

# de.NBI Quarterly Newsletter

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

## de.NBI Cloud Certification



On June 22nd 2021, the de.NBI Cloud site at Bielefeld University, Germany, has been certified for implementing and maintaining an information security management system that fulfills the requirements of the ISO/IEC 27001: 2017 standard. The successful certification confirms the professional level of management

and administration of the cloud infrastructure, which reinforces the basis for secure handling of sensitive research data in the future.

The de.NBI Cloud site at Bielefeld University is one of the first German scientific cloud providers to achieve ISO 27001 certification and thereby underlines its claim to offer state-of-the-art computational infrastructure, data storage and data protection standards to German researchers in the Life Sciences.

This first success also paves the way for the upcoming certifications of the other de.NBI Cloud sites in 2021 and 2022, which will continue to substantiate the federated de.NBI Cloud as a trustworthy resource for handling of sensitive data according to the GDPR regulations.

The de.NBI Cloud provides compute and storage resources free of charge for academics.

Find further details at: <https://cloud.denbi.de/>



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## Article on the Continuation of the de.NBI Network by A. Pühler

The article "Continuation of the de.NBI network" in the latest issue of the journal "Biologie in unserer Zeit" (BIUZ) by the de.NBI coordinator, Alfred Pühler, reports on the achievements of the network and the planned continuation within the Helmholtz Association. In almost seven years, the de.NBI network has built up an extensive infrastructure that helps all researchers of the life science area to analyse large experimental data sets via service and training offers. This has been achieved through BMBF funding, which brought together the best-known bioinformatics groups focused on service and training in Germany in a network. In addition, a cloud resource has been established at six locations that can be used free of charge for the analysis of life science datasets. On international level, the de.NBI network is integrated into the ELIXIR consortium via the German node. Since the BMBF project funding of the de.NBI network will expire at the end of this year, the established bioinformatics infrastructure has been struggling for sustainable continuation. The main impulse came from the German government, which at short term provided the Jülich Research Centre with funding to continue the de.NBI network. The task is now to transfer the established bioinformatics infrastructure into the Helmholtz Association and to ensure that both, the service and training offers, as well as the cloud resources remain functional and that membership in the ELIXIR consortium can be continued seamlessly. Due to time constraints this transformation procedure is a demanding challenge. The de.NBI coordinator hopes that a satisfactory solution can be found for all participants of the de.NBI network.

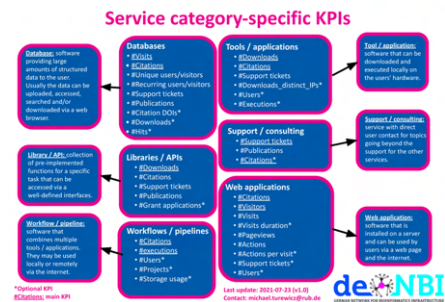
Find the publication at: <https://www.biuz.de/index.php/biuz/article/view/4634>

## Semi-automatic system for KPI collection

The Special Interest Group 2 Service and Service Monitoring announced the development of a Key Performance Indicator (KPI) collection system. The goal is to simplify the collection and visualization of KPI data from inside the de.NBI network. Providers of de.NBI services, the SIG 2 and the de.NBI administration will benefit from this KPI collection system as it serves as a centralized system for the collection of KPIs. A prototype of the KPI collection System has been developed by the service unit GCBN and successfully tested with example data. The system enables user management and relies on ELIXIR AAI for access control. KPI data can be entered into the system via a REST webservice, by upload of CSV files or manually by hand. In the next step all service units will test the KPI collection system with their (manually collected) KPI data to see how it will perform with larger amounts of data and users.

As the topic of KPIs is rather complex, the SIG 2 designed a KPI Cheat Sheet to support providers of de.NBI services even further. The KPI Cheat Sheet gives an overview about all de.NBI KPI categories as well as KPI regulations.

The KPI Cheat Sheet is openly available at: [https://www.denbi.de/images/Service/20210624\\_KPI\\_Cheat\\_Sheetpptx.pdf](https://www.denbi.de/images/Service/20210624_KPI_Cheat_Sheetpptx.pdf)



## 2<sup>nd</sup> Annual Meeting of the de.NBI Industrial Forum 2021

The annual meeting of the de.NBI Industrial Forum will take place for a second time since its founding in 2019. The topics from 2020 covered recent developments in plant bioinformatics as well as the still ongoing coronavirus crisis.



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

This year the annual meeting will focus on the high relevance topics Artificial Intelligence (AI) and the NFDI (Nationale Forschungsdateninfrastruktur). Furthermore a representative of the Helmholtz Association will give insights about the future of the de.NBI Industrial Forum. The annual meeting of the de.NBI Industrial Forum will be an online event on November 25th 2021 from 1 – 4:30 pm (CET). The program as well as the registration will be available in the next weeks.

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

Event website: <https://www.denbi.de/events/1284-virtual-2nd-annual-meeting-of-the-de-nbi-industrial-forum>

## Two de.NBI Summer Schools in 2021

This year de.NBI will conduct two summer schools:

- 🧑‍🎓 **Data Analysis of Mass Spectrometry based Proteomics, Lipidomics and Metabolomics** (27-30 Sep 2021) and
- 🧑‍🎓 **Analysis of Microbial Communities** (04-08 Oct 2021).

The summer schools have the aim to give PhD students and postdocs in computer science/bioinformatics/life sciences deeper insights into algorithms or software systems in the proteomics, lipidomics and metabolomics, and metagenomics and metaproteomics, respectively. Participants will use existing tools to analyze and visualize real-world datasets (data specifically prepared for the tutorials as well as the participants' own data) and will be instructed by keynote and de.NBI speakers. Beyond that, participants will be put into a position to be able to combine existing and future algorithms or tools with other solutions as well as to integrate them into a sustainable software system.

Further information and registration at:

- 1) <https://www.denbi.de/training/1150-de-nbi-summer-school-2021-proteomics-lipidomics>; Registration deadline 31 Aug 2021
- 2) <https://www.denbi.de/training/1269-de-nbi-summer-school-2021-part-2-microbial-community-analysis>; Registration will open soon.

## New ELIXIR Community-led Implementation Studies

Seven new Community-led Implementation Studies were launched on 1 June 2021 that aim to integrate Community-oriented resources with the ELIXIR Platforms and other Communities. These projects were collectively awarded € 1.5million from the ELIXIR core budget, and will run until 2023. The seven new Community-led Implementation Studies relate to ELIXIR's 3D-BioInfo, Plant Sciences, Galaxy, Intrinsically Disordered Proteins (IDP), human Copy Number Variation (hCNV), and Proteomics Communities Germany is involved in six out of seven studies, with a total of 13 person months distributed among the eleven ELIXIR-DE members actively engaged in these studies.

In particular, the ELIXIR-DE members at Ruhr University Bochum have a leading role within the implementation study "Increasing the translational value of public proteomics datasets: Automatic metadata-driven reanalysis in cloud infrastructures" by the ELIXIR Proteomics Community.

Details at: <https://elixir-europe.org/news/elixir-funds-seven-new-life-science-data-projects>



## Update on ELIXIR Germany Service Provision



A main goal of the German ELIXIR Node is to provide bioinformatics services and resources for life sciences research in academia and industry. The academic members of ELIXIR Germany maintain and develop further more than 100 software tools. This impressive service portfolio has recently been updated and is now available as a list on the ELIXIR Germany website.

In particular, ELIXIR Germany members at Heidelberg University, EMBL Heidelberg, DKFZ Heidelberg (Deutsches Krebsforschungszentrum) and Charité Berlin have added 27 new tools for data analysis in human bioinformatics. A prominent example is *Magellan* that is a web application for the display and analysis of next-generation sequencing data with a focus on COVID-19. The goal of *Magellan* is to provide easy and open access to highly relevant data of COVID-19 patients for the research community.

A complete list of ELIXIR services with search functions is available at: <https://elixir-europe.org/services/list>

Find *Magellan* at: <https://www.denbi.de/services/1189-magellan-display-and-analysis-of-next-generation-sequencing-data-with-a-focus-on-covid-19>

## ELIXIR Annual Report 2020

ELIXIR has published its 2020 Annual Report – A Story of Collaboration, Innovation and Preparedness, detailing the scientific developments and showcases the impact of ELIXIR's activities in various areas, including COVID-19. This report is the second to be published within the ELIXIR 2019-2023 Scientific Programme and details the progress that has been made against the long-term strategic objectives. The annual report also highlights the participations of the European nodes. Germany has participated in a total of 15 ELIXIR implementation studies and six ELIXIR publications since the beginning of its activities.

For more information, the annual report is available for download via: <https://elixir-europe.org/news/elixir-2020-publishes-annual-report>



## For better patient care: Cooperation between MIRACUM and de.NBI

de.NBI and MIRACUM (Medical Informatics in Research and Care in University Medicine), the largest consortium within the the Medical informatics Initiative, have joined forces to integrate analysis techniques into patient care in the form of bioinformatics workflows by making use of the possibilities of the de.NBI Cloud and especially the Galaxy framework. The concrete use case is "From Knowledge to Action - Support for the Molecular Tumor Board". From de.NBI side, Freiburg university, member in both, Miracum and de.NBI, is driving the effort.



de.NBI and the projects funded by the Medical Informatics Initiative complement each other and build on each other in order to ensure a reliable and secure IT infrastructure between research and patient care in Germany.

Find more information at: <https://www.denbi.de/news/1279-for-better-patient-care-cooperation-between-miracum-and-the-german-network-for-bioinformatics-infrastructure-de-nbi>

Find information on MIRACUM at: <https://www.miracum.org/>

## A look back at the event WiDS - Perspectives in Industry and Academia

The Joint Bayer AG & de.NBI/ELIXIR Germany online conference “Women in Data Science - Perspectives in Industry and Academia” on 18 June 2021 was attended by 150 participants from all over the world. Six spokeswomen from Bayer Crop Science Division, de.NBI and ELIXIR addressed the gender gap in data science and reported on efforts towards equal employment opportunities at all levels, starting with professionals up to executives. The panel discussion addressed collaborations between researchers in academia and industry and shed more light on the speakers’ personal career experiences. These efforts are vital, but more attention needs to be paid in the future on



how gender biases can be addressed more efficiently.

As there is a underrepresentation of women in computer and data science, more women need to be attracted to and subsequently to be retained in the field to contribute their skills and perspectives, whether it is industry or academia.

Due to the great interest in our first event, the de.NBI administration office is planning a follow-up event in autumn 2021.

More information at: <https://www.denbi.de/events/1226-women-in-data-science-2021-perspectives-in-industry-and-academia>

The slides of B. Batut’s talk are available at <https://bit.ly/bebatut-women-data-science-2021>

Voices from the anonymous feedback survey:

*Thank you for organizing an amazing and inspiring event. I learned of new job opportunities in data science from both industry and academic perspective. The talks were insightful and encouraging well.*

*The talks were very informative. The speakers had a positive attitude and answered all questions very well.*

*Very instructive to have other women experiences and points of view.*

## de.NBI supported the ISMB/ECCB 2021

From 25-30 July 2021, the ISMB/ECCB 2021 conference took place as a virtual event. The ISMB/ECCB with more than 2100 participants from all over the world is the largest meeting of scientists working in computational biology and provides an intense multidisciplinary forum for disseminating the latest developments in computational tools for data driven biological research. This year, de.NBI hosted at a virtual booth, presenting the de.NBI service and training program, the network’s activities, the de.NBI Cloud and ELIXIR Germany. Furthermore, de.NBI member Renato Alves presented a technical talk about the de.NBI training program. The Senior Scientist Award Keynote “Analyzing microbes in us and on our planet” was given by Peer Bork (HD-HuB/EMBL Heidelberg). In addition, several de.NBI members gave lectures in the Microbiome COSI (Communities Of Special Interest), e.g. Alexander Sczyrba (Bielefeld University/BiGi) and Thilo Muth (Associated Partner at BAM, Berlin)

Find more information at: <https://www.iscb.org/ismbecb2021>

## 2000<sup>th</sup> de.NBI Twitter follower, 1000<sup>th</sup> de.NBI LinkedIn follower and webpage record

We are pleased to announce that Theresa Cavasin is our 2000<sup>th</sup> de.NBI Twitter follower. She is working at the Center for Bioinformatics (ZBH) in Hamburg and became aware of the current de.NBI activities through our Women in Data Science (WIDS) event that was recently hosted together with the Bayer AG. The de.NBI Administration office sent Theresa Cavasin a de.NBI goody bag including a set of de.NBI brochures and some de.NBI merchandise articles.

On average, the de.NBI Twitter channel welcomes one new follower per day. Interestingly, the 1,000-follower-mark on LinkedIn was passed on the same day and also the de.NBI webpage achieved a new visitor record. Almost **4,000 unique users** visited the page in June. This shows the great interest in news about bioinformatics service and training in the German and European life sciences communities. It is also proof of the high level of acceptance and importance of de.NBI that has been achieved during almost seven years of work.



## News from the de.NBI Office

**David Weinholz** is the new member of the de.NBI Administration Office(AO). He holds a Bachelor's degree in Cognitive Informatics and has a Master's degree in Intelligent Systems from Bielefeld University. During his studies, he has already been involved in the development of the de.NBI Cloud Portal and SimpleVM. As part of the de.NBI Cloud Governance, he will now expand the portal functionality to further meet the needs of the life sciences community.











We welcome David 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.](https://denbi.de/services)

-  **BacDive** has been updated with homepage relaunch, Modular Advanced Search, searchable NCBI tax ID, Integration of links to BacMedia and BRENDA's Enzymedetector, 1500 new strain pictures. Find the service at: <https://www.denbi.de/services/347-bacdive>. Furthermore, BacDive has hit 100,000 unique users per year in July.
 
-  **COPASI 4.32** (Build 245) released. Find the service at: <https://www.denbi.de/services/373-copasi-creating-and-solving-mathematical-models-of-biological-processes>

-  **SeqAn 3.0.3**, New release of the modern #C++P library for sequence analysis. Find out more about it at <https://seqan.de/release/2021/05/28/seqan-3-0-3-release>.
 
-  **PiGx**: Pipelines in Genomics. A SARS-CoV2 wastewater sequencing pipeline created. Sequencing is one of the bestways of monitoring. We built a reproducible analysis pipeline for that. Find the pipeline at: [https://github.com/BIMSBbioinfo/pigx\\_sarscov2\\_ww](https://github.com/BIMSBbioinfo/pigx_sarscov2_ww)


### Recent Publications by de.NBI partners:

-  Pühler, A. (2021). **Verstetigung des de.NBI-Netzwerks**. *Biologie in Unserer Zeit*, 51(3), 221–222. <https://doi.org/10.11576/biuz-4634>
-  Eggers B, Schork K, Turewicz M, Barkovits K, Eisenacher M, Schröder R, Clemen CS, Marcus K. **Advanced Fiber Type-Specific Protein Profiles Derived from Adult Murine Skeletal Muscle**. *Proteomes*. 2021 Jun 8;9(2):28. <https://doi.org/10.3390/proteomes9020028>.
-  Maslova, M., Herden, H., Schork, K., Turewicz, M., Eisenacher, M., Schroers, R., Baraniskin, A., & Mika, T. (2021). **Computertomography-Based Prediction of Complete Response Following Neoadjuvant Chemoradiotherapy of Locally Advanced Rectal Cancer**. *Frontiers in oncology*, 11, 623144. <https://doi.org/10.3389/fonc.2021.623144>
-  Schork K, Podwojski K, Turewicz M, Stephan C, Eisenacher M. **Important Issues in Planning a Proteomics Experiment: Statistical Considerations of Quantitative Proteomic Data**. *Methods Mol Biol*. 2021;2228:1-20. [https://doi.org/10.1007/978-1-0716-1024-4\\_1](https://doi.org/10.1007/978-1-0716-1024-4_1)
-  Vvedenskaya O, Rose TD, Knittelfelder O, Palladini A, Wodke JAH, Schumann K, Ackerman JM, Wang Y, Has C, Brosch M, Thangapandi VR, Buch S, Züllig T, Hartler J, Köfeler HC, Röcken C, Coskun Ü, Klipp E, von Schoenfels W, Gross J, Schafmayer C, Hampe J, Pauling JK, Shevchenko A, **Non-alcoholic fatty liver disease Stratification by Liver Lipidomics**, *Journal of Lipid Research* (2021), <https://doi.org/10.1016/j.jlr.2021.100104>.

## 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.

## de.NBI supported conferences in the near future



### 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, a poster and invited industry talks.



On 08-09 September will be dedicated to a number of workshops where de.NBI Partners will teach the tutorials:

- Cell segmentation using KNIME Analytics Platform and its Tensorflow2 Integration; J. Mothes, T.H. Dadi, Konstanz (CIBI)
- 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. Ehrh, 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>

## ELIXIR events



**ELIXIR Innovation and SME Forum:** Building the learning ecosystem of health: from data tracking to preventive medicine, 13 September | Hybrid, [BC]2 Conference in Basel

Join ELIXIR at the [BC]2 Basel Computational Biology Conference for this event all about health and preventive medicine. Including three fantastic keynotes including Serena Scollen (B1MG), Bogi Eliassen (Faroese genome sequencing project) and Nicolas Loeillot (Group Mutuel) and a showcase of exciting tech and pharmaceutical advancements from start-ups, SMEs and established companies.



Register before the 9 September at: <https://elixir-europe.org/events/learning-ecosystem-health-2021-BC2>



**BioHackathon Europe** 8-12 November 2021 | Hybrid, Barcelona

With close to 40 exciting bioinformatics, training and life science data related projects to choose from, there's something for everyone at this year's BioHackathon Europe. Don't miss this unique opportunity to network, learn and have fun with enthusiastic developers from across the world!



Register before 15 September at: [https://bit.ly/BHE\\_2021](https://bit.ly/BHE_2021)



## Overview of upcoming de.NBI events

Date	Event	City	Organizer
Aug-Sep 2021	Computational genomics course for hands-on data analysis 2021 - Machine Learning for Genomics	Online	RBC
23 Aug 2021	5th BioInfra.Prot Tool-Training for Proteomics & Community Meeting	Online	RBC
24-26 Aug 2021	The Linux Command Line: From Basic Commands to Shell Scripting 2-2021	Online	Ass. Partner UKE Hamburg
06-07 Sep 2021	Software Carpentry Workshop 02 2021	Online	Ass. Partner ZB MED
08 Sep 2021	Cell segmentation using KNIME Analytics Platform and its Tensorflow2 Integration - GCB 2021	Online	CIBI
08 Sep 2021	BioC++ - solving daily bioinformatic tasks with C++ efficiently - GCB 2021	Online	CIBI
08 Sep 2021	Bioinformatics tools for analyzing clinical metaproteomics samples of the human gut - GCB 2021	Online	BiGi
08 Sep 2021	Exploring Target Structures with ProteinsPlus - GCB 2021	Online	BioData
08 Sep 2021	Non-targeted label-free Proteomics - GCB 2021	Online	CIBI

Date	Event	City	Organizer
13 - 21 Sep 2021	CIBI User Meeting 2021	Online	CIBI
13 Sep 2021	Data management plan for Beginners	Online	RBC, CAU, GCBN
27-30 Sep 2021	de.NBI Summer School 2021 - Analysis and integration of Mass Spectrometry based omics data in Proteomics, Metabolomics and Lipidomics	Online	BioInfra.Prot/CIBI
01 Sep 2021	2nd BioInfra.Prot Community Meeting -Talks and tutorials for an easy introduction into omics analyses	Online	BioInfra.Prot/CIBI
04-08 Oct 2021	de.NBI Summer-School-2021 - Microbial Community Analysis	Online	BiGi / HD-HuB
05 Oct 2021	LIFS Course - ILS 2021 & LipidomicsForum 2021	Regensburg	BioInfra.Prot/LIFS
28 Oct 2021	6. ELIXIR-DE CCU Meeting	Online	CAU
28 Oct 2021	28. CCU Meeting	Online	CAU
22-24 Nov 2021	3rd de.NBI/ELIXIR-DE metaRbolomics Hackathon	Wittenberg	CIBI/MASH

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

## IMPRESSUM

### RESPONSIBLE FOR CONTENTS

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