi.de/elixir-germany>



New Lead for SIG 6 de.NBI Cloud

Since its start in 2017, the establishment of the de.NBI cloud has successfully been steered by the SIG 6 de.NBI cloud headed by Christian Lawerenz, Heidelberg/Berlin, and Alexander Sczyrba, Bielefeld, as deputy. At the beginning of this year, Chris Lawerenz announced that he would like to step down from his leading position in SIG 6. Fortunately, Alexander Sczyrba, professor at Bielefeld University and head of the Computational Metagenomics group, has agreed to act as a candidate for the chair position and was finally elected by the CCU on 21 April 2020. For the deputy position Ivo Buchhalter has been proposed by the service center HD-HuB. Ivo Buchhalter is head of Omics IT and Data Management Core Facility at the German Cancer Research Center (DKFZ) in Heidelberg. He holds two PhD degrees, one in biology and the other in computational biology. Since he is very well trained in cloud computing, he represents the ideal candidate for the deputy position. Following the



Alexander Sczyrba
SIG 6 chair

SIG 6
de.NBI cloud



Ivo Buchhalter
SIG 6 co-chair

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recommendation of the SIG 6, the CCU elected Ivo Buchhalter as the new co-chair of the Special Interest Group “de.NBI cloud” in their 23rd meeting on 30 June 2020. Thus, both SIG 6 management positions could be newly filled and the de.NBI cloud can continue its successful development.

Finally, the de.NBI coordinator would like to thank **Chris Lawerenz** for his long-standing great commitment in setting up the de.NBI cloud, which has reached an impressive level.

A Framework to Assess the Quality and Impact of Bioinformatics Training across ELIXIR

A new publication from 23 July 2020 the ELIXIR Training Platform, led by the ELIXIR EXCELERATE Quality and Impact Assessment Subtask in collaboration with the ELIXIR Training Coordinators Group, describes the implementation of an assessment strategy to measure quality and impact of its entire training portfolio. The analysis is based on an overview of the ELIXIR training data collected over the past 4 years.

As ELIXIR-DE representative Daniel Wibberg contributed to this publication.

Full quotation: Gurwitz KT, Singh Gaur P, Bellis LJ, Larcombe L, Alloza E, et al. (2020) *A framework to assess the quality and impact of bioinformatics training across ELIXIR*. PLOS Computational Biology 16(7): e1007976. <https://doi.org/10.1371/journal.pcbi.1007976>

Number of training events	986
Number of days of training	2,792
Number of trainers/facilitators	3,247
Number of individuals trained	21,841
Number of feedback responses received (corresponding to the quality metrics set of data)	8,157
Number of events for which feedback was collected	499
Percentage of participants who provided feedback for events in which feedback was collected (corresponding to the quality metrics set of data)	68%

ELIXIR-wide training event statistics (data accessed from the training metrics database on 6 August 2019). <https://doi.org/10.1371/journal.pcbi.1007976.t001>

Much More Needs to Happen – An Interview with A. Pühler

In an interview entitled “Es muss sehr viel mehr passieren” with the DUZ (Deutsche Universitätszeitung) published on 17 July 2020, issue 7.2020, de.NBI Coordinator Alfred Pühler, in his function as a Leopoldina member, communicated that life sciences in Germany need a modern IT infrastructure to better exploit their potential. He underlined the necessity to build up distributed research infrastructures for life sciences in Germany combined with an appropriate funding.

Link to the interview: <https://www.duz.de/beitrag/!/id/865/es-muss-sehr-viel-mehr-passieren>

Julio Saez-Rodriguez Affiliated as Associated de.NBI Partner

In June 2020, the Central Coordination Unit (CCU) of de.NBI unanimously approved the application of Prof. Dr. Julio Saez-Rodriguez (Heidelberg University) to become an Associated Partner of the de.NBI consortium. The research group of Julio Saez-Rodriguez at the Medical Faculty of Heidelberg University (Institute for Computational Biomedicine) aims to acquire a functional understanding of the deregulation of signaling networks in disease and to apply this knowledge to develop novel therapeutics. Towards this end, the group develops computational approaches that integrate biological knowledge with diverse types of omics data, with a recent focus on single-cell technologies.

The services offered by the Saez-Rodriguez group for de.NBI include a series of tools to perform pathway- and network-based analysis of omics data. The services include Omnipath (<http://omnipathdb.org/>), a meta resource of literature-curated knowledge, PROGENy (<https://saezlab.github.io/progeny/>) and DOROTHEA (<https://saezlab.github.io/dorothea>) for the estimation of pathway and transcription activity, respectively, and CARNIVAL (<https://saezlab.github.io/CARNIVAL>) to find causal paths in large signaling networks. The methods are implemented in various software, mostly available as R-packages (and in Bioconductor). Due to the geographical proximity as well as the complementary research focus of the Saez-Rodriguez group to members of HD-HuB, contributions of this associated partner, also to training, will be aligned with activities of the HD-HuB service center.



Photo: J. Saez-Rodriguez

Find more information at: <https://www.denbi.de/network/associated-partners/21-about/948-research-group-of-julio-saez-rodriguez> and <https://saezlab.org>





3rd de.NBI Cloud User Meeting



CLOUD USER MEETING ONLINE 2020

The 3rd de.NBI Cloud User Meeting will take place as a virtual conference from **8-14 October 2020**. Learn about actual de.NBI Cloud projects and participate in multiple workshops, which will instruct users to develop or extend their own services and tools to the cloud computing environment in de.NBI Cloud. For beginners, there will be a pre-course on basic Unix commands on 7 October 2020.

This year's lectures will feature the use cases:

-  Cov-seq: An amplicon sequencing protocol for Sars-CoV-2 (Daniel Hübschmann – German Cancer Research Center)
-  Leveraging the de.NBI Cloud for large-scale human genome assembly (Peter Ebert – Max-Planck-Institut für Informatik, Algorithms for Computational Genomics)
-  BIIGLE – Large-scale image annotation in the de.NBI Cloud (Martin Zurowietz – Bielefeld University, Biodata Mining)
-  MetaProteomeCloud – Microbial community proteomics using cloud technologies (Kay Schallert – Otto von Guericke University Magdeburg, Institute for Process Engineering)

and workshops on:

- Running Snakemake Workflows in the de.NBI Cloud
- OpenStack Introduction
- Extensible Cluster Setup in the Cloud with BibiGrid and Ansible
- Using Terraform to define infrastructure as code
- BioConda and BioContainers
- Kubernetes Introduction
- Deploying Web Services in the de.NBI Cloud

Registration is open now!!

Find more information and registration at: <https://cloud.denbi.de/3rd-de-nbi-cloud-user-meeting/>

New Members and Developments in the de.NBI Industrial Forum

Since its founding event in November 2019, the de.NBI Industrial Forum's membership numbers have increased continuously. In 2020 four companies have joined the de.NBI Industrial Forum rising the membership numbers to 29 in total, namely:



Wiens Synefex GmbH
(Lage)



HTK Hygiene Technologie
Kompetenzzentrum GmbH
(Bamberg)



Carl Zeiss Microscopy
GmbH (Jena)



Biocrates Life Sciences AG
(Innsbruck)

The industry forum is becoming more and more international. In addition to the Luxembourg company ITTM S.A., the Austrian company Biocrates Life Sciences AG is now also a member.

The industry forum now offers the opportunity to present services from industry members on the de.NBI website. The service APEER from Carl Zeiss Microscopy GmbH has made the markup. APEER is a comprehensive web service for the analysis and evaluation of image data, such as microscopy images. The service is free of charge for non-profit users. Member companies who would also like to present their own services on www.denbi.de, please contact the de.NBI Coordinator.



More Information on the de.NBI Industrial Forum at: <https://www.denbi.de/industrial-forum>

Find the service at: <https://www.denbi.de/industrial-forum/industrial-forum-services>

News from the de.NBI Office

Since July 2020, **Nils Christian Lübke** is the newest member of the de.NBI Administration Office (AO). Nils holds a Bachelor's degree in Molecular Biotechnology and has a Master's in Genome Based Systems Biology from Bielefeld University. His research interests comprise topics in industrial biotechnology and systems biology as well as a keen interest in synthetic biology. The latter one depicted in a decade of experience in the international genetically engineered machine (iGEM) competition.












Nils Christian's work will include expanding the de.NBI activities in new communities. Additionally, he will support the de.NBI AO activities in the SIG 2 Service & Service Monitoring.

We welcome Nils Christian in our team and look forward to a successful cooperation!










Recent Updates of de.NBI Services

New features or versions of various de.NBI services and tools have been released in the last months:





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BacDive: The bacterial diversity metadatabase is now amended with a dashboard Explore microbial data in a new interactive way! Find the service at: <https://www.denbi.de/services/347-bacdive-the-bacterial-diversity-metadatabase-focuses-providing-organism-linked-information-covering-the-multifarious-aspects-of-bacterial-biodiversity>

- 
e!DAL-PGP: A new video explains data publication with plant genomics & phenomics research data repository. Find service and video at: <https://www.denbi.de/services/513-e-dal-pgp-plant-genomics-and-phenomics-research-data-repository>

- 
STAMPS: A new webpage has been launched for the Simple Targeted Assays for Metabolic Pathways & Signaling (STAMPS) database. The service provides a pathway-based approach to access proteomics assays for targeted proteomics. Find the service at: <https://www.denbi.de/services/335-stamps>

- 
COPASI: New version of the complex pathway simulator COPASI 4.28 is ready for download. Find the service at: <https://www.denbi.de/services/373-copasi-creating-and-solving-mathematical-models-of-biological-processes>

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UseGalaxy.eu: Galactic Circos, a Galaxy wrapper providing a GUI for the Circos tool has been integrated into the galaxy.eu platform. Circos is a software package for visualizing data and information in a circular layout. Publication: H Rasche, S Hiltmann, *Galactic Circos: User-friendly Circos plots within the Galaxy platform*, *GigaScience*, Volume 9, Issue 6, June 2020, g1aa065, <https://doi.org/10.1093/gigascience/g1aa065>. Find the service at: <https://www.denbi.de/services/357-european-galaxy-server-transcription-analysis>. A training package is available at: <https://training.galaxyproject.orgF/training-material/topics/visualisation/tutorials/circos/tutorial.html>

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GLASSgo: sRNA Homolog Finder has been updated to version 1.5.2, that is fully incorporated into the workflow management system GALAXY. The improved version contains a new feature for extracting the upstream regions, allowing the search for conserved promoter elements. New Publication: RA Schäfer, SC Lott, J Georg, BA Grüning, WR Hess, B Voß, *GLASSgo in GALAXY: high-throughput, reproducible and easy-to-integrate prediction of sRNA homologs*, *Bioinformatics*, btaa556, <https://doi.org/10.1093/bioinformatics/btaa556>. Find the service via: <https://www.denbi.de/services/356-freiburg-rna-tools-webserver>.

New services provided by de.NBI members and associated partners:

- 
SemLookP: Tool for metadata annotation & data search in the area of translational medicine. It is provided by our associated partner ZB MED. Find the service at: <https://www.denbi.de/services/927-semlookp-metadata-annotation-data-search-in-the-area-of-translational-medicine>

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PUBLISSO: Open access publishing platform for research articles. It is provided by our associated partner ZB MED. Find the service at: <https://www.denbi.de/services/926-publisso-open-access-publishing-platform-for-research-articles>

- 
LIVIVO: Interdisciplinary discovery service for literature and information It is provided by our associated partner ZB MED. Find the service at: <https://www.denbi.de/services/925-livivo-interdisciplinary-discovery-service-for-literature-and-information>

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CalibraCurve: Automated batch-mode determination of dynamic linear ranges and quantification limits. Publication: *CalibraCurve: A Tool for Calibration of Targeted MS-Based Measurements and quantification limits*, M Kohl, M Stephat, T Bracht, D A Megger, B Sitek, K Marcus, M Eisenacher, *Proteomics* 2020, 20, <https://doi.org/10.1002/pmic.201900143>. Find the service at: <https://www.denbi.de/services/921-calibracurve-automated-batch-mode-determination-of-dynamic-linear-ranges-and-quantification-limits>

-  **BIONDA:** Database for biomarker-disease relationships. It enables search for potential COVID-19 biomarkers. A new tool provided by BioInfra.Prot - Bochum. Find the service at: <https://www.denbi.de/services/920-bionda-database-for-biomarker-disease-relationships>
-  **MeDeCom:** MeDeCom is a computational method for decomposition of heterogeneous DNA methylomes. It applies matrix factorization with biologically motivated constraints and regularization to discover and quantify latent components in methylomes of multi-cellular samples. The tool is provided by HD-HuB-epi. Find the service at: <https://www.denbi.de/services/915-medecom-decomposition-of-heterogeneous-dna-methylomes>
-  **APEER:** A cloud-based digital microscopy platform that helps bridging the gap between researchers and developers. It facilitates the creation of fully automated image processing workflows. It is the first Service by a member of the industrial forum. Find the service at: <https://www.denbi.de/industrial-forum/industrial-forum-services>

Recent Publications by de.NBI partners:

-  VA Padilha, OS Alkhnabashi, SA Shah, ACPLF de Carvalho, R Backofen, *CRISPRcasIdentifier: Machine learning for accurate identification and classification of CRISPR-Cas systems*, GigaScience, Volume 9, Issue 6, June 2020, g1aa062, <https://doi.org/10.1093/gigascience/g1aa062>
-  O Schwengers, P Barth, L Falgenhauer, T Hain, T Chakraborty, A Goesmann. *Platon: identification and characterization of bacterial plasmid contigs in short-read draft assemblies exploiting protein sequence-based replicon distribution scores*, Microbial Genomics (2020), 95, 295, <https://doi.org/10.1099/mgen.0.000398>, Link to software: <https://www.uni-giessen.de/fbz/fb08/Inst/bioinformatik/software/platon>
-  W Kopp, R Monti, A Tamburrini, U Ohler, & A Akalin. *Deep learning for genomics using Janggu*. Nat Commun 11, 3488 (2020). <https://doi.org/10.1038/s41467-020-17155-y>. Link to press release: <https://www.mdc-berlin.de/news/press/maui>. Link to the tool: <https://github.com/BIMSBbioinfo/janggu>
-  T van Rossum, P Ferretti, OM Maistrenko, P Bork. *Diversity within species: interpreting strains in microbiomes*. Nat Rev Microbiol (2020), <https://doi.org/10.1038/s41579-020-0368-1>

de.NBI @ CONFERENCES

de.NBI supported conferences in the near future

GCB 2020 – German Conference on Bioinformatics, 14-17 September 2020 – Virtual Conference

This year's conference is organized by a committee from Frankfurt, Mainz and Bingen. Due to the corona pandemic the meeting will be held virtually. The de.NBI will be present with a virtual booth. The first day will be dedicated to a number of workshops.

de.NBI Partners will teach the tutorials:

- BioC++ - solving daily bioinformatic tasks with C++ efficiently; R. Rahn, S. Mehringer, M. Ehrhardt, FU Berlin
- Protein Structure Fundamentals: Searching – Analyzing – Modelling; K. Schöning-Stierand, M. Rarey, Uni Hamburg

General information and registration at: <https://gcb2020.de/>



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.


Due the corona pandemic and the social distancing measures in effect since 25 March 2020, a number of de.NBI training courses have been cancelled or postponed. The network is continuously developing alternative forms of training.










Have also a look into our online training library, which is continuously expanded.

Under the actual conditions, please consult the de.NBI training program for updates.

Overview of upcoming de.NBI events



Date	Event	City	Organizer
 31 Aug – 01 Sep 2020	Software Carpentry 1.2020	online	Assoc. Partner ZB MED

Date	Event	City	Organizer
 02 Sep 2020	6th de.NBI Genomics training course	online	BiGi
 14 Sep 2020	BioC++ - solving daily bioinformatic tasks with C++ efficiently	online	CIBI
 14 Sep 2020	ProteinsPlus at the German Conference for Bioinformatics (GCB)	online	BioData
 21-23 Sep 2020	Tools for Systems biology modeling and data exchange: COPASI, CellNetAnalyzer, SABIO-RK, FAIRDOMHub/SEEK 2020	online or Magdeburg	de.NBI-SysBio
 23-25 Sep 2020	Computational genomics course for hands-on data analysis 2020	online	RBC/epi
 8-14 Oct 2020	3rd de.NBI Cloud User Meeting	online	CAU, SIG 6, de.NBI Cloud group
 20 Oct 2020	Computing Skills for Reproducible Research: Software Carpentry Course 2020	online	HD-HuB
 23 Oct 2020	24. CCU Meeting	online	CAU, RBC
 02 Nov 2020	5th Differential analysis of quantitative proteomics data using R	online	BioInfra.Prot
 09 Nov 2020	2nd Advanced analysis of quantitative proteomics data using R	online	BioInfra.Prot
 15-19 Mar 2021	de.NBI Spring School 2021 - Metagenomics	Gießen	BiGi et al.

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

IMPRESSUM

RESPONSIBLE FOR CONTENTS

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