# de.NBI Quarterly Newsletter

This de.NBI Quarterly Newsletter in **May 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/

## ELIXIR-CONVERGE releases the Research Data Management Kit

ELIXIR-CONVERGE, a three-year Horizon 2020 project, brings together data management experts from all 23 ELIXIR Nodes, representing 29 research institutes and 22 countries across Europe, to work collaboratively on some major challenges around accessing, provisioning and distributing data. The development of a data management toolkit sits at the core of the project, providing researchers with a strategy to manage their data to international standards.

As a result, on 31 March 2021, the ELIXIR-CONVERGE project launched a new platform for research data management: the **RDMkit** (https://rdmkit.elixir-europe.org).

Developed and managed by experienced scientists, who work with life science data on a daily basis, this research data management kit provides a comprehensive guide of best practices applicable to projects from start to finish. The RDMkit lists tools and resources that can help solve common problems related to data management in life sciences. With the fundamental goals (I) to empower researchers developing and executing project data management plans, (II) to recommend FAIR data and (III) to facilitate the adoption of best practices of research data management by academia and industry the new tool is designed for a wide variety of users across Europe.

The content of the RDMkit is subdivided into six different sections:
- The research data life cycle
- The user's role
- The research domain
- The data management problem
- The tools and resources needed
- The practical examples for tools assembly

The RDMkit is a community-driven effort that welcomes contributions to improve its usability and content, expand to other domains or represent different user roles. If you want to contribute to this open-source toolkit, your support will be officially recognised on the site. To find out more, visit the RDMkit page for contributions.

For more information please visit https://rdmkit.elixir-europe.org

## Women in Data Science – Perspectives in Industry and Academia

The thematic field of data science has grown significantly over the last two decades, but even with this expansion of opportunities, women are still underrepresented in this field. What are the opportunities, but also the obstacles that women face if they decide to enter this field? Actually, there are plenty of opportunities for women in data science to

*Joint Bayer AG and de.NBI / ELIXIR Germany Event*
**Women in Data Science – Perspectives in Industry and Academia**

*June 18th 2021*
*3:00 – 5:30 pm*

**Register Online: HERE**

*Agenda*

// **3:00 pm:** Opening Address
// WiDS network at Bayer AG - **Arwa Al-Dilaimi**, Bayer AG, Monheim, DE
// German Network for Bioinformatics Infrastructure (de.NBI) - **Tanja Dammann-Kalinowski**, de.NBI, Bielefeld, DE

// **3:15 pm:** Data Science - Perspectives in Industry
// Where great minds can make a difference: Working for Bayer - **Veronica Lopez Ramua**, Bayer AG, Monheim, DE
// Digitally capable: How science, technology and innovation helps you to build a resilient career - **Catherine Sirven**, Bayer AG, Lyon, FR
// My career experience as biostatistician and project manager - **Erica Maresso**, Bayer AG, Frankfurt am Main, DE

// **4:00 pm:** Data Science - Perspectives in Academia
// ELIXIR - Data for Life - **Katharina Lauer**, ELIXIR, Hinxton, UK
// How I developed my career in data science: role models, training, mentoring and community - **Bérénice Batut**, de.NBI/ELIXIR Germany, University of Freiburg, DE
// Women power in data curation and data management - **Ulrike Wittig**, de.NBI/ELIXIR Germany, Heidelberg Institute for Theoretical Studies, Heidelberg, DE

// **4:45 pm:** Panel Discussion
// **5:15 pm:** Closing Remarks

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linkedin.com/company/bayer   linkedin.com/company/de-nbi

thrive. To show how attractive and diverse the job of a data scientist can be, regardless of whether it is industry or academia, Bayer AG and de.NBI/ELIXIR Germany are organizing joint online event entitled 'Women in Data Science - Perspectives in Industry and Academia', to be virtually held on 18th June 2021. Six female speakers from Bayer AG, de.NBI and ELIXIR active in the vast field of data science will share their experiences, the challenges they face, and the opportunities for advancement. In conclusion, a panel discussion will focus on the promotion of women and the recognition of 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/1226-women-in-data-science-2021-perspectives-in-industry-and-academia

# Establishment of the ELIXIR Germany Code of Conduct



The ELIXIR Germany Code of Conduct contains important and binding rules for all event attendees across confidentiality and safety, professional integrity and personal conduct. The aim of the Code is to ensure the compliance and the commitment of all participants to these values and principles at all ELIXIR Germany events, as an integral part of the way we can all support the development of ELIXIR Germany and each other. The ELIXIR Germany Code of Conduct Oversight Group is responsible for enforcing the Code of Conduct and is supported by "ELIXIR Germany Allies", who are assigned responsibility for an individual event.

For more information, please visit https://www.denbi.de/code-of-conduct

Attribution & Acknowledgements:
The Code of Conduct has been adopted and modified for ELIXIR Germany based on ELIXIR CoC under the CC-BY 4.0 license.



**1 DIVERSITY**

**3 FOSTER TRUST AND COLLABORATION**

**2 ACT ETHICALLY AND WITH INTEGRITY**

**4 RESPECT AND SHOW COURTESY TO EACH OTHER**

# de.NBI Cloud @ ELIXIR Compute Platform

On 14 May 2021, Nils Hoffmann, the de.NBI ELIXIR-DE Compute and Interoperability Platform Coordinator, presented an overview of the de.NBI Cloud as part of the bi-monthly ELIXIR Compute Platform call. His presentation covered many relevant topics, such as the organisation of the cloud federation, its development and growth over the past five years, as well as current activities like the introduction



of a user-credits system and the ongoing efforts to certify all cloud locations according to the ISO 27001 information security management standard. Further topics included the contributions of the de.NBI cloud to various ELIXIR activities, COVID-19 related research, the European Open Science Cloud (EOSC-Life), Global Alliance for Genomic Health (GA4GH) , and national research infrastructure programmes, such as GAIA-X and Nationale Forschungsdateninfrastruktur (NFDI). The presentation was well received and sparked a lively discussion about organisational, technical and legal challenges involved with the operation of a federated scientific cloud infrastructure.

For more information please visit: https://cloud.denbi.de/

## Towards a de.NBI Plant Bioinformatics Community

The service center German Crop BioGreenformatics Network (GCBN) organized a user meeting on 11 March 2021 embedded in the framework of the "Plant2030 Statusseminar 2021". Based on the survey among potential members of the Plant Bioinformatics Community conducted beforehand, the session comprised general information on services and training offered by the de.NBI network and, in particular, the service and training portfolio of the GCBN. In the subsequent discussion the participants gave a lively feedback. The collected suggestions from the survey and the meeting will be used to adapt and improve the Services and Training activities offered by the GCBN accordingly. In addition, the user meeting will mark a starting point for the establishment of a forum for the de.NBI Plant Bioinformatics Community.

Further information on the GCBN service center can be accessed here: https://www.denbi.de/network/german-crop-biogreen-formatics-network-gcbn

## Peer Bork awarded 2021 Novozymes Prize for sharing scientific tools

Peer Bork, Director of EMBL Heidelberg and coordinator of the de.NBI Service Center for Human Bioinformatics (HD HuB) receives the Novozymes Prize 2021 for developing groundbreaking, publicly available bioinformatics tools. His original tools, databases and web servers have enabled the collection and analysis of biological data in a vast variety of fields like health environment and climate for hundreds of thousands of researchers. With STRING, STITCH, SMART, eggNOG and iTOL, all of them in the de.NBI service portfolio, Peer Bork and colleagues have developed tools for researchers, so they can now more easily analyse the many data open source.
Congratulations from the de.NBI community!!

More information at: https://embl.org/news/lab-matters/peer-bork-honoured-for-innovative-scientific-tools/
and https://novonordiskfonden.dk/en/news/biologisk-pioner-prisbeloennes-for-at-dele-sine-videnskabelige-vaerktoejer/
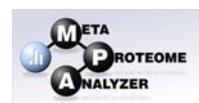
## de.NBI Project MetaProtServ in Final at the Hugo Junkers Prize 2020

The Hugo Junkers Prize for Research and Innovation is Saxony-Anhalt's most highly endowed research and innovation prize. Innovative projects in application-oriented research from science and industry are the main focus. The de.NBI project MetaProtServ participated in this year's competition and reached the final among almost 100 competitors. The team around Dr. Dirk Benndorf, Dr. Robert Heyer, Kay Schallert, Prof. Dr. Udo Reichl and Prof. Dr. Gunter Saake presented the metaproteome analysis and bioinformatics workflow for functional high-throughput monitoring of microbiomes in medicine, technology and the environment. So far, microbiome analyses have not been used in the clinic for diagnosing diseases or in biotechnology for process monitoring. The workflow developed by Bennorf and colleagues allows the taxonomic and functional analysis of a wide variety of samples within 24 hours, which is much faster compared to existing methods on the market. The de.NBI partners from Magdeburg were among the finalists of the Hugo Junkers Prize 2020 competition in the category 'innovative fundamental research'.

More information on the contest at: https://www.hugo-junkers-preis.de/startseite

Find the service MetaProteomeAnalyzer at: https://www.denbi.de/services/323-metaproteomeanalyzer-identification-of-taxonomic-and-functional-relationships-between-identified-proteins

## After the hackathon is before the hackathon

<span style="float:right">*by S. Neumann*</span>

The 2nd de.NBI/ELIXIR-DE metaRbolomics workshop was held online from 22-24 March 2021, with more than 40 participants from Germany, Europe and the rest of the planet; across all career levels including two participants from Industry.

A lot of ground was covered. For example developments on metabolomics data processing packages in the RforMassSpectrometry community, efforts on quality control (QC) reporting in the Proteomics Standards Initiative (PSI) mzQC standard or proposals for the upcoming ELIXIR BioHackathon 2021 in November.

It was exciting to see how the participants interacted in the videoconference, breakout rooms, chat channels and joint documents, which had a lot of momentum, just as you want a hackathon to be.



*Figure 1: Participants with activated cameras during the group screenshot*

After the hackathon is before the hackathon, the next de.NBI / ELIXIR-DE metaRbolomics gathering has already been scheduled for November this year in the venerable Leucorea Wittenberg. The registration will open in September.

For details, please see https://www.denbi.de/training/1177-3rd-de-nbi-elixir-de-metarbolomics-hackathon

## News from the de.NBI Office

**Nils Hoffmann** is the new member of the ELIXIR Germany Administration Office (AO). He holds a PhD in bioinformatics for mass spectrometry based metabolomics and a diploma in informatics in the natural sciences, both from Bielefeld University. He has worked as a solution engineer and technical project manager for semantic search applications before rejoining academia as a project coordinator for the de.NBI associated project lipidomics informatics for life sciences (LIFS) and post-doctoral researcher for bioinformatics in lipidomics at the Leibniz Institut für Analytische Wissenschaften -ISAS- e.V., in Dortmund. His research interests include algorithms for mass spectrometry analysis of small molecules, data standardization and integration, as well as biological and clinical applications of lipidomics and metabolomics.

As a Compute and Interoperability Platform Coordinator, Nils will support the ELIXIR-DE activities in the ELIXIR Compute Platform as part of SIG 6 de.NBI Cloud, and in ongoing and upcoming ELIXIR interoperability projects.

We welcome Nils 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. Check our services at https://denbi.de/services.

- **EDGAR 3.0** provides new scalable infrastructure based on the de.NBI Cloud for comprehensive microbial comparative gene content analysis. Find the service at: https://www.denbi.de/services/314-edgar-comparative-genomics-platform. The new version is presenteted in: M Dieckmann, S Beyvers, RC Nkouamedjo-Fankep, P Hanel, L Jelonek, J Blom, AGoesmann, **EDGAR3.0: comparative genomics and phylogenomics on a scalable infrastructure**, Nucleic Acids Research, 2021, gkab341, https://doi.org/10.1093/nar/gkab341

- **COPASI 4.31** (Build 243) released. Find the service at: https://www.denbi.de/services/373-copasi-creating-and-solving-mathematical-models-of-biological-processes
The Linux installation has been transformed to a self-extracting interactive archive. Furthermore there has been a speedup since version 4.30 and many more amendments so that an upgrade is worth trying.

- **iTOL:** The new version iTOL v6 available at https://www.denbi.de/services/274-itol-display-and-manipulation-of-phylogenetic-trees. Furthermore find the latest publication on the service: I Letunic, P Bork, **Interactive Tree Of Life (iTOL) v5: an online tool for phylogenetic tree display and annotation**, *Nucleic Acids Research*, 2021, gkab301, https://doi.org/10.1093/nar/gkab301

- **LipidCreator 1.2.0** is a lipid building block-based workbench and knowledge base for the automated generation of targeted lipidomics mass spectrometry. The new version is now available via the skyline store at https://www.denbi.de/services/340-lipidcreator-computing-precursor-and-fragment-masses-formulas-for-lipids-for-targeted-lipidomics

Accompanying documentation: Kopczynski D, Peng B, Hoffmann N, Pratt B &Ahrends R. (2021, April 20). **LipidCreator 1.2.0.772** (Version 1.2.0.772). Zenodo. http://doi.org/10.5281/zenodo.4705456

- **plaBiPD:** The comprehensive platform for genomes of crop plants has now added support for the Brassica species Camelina sativa. Find the service at: https://www.denbi.de/services/355-plabipd-functional-annotation-of-plant-genomes

- **Galaxy.eu** is celebrating 30,000 registered users End of April. Additionally, the European Galaxy Server is now listed in the Catalogue of Research Infrastructure Services (CatRIS). CatRIS is a portal for services and resources provided by Research Infrastructures across Europe. The European scientific community can find it under the following categories *Compute, Software, Services, Applications, Consultancy & Support, Data Analysis, Data* Management, Education & Training for different scientific categories. All the different European Galaxy Flavours are also included as use cases.

- **>BIOC::Code explore**: Many de.NBI tools such as BioMaRt,DeSeq, DEXseq Ypasa… are written in R. Thus the new development at https://code.bioconductor.org enables browsing the contents and git history of all software packages. Search for across all software packages at once, and filter results by file names, types, or packages.

### Recent Publications by de.NBI partners:

- Videm, P, Kumar A, Zharkov O, Grüning BA, Backofen R., **ChiRA: an integrated framework for chimeric read analysis from RNA-RNA interactome and RNA structurome data**, GigaScience, Volume 10, Issue 2, February 2021, giaa158, https://doi.org/10.1093/gigascience/giaa158

- Gallardo-Alba C, Grüning B, Serrano-Solano B (2021) **A constructivist-based proposal for bioinformatics teaching practices during lockdown.** PLoS Comput Biol 17(5): e1008922. https://doi.org/10.1371/journal.pcbi.1008922

- Serrano-Solano B, Föll MC, Gallardo-Alba C, Erxleben A, Rasche H, Hiltemann S, et al. (2021) **Fostering accessible online education using Galaxy as an e-learning platform.** PLoS Comput Biol 17(5): e1008923. https://doi.org/10.1371/journal.pcbi.1008923

- Batut B., van den Beek M., Doyle M.A., Soranzo N. (2021) **RNA-Seq Data Analysis in Galaxy**. In: Picardi E. (eds) RNA Bioinformatics. Methods in Molecular Biology, vol 2284. Humana, New York, NY. https://doi.org/10.1007/978-1-0716-1307-8_20

- The results of two major international projects on the **rye** and **barley** genomes with participation of GCBN members have been published. Data are integrated in the GCBN tool suite **CATS**:

  - M Mascher, …H Gundlach, …U Scholz, KFX Mayert, *et al.* (2021), ***Long-read sequence assembly: a technical evaluation in barley***. The Plant Cell. DOI: 10.1093/plcell/koab077

  - T Rabanus-Wallace, …H Gundlach, …KFX Mayer, …U. Scholz, *et al.* (2021), **Chromosome-scale genome assembly provides insights into rye biology, evolution, and agronomic potential**. Nature Genetics. DOI: 10.1038/s41588-021-00807-0

- T Van Den Bossche, …K Schallert, …D Benndorf, S Fuchs, …R Heyer, …A Scryba, …T Muth. **Critical Assessment of Metaproteome Investigation (CAMPI):** *A Multi-Lab Comparison of Established Workflows,* bioRxiv 2021.03.05.433915; DOI: 10.1101/2021.03.05.433915
  This publication summarizes results of a multi-lab benchmarking study in metaproteomics applying established de.NBI tools like MetaproteomeAnalyzer, SearchGUI/Peptide Shaker, Prophane, eggNOG or mOTUs. The study has been conducted as a community challenge during the 3ʳᵈ international metaproteomis symposium (Dec 2018).

# 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.

<div align="center">Please consult the de.NBI training program for updates.</div>

## de.NBI supported conferences in the near future

**ISMB/ECCB 2021, 25-30 July 2021, virtual conference**
The de.NBI office will be presented with a virtual booth and a tech talk introducing the network and our training program.
General information at: https://www.iscb.org/ismbeccb2021

**GCB 2021 – German Conference on Bioinformatics, 06-08 September 2021 – virtual conference**
This year's conference is organized by the bioinformaticians from Halle, Leipzig, Gatersleben und Quedlinburg. Again the meeting will take place virtually due to the pandemic situation. The de.NBI will be present with a virtual booth. de.NBI Partners will teach the tutorials:
- Bioinformatics tools for analyzing clinical metaproteomics samples of the human gut; R. Heyer, K. Schallert, D. Benndorf (OVGU Magdeburg), S. Fuchs (RKI Berlin), T. Muth – BAM Berlin (BiGi)

- Exploring target Structures with ProteinsPlus; K. Schöning-Stierand, C. Ehrt, M. Rarey, Uni Hamburg (BioData)
- Non-targeted label free proteomics; T. Sachsenberg, Uni Tübingen (CIBI)
- BioC++ - solving daily bioinformatic tasks with C++ efficiently; M. Ehrhardt, R. Rahn, E. Seiler, FU Berlin (CIBI)

General information and registration at: https://gcb2021.de

## ✳ Overview of upcoming de.NBI events

| | Date | Event | City | Organizer |
|---|---|---|---|---|
| | 17-20 May 2021 | Ontologies - statistics, biases, tools, networks, and interpretation 2021 | Online | HD-HuB |
| | 20 May 2021 | GeoMine @ ProteinsPlus - Versatile Tools for Structural Investigations | Online | BioData |
| | 08-10 Jun 2021 | The Linux Command Line: From Basic Commands to Shell Scripting | Online | Ass. Partner UKE Hamburg, M. Alawi |
| | 11 Jun 2021 | EDGAR User Meeting - Use Case Reports and Software Updates | Online | BiGi |
| | 01 Jul 2021 | BRENDA – The comprehensive Enzyme Information System (Webinar) | Online | BioData |
| | Aug-Sep 2021 | Computational genomics course for hands-on data analysis 2021 - Machine Learning for Genomics   -> Application Deadline 30 Jun 2021 | Online | CIBI |
| | 2021-08-23 | 5th BioInfra.Prot Tool-Training for Proteomics & Community Meeting | Online | RBC |
| | 15 Jul 2021 | 5. ELIXIR-DE CCU Meeting | Online | CAU |
| | 15 Jul 2021 | 27. CCU Meeting | Online | CAU |
| | 27 Sep–01 Oct 2021 | de.NBI Summer School 2021 - Analysis and integration of Mass Spectrometry based omics data in Proteomics, Metabolomics and Lipidomics | Online | BioInfra.Prot/ CIBI |
| | 05 Oct 2021 | LIFS Course - ILS 2021 & LipidomicsForum 2021 | Regensburg | BioInfra.Prot/ LIFS |
| | 22-24 Nov 2021 | 3rd de.NBI/ELIXIR-DE metaRbolomics Hackathon | Wittenberg | CIBI/MASH |

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

## IMPRESSUM

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