

# de.NBI Quarterly Newsletter

This de.NBI Quarterly Newsletter in November 2019 informs about recent developments and current events in the project

**German Network for Bioinformatics Infrastructure – de.NBI.**

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

## de.NBI INDUSTRIAL FORUM KICKOFF MEETING

The Kick-off Meeting of the de.NBI Industrial Forum took place in Berlin on 26 November 2019. In total, nearly 60 participants from industry and academia attended a well-structured program which started with welcome addresses by M. Kölbl, BMBF, and S. Kleinsimon, HealthCapital. In the opening session, talks on the de.NBI network, the ELIXIR industry strategy and the LifeTime project informed on activities within Germany and Europe. A highlight of the meeting was the flash talk session, in which industry representatives presented their company profiles. The contributors were: ITTM S.A., Esch-sur-Alzette, LU; Ribocon GmbH, Bremen; b.experts GmbH, Dortmund; Merantix AG, Berlin; MVZ Dr. Eberhard & Partner ÜBAG, Dortmund; geneXplain GmbH, Wolfenbüttel; KWS SAAT SE, Einbeck; Kairos GmbH, Bochum.



The main session of the meeting was then reserved for contributions dealing with de.NBI activities, namely service and training as well as cloud computing. A very special event was the presentation by U. Ohler, MDC Berlin, highlighting the role of artificial intelligence in the life science area. In the general discussion at the end of the meeting, it was pointed out that researchers from industry have many opportunities to use the various offers of the de.NBI. In particular, industrial researchers may attend training courses on important tools. In addition, there will be opportunities to learn

more about cloud computing including conditions under which the de.NBI Cloud can be used. The de.NBI network is also happy to respond to the wishes of forum members. For example, industrial researchers should define research questions that can be investigated in cooperation with academia and industrial partners.

Further information and program of the kick-off meeting at: <https://www.denbi.de/industrial-forum>

## CELEBRATING THE 5<sup>TH</sup> ANNIVERSARY OF THE GERMAN NETWORK FOR BIOINFORMATICS INFRASTRUCTURE



In March 2020, the de.NBI network celebrates its 5<sup>th</sup> anniversary. To mark this event the de.NBI will hold a symposium on 13 February 2020 at the Seminaris CampusHotel in Berlin. The first session will showcase the current state of development of the network. The de.NBI coordinator will start with an overview of the de.NBI highlights, followed by three selected presentations focusing on bioinformatics for humans, plants and microbes. In the second part of the symposium, external experts will present their views on specific aspects of the de.NBI network. The ELIXIR director **Niklas Blomberg** will talk about „ELIXIR and its cooperation with de.NBI“. **Rolf**

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**Apweiler**, the director of EMBL-EBI, will give a special lecture on „The future of digital medicine in Germany and Europe“. Last but not least, **Dietrich Rebholz-Schuhmann**, the director of ZB MED – Information Centre for Life Sciences, will present the topic „Handling of research data in the life sciences“.

All members of the forty **de.NBI projects** within the eight service centers and the **Scientific Advisory Board** are welcome at the symposium. In addition, the members of **reviewer team** and the representatives of the **de.NBI Industrial Forum member** companies are invited. Thus most people involved in the success of the de.NBI network will meet to celebrate the 5<sup>th</sup> anniversary.

For members of the de.NBI network and the SAB the symposium will take place together with the SAB- and plenary meetings at the same venue which are scheduled for 13 and 14 February 2020.



Deutsches Netzwerk für Bioinformatik-Infrastruktur  
**5-Year Event | 4<sup>th</sup> SAB Meeting | Plenary Meeting**  
13-14 February 2020, Berlin

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

Registration link for de.NBI consortium has been distributed via e-mail. Registration is open until 20 January 2020.

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## RBC FREIBURG HOSTS THE HUMAN CELL ATLAS GALAXY INSTANCE

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The Human Cell Atlas Galaxy instance contains tools for Single Cell Clustering, Trajectories analysis and interactive visualization, allowing simple data analysis through the Galaxy user interface. It also includes facilities to import matrix data from the Human Cell Atlas and the EBI Single Cell Expression Atlas, for re-analysis. The portal runs as part of the larger usegalaxy.eu infrastructure (<https://usegalaxy.eu>) and has access to thousands of cores and terabytes of memory and storage, hosted by Galaxy Team of the University of Freiburg. The Freiburg Galaxy server with more than 10,000 users is part of the de.NBI Cloud and is the biggest Galaxy instance in Europe, and one of the biggest worldwide. It provides access to more than 2,000 bioinformatics tools, covering most of the bioinformatics topics in the life sciences.

More information at: <https://data.humancellatlas.org/analyze/portals/hca-galaxy-instance>

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## NEW ELIXIR-DE TECHNICAL COORDINATOR DEPUTIES

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Björn Grüning (RBC Freiburg) is the technical coordinator of ELIXIR Germany (see Issue 1/2019). The national team for technical coordination of the German ELIXIR Node has now been supplemented by the CCU during their meeting in October 2019 in Bielefeld. The CCU elected two new deputy members of ELIXIR's Technical Coordinator's Group: Marius Dieckmann from BiGi Gießen and Sebastian Jünemann from BiGi Bielefeld. The Technical Coordinator's Group (TeCG) is comprised of technical representatives from each ELIXIR Node. The members of the TeCG meet regularly to share information and expertise and to support implementing the ELIXIR Platforms.

More information at: <https://www.denbi.de/elixir-germany>

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## THE de.NBI/ELIXIR-DE TRAINING PLATFORM

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The de.NBI/ELIXIR-DE training platform also known as special interest group 3 (SIG 3) "Training & Education" has published the article *The de.NBI/ELIXIR-DE training platform - Bioinformatics training in Germany and across Europe within ELIXIR* in the F1000 ELIXIR channel. The paper presents the high-quality, coherent, timely, and impactful training program across the eight de.NBI service centers. Since 2015, more than 250 training courses have been conducted with more than 5,400 participants and these courses received recommendation rates of almost 90% (Status October 2019). In addition to face-to-face training courses, online training was introduced on the de.NBI website in 2016 and guidelines for the preparation of e-learning material were established in 2018. The de.NBI/ELIXIR-DE training platform is closely linked to ELIXIR training activities, advertising training courses via TeSS and discussions on the exchange of data for training events which are essential for the quality assessment on both the technical and administrative levels.

Citation: Wibberg D, Batut B, Belmann P et al. The de.NBI / ELIXIR-DE training platform - Bioinformatics training in Germany and across Europe within ELIXIR. F1000Research 2019, 8(ELIXIR):1877 (<https://doi.org/10.12688/f1000research.20244.1>)

## de.NBI SUMMER SCHOOL (BIO)DATA SCIENCE - REVIEW

The 5<sup>th</sup> de.NBI Summer School “(Bio)Data Science” was hosted from 02 - 06 September 2019 at IPK Gatersleben. The training event was conducted by the Service Centers GCBN, BiGi, BioData, BioInfra.Prot, CIBI and de.NBI-SysBio.

During the one-week event, 17 participants learned that modern high-throughput -omics technologies in the life science field produce large quantities of high-dimensional data. Besides new challenges for analyzing and visualizing big amounts of data, the management and sharing have become an important issue in the daily research process.



Photo: IPK Gatersleben, Himpe

The 2019 Summer School gave an overview of possibilities for a FAIR data sharing and their benefits for both, data producers and data consumers. Furthermore, de.NBI trainers provided introductions to recent technologies for processing and inspecting these data, e.g. the de.NBI Cloud or KNIME. A full day was dedicated to deep learning & image analysis with the kind support of Axel Mosig (Ruhr University Bochum).

The Summer School covered a number of interesting lectures and hands-on sessions by de.NBI speakers and renowned experts. Doris Wedlich (Karlsruhe Institute of Technology) gave the keynote lecture “Orientation in the Jungle – The RfII: A council dedicated to scientific information infrastructures in Germany” and Mathias Wilhelm (Technical University of Munich) contributed with a keynote on “ProteomicsDB”.

The week of intensive training was accompanied by a social program featuring guided tours of the IPK plant cultivation hall and seedbank, a barbecue party and a sightseeing tour of the beautiful world heritage site in Quedlinburg.

de.NBI will follow up its successful summer school training program with a summer school on Metagenomics planned for September 2020.

Find the detailed program at: <https://meetings.ipk-gatersleben.de/denbi-summer-school-2019/program/>

## GOING TO THE LAB ON VACATION! – BIOBYTE 2019

The de.NBI supported the BioByte 2019 from 15-19 July 2019, a Summer School for high school students that was organized by MLU Halle in cooperation with the de.NBI partners at IPK Gatersleben (U. Scholz) and IPB Halle (S. Neumann). It is part of de.NBI’s outreach activities for promoting bioinformatics in Germany. For one week pupils of the 10th and 11th grades had the opportunity to see what is actually behind the subject “Bioinformatics”. The day at the IPB focused on how plant constituents can be determined. The 21 participants first had a guided tour through the greenhouses and phytochambers as well as to a mass spectrometry (MS) laboratory. For the subsequent laboratory test, MS experts provided various fruits, such as raspberries and grapes, from which an extract for MS analysis was to be produced. The innumerable signals from chemical compounds and their fragments that a mass spectrometer delivers must then be evaluated. Together with the staff of the Bioinformatics and Mass Spectrometry working group the pupils created an evaluation workflow on the computer and had to clarify the question “Does the sample contain blood or ketchup?”

Hopefully the initiative will help the participants with their career orientation and that one or the other will be inspired to study a subject in the MINT field - perhaps even in plant research.

Find more Details at: <https://www.ipb-halle.de/oeffentlichkeit/veranstaltungen/veranstaltung-detail/in-den-ferien-ins-labor-na-klar/>



## 2<sup>nd</sup> de.NBI Cloud USER MEETING - REVIEW



**CLOUD  
USER  
MEETING<sup>2</sup>  
HEIDELBERG**

This year, the de.NBI Cloud user meeting entered the second round in Heidelberg. After the premiere at the CeBiTec in Bielefeld, the second meeting was organized at the BioQuant at Heidelberg University. In a cozy atmosphere, experienced and novice de.NBI Cloud users learned how to apply the cloud in their daily work.

Talks such as “SILVAngs with the de.NBI Cloud” and “Environmental microbial bioinformatics in the cloud” presented the capabilities of a de.NBI Cloud project, whereas the workshops on the second and third day provided the necessary know-how.

Six hands-on sessions, e. g. “Introduction to Bibigrd” or “Kubernetes Hands-On” were organized for providing knowledge in a variety of tools and software solutions that are not only used in the cloud computing ecosystem.

As last year, participants met the developers and admins behind the screen in person to discuss best practices and already realized de.NBI Cloud projects.

In a closing discussion session, the participants expressed their wishes for more use case oriented workshops and an additional introductory level session for beginners. We appreciate all user comments, which will definitely be included in the future planning.

We enjoyed seeing the increased interest in using the de.NBI Cloud and look forward to the de.NBI Cloud user meeting 2020 with more workshops and fruitful discussions!

More information and program at: <https://cloud.denbi.de/2nd-de-nbi-cloud-user-meeting/>

## 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:

- 🔗 **LipidXplorer 1.2.8:** Release note LipidXplorer is a software that supports a variety of untargeted shotgun lipidomics experiments and experiments from LC/MS lipidomics. It is designed to support bottom-up and top-down shotgun lipidomics experiments performed on all types of tandem mass spectrometers. Lipid identification does not rely on a database resource of reference or simulated mass spectra. Al Machot, F, Hoffmann, N, Miranda Ackerman, J, & Schwudke, D. (2019, October 14). *LipidXplorer 1.2.8* (Version 1.2.8). Zenodo. <http://doi.org/10.5281/zenodo.3483977>
- 🔗 **IntaRNA v3:** Efficient RNA-RNA interaction prediction incorporating accessibility and seeding of interaction sites. V3 was uploaded in September. The software features multiple personalities and helix based RNA interaction (<https://doi.org/10.5220/0007689701310140>); Find the service at: <https://github.com/BackofenLab/IntaRNA/>
- 🔗 **BacDive** has hit 100,000 unique users this year in October. This is a new peak value for the bacterial meta-data base. <https://www.denbi.de/services/347-bacdiver-the-bacterial-diversity-metadatabase-focuses-providing-organism-linked-information-covering-the-multifarious-aspects-of-bacterial-biodiversity>
- 🔗 **OpenMS:** A new openMS application with publically available workflow has been published: *MHCquant: Automated and Reproducible Data Analysis for Immunopeptidomics*, L Bichmann, A Nelde, M Ghosh, L Heumos, C Mohr, A Peltzer, L Kuchenbecker, T Sachsenberg, JS Walz, S Stevanović, HG Rammensee, and O Kohlbacher Journal of Proteome Research 2019, <https://doi.org/10.1021/acs.jproteome.9b00313>

### Publications

- 🔗 **SIG 3 training and education:** *The de.NBI/ELIXIR-DE training platform - Bioinformatics training in Germany and across Europe within ELIXIR*, Wibberg D, et al. F1000Research 2019, <https://doi.org/10.12688/f1000research.20244.1>

## de.NBI @ CONFERENCES

CAU members have been present on a variety of conferences

### ICRC 2019 – International CeBiTec Research Conference

This year’s International CeBiTec Research Conference” in Bielefeld, 23-25 September 2019, promoted scientific excellence in microbial biotechnology. It focused on “Renewable feedstocks and synthetic pathways for production of fine chemicals”. The major topics were aroma biotechnology, synthetic pathways, and a podium discussion on white biotechnology, alternative feedstocks, and C1 utilization. The de.NBI office was present with a booth to introduce de.NBI services into this community.

Find a review of the conference at: <https://www.cebitec.uni-bielefeld.de/localmedia/downloads/quarterly/CeBiTec-Quarterly-2019-3.pdf>



**Advances in Industrial Biotechnology:**  
Renewable feedstocks and  
synthetic pathways for  
production of fine chemicals

Center for Interdisciplinary Research (ZiF)  
Bielefeld University  
September 23<sup>rd</sup> – 25<sup>th</sup>, 2019



## German Conference on Synthetic Biology (GCSB 2019)

The German Conference on Synthetic Biology (GCSB), which is organized since 2017 by the German Association for Synthetic Biology (GASB) was held at RWTH Aachen from 12-13 September 2019. The conference covered classical metabolic and protein engineering topics up to novel genetic tools for genome modification. Additional sessions focused on synthetic biology in plants and mammalian cells. The developments on minimal cells and cell-free environments were also covered which completed the conference program on all aspects of synthetic biology. de.NBI took part in the poster session by presenting relevant services as well as training courses for the synthetic biology community. During the networking breaks, a representative from the de.NBI network gave support to researchers regarding bioinformatics issues and recommended the de.NBI Cloud to scientists with highly demanding computational tasks.

Find the full program at: [https://registration.gcsb.info/conferences/gcsb2019/schedule/events?pk\\_kwd=frmgcsbnf](https://registration.gcsb.info/conferences/gcsb2019/schedule/events?pk_kwd=frmgcsbnf)



## GCB 2019

The de.NBI supported the scientific program of the GCB 2019, 16-19 September in Heidelberg. The GCB (German Conference on Bioinformatics) is the annual conference devoted to all areas of bioinformatics in Germany. This year, the focus was set on *Precision Medicine—where Bioinformatics & Medical Informatics meet*. The GCB featured a special de.NBI session with a keynote by Oliver Kohlbacher (CIBI): From Omics Data to Therapies – Personalizing Treatments. Further presentations in the session were given by Pavankumar Videm, Mario Looso, Björn Grüning and Enio Gjerga. At the de.NBI booth, questions concerning de.NBI, the de.NBI Cloud and the Industrial Forum were answered by the training and web coordinator Daniel Wibberg. Furthermore, several de.NBI partners taught workshops on:



- Getting started with the de.NBI Cloud
- Proteomics and metabolomics with OpenMS and pyOpenMS
- de.NBI showcase: Combining workflows, tools and data management
- Integrating computational meta-omics for microbiome research
- Multi Omics Factor Analysis (MOFA)

Further information is available at: <https://gcb2019.de/>

## de.NBI supported conferences in the next time

### 6<sup>th</sup> 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. After the successful conduction of 80 training events in 2019 the actual list of scheduled courses is currently quite short. A number of training events are in the pipeline but not yet scheduled. Please consult the de.NBI training program for updates.

## Major de.NBI events – Save the Dates

- **5-Year Event | de.NBI SAB Meeting | Plenary Meeting 2020, 13-14 February 2020, Berlin.** The venue is the Seminaris Campus Hotel Berlin. This meeting is the obligatory annual assembly of the de.NBI consortium. The meeting will simultaneously celebrate five years of de.NBI. The registration is open to de.NBI consortium only and the link has been distributed by email.



## Overview of upcoming de.NBI events

Date	Event	City	Organizer
 16 Jan 2020	<a href="#">ELIXIR Guest Webinar supported by de.NBI: ISO interoperability standards in Biotechnology</a>	online	de.NBI-SysBio
 22 Jan 2020	22. CCU Meeting	Bielefeld	CAU
 28-30 Jan 2020	<a href="#">Data Carpentry Workshop 2020</a>	Heidelberg	HD-HuB
 13-14 Feb 2020	<a href="#">de.NBI 5-Year Event   SAB Meeting   Plenary Meeting</a>	Berlin	CAU
 17-20 Feb 2020	<a href="#">9th Galaxy workshop on HTS data analysis</a>	Freiburg	RBC

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

## IMPRESSUM

### RESPONSIBLE FOR CONTENTS

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