

de.NBI Quarterly Newsletter

EDITORIAL

Dear de.NBI members, dear de.NBI followers,

It is a pleasure to present the 4th issue of the de.NBI Quarterly Newsletter of the current year. Again, this newsletter informs on important events of the last three months and on the activities which are planned for the future.

As an important step to start an industrial branch of the de.NBI network, the symposium “Data Driven Innovation in Industrial Biotechnology” was held in Frankfurt and jointly organized by ELIXIR, de.NBI and DECHEMA. Looking to the future, the scientific Advisory Board (SAB) and Plenary Meeting is scheduled for the end of November 2018. One of the main purposes of this meeting is to present the de.NBI activities of the last year to the SAB and to receive valuable recommendations for the further development of the network.

In the third year of its existence the de.NBI Cloud is again supported with a significant BMBF grant, which will be used to close hardware gaps and to invest in cloud computing security and certification. Another highlight for the de.NBI Cloud was the 1st de.NBI Cloud user meeting that took place at Bielefeld University. Almost 50 participants exchanged ideas on cloud computing projects and demonstrated their interest in the newly established infrastructure.

Finally, the newsletter reports on the launch of the completely new de.NBI web page, which has been designed to increase user-friendliness. In particular, the new web page now represents a common entrance gate to the de.NBI network. To reach the public, de.NBI released the de.NBI impact flyer and published an article on Wikipedia.

Last but not least as de.NBI coordinator I hope that this newsletter contains valuable information for de.NBI members and followers.




A. Pühler (de.NBI Coordinator)

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

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FIRST STEPS TO A de.NBI INDUSTRIAL FORUM

One of the major tasks of the de.NBI network concerns the development of an industrial branch. This task has successfully been started with the joint symposium **"Data Driven Innovation in Industrial Biotechnology"** from 15 – 16 October 2018 in Frankfurt/Main. At the end of the symposium the foundation of the de.NBI Industrial Forum for large, medium-sized and small companies dealing with big data sets in the life sciences field has been announced.



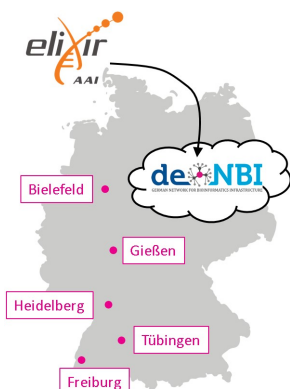
The participants of the symposium "Data Driven Innovation in Industrial Biotechnology" (Foto: ELIXIR)

The symposium was jointly organized by ELIXIR, de.NBI and DECHEMA. It was a continuation of ELIXIR's event series entitled "Innovation and SME Forum", which tours all over Europe with specific national thematic priorities.

Thankfully, DECHEMA provided their conference facilities and organizational know-how. Altogether, nearly 100 participants from academia and industry convened and followed the contributions, many of them presented by speakers from industry. The de.NBI network specifically reported on tools and services in plant phenotyping, proteomics, microbial bioinformatics, Galaxy frameworks, de.NBI Cloud, and systems biology considered to be of interest for industry. The general conclusion at the end of the symposium was that the success of the event resulted from the excellent collaboration of the three partners.

The program and slides are available at: <https://www.elixir-europe.org/events/sme-event-frankfurt>

FURTHER FINANCIAL SUPPORT FOR THE de.NBI CLOUD



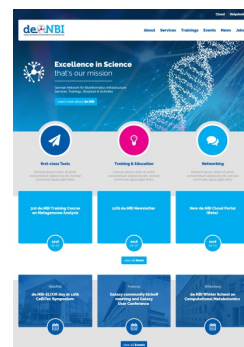
The de.NBI Cloud located at five universities, namely Bielefeld, Freiburg, Gießen, Heidelberg and Tübingen, was started in the year 2016. The de.NBI Cloud is financed by BMBF grants. In the past, BMBF provided financial support to establish a compute and storage component. Now in 2018, the BMBF announced to invest again in the de.NBI Cloud. This time, the existing de.NBI cloud sites will receive financial support to close hardware gaps. In addition, the grant will also be used to invest in cloud computing security and certification of the de.NBI Cloud.

At the moment, the federated de.NBI cloud consists of more than 16,000 cores, 170 TB RAM and 38 PB storage capacity. A cloud portal represents the central access point to the federated de.NBI Cloud platform. The whole system is accessible through single sign-on and is based on the ELIXIR Authentication and Authorization Infrastructure (ELIXIR-AAI). Since it became productive in spring 2017, the federated cloud is already used by a larger group of scientists from the life sciences area for the analysis of big data sets.

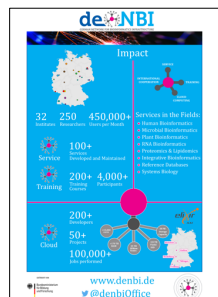
LAUNCH OF THE NEW de.NBI WEBSITE

The de.NBI office is proud to present the new de.NBI website. The new website is a complete redesign focused on lucidity and usability to drastically increase the user-friendliness. To address the users directly, the user-relevant information, like the de.NBI services, training courses and cloud, is now presented at front. In addition, the new website has a responsive design, which allows a smooth display on smaller screens like mobile devices. All in all, the new de.NBI website is designed to become the entrance gate for life scientists and bioinformaticians to the bioinformatics infrastructure in Germany.

The new de.NBI website can be found at <https://www.denbi.de>



RELEASE OF THE de.NBI IMPACT FLYER



The recently released de.NBI Impact Flyer gives an overview of the de.NBI service, training and cloud portfolio and presents the great impact of de.NBI on the Life Science and Bioinformatics communities in Germany. The Impact Flyer summarizes facts and figures about de.NBI, making it easy for new researchers to get an overview of the key benefits of using de.NBI services and resources. Requests for printed copies for further distribution are welcomed by the de.NBI office.

The de.NBI impact flyer can be found at <https://www.denbi.de/downloads>

THE de.NBI ARTICLE ON WIKIPEDIA









WIKIPEDIA

de.NBI is now represented in the largest online encyclopedia – Wikipedia. The de.NBI Wikipedia article gives insights into the activities and structure of the network, and encourages further reading. Additionally, the article complements the efforts taken to increase the online visibility of the de.NBI. Together with the Wikipedia article, the new website and the activities in social media (on Twitter and YouTube), the de.NBI network is well equipped to increase the reach in the area of life sciences and bioinformatics. Further editing of the Wikipedia article is welcome.

The de.NBI Wikipedia article can be found at <https://en.wikipedia.org/wiki/de.NBI>

RECENT UPDATES OF de.NBI SERVICES

New versions of various de.NBI services and tools have been released in the last months accompanied by the respective publications:

-  **COPASI 4.24.** COPASI is a software application for simulation and analysis of biochemical networks and their dynamics. COPASI 4.24 (Build 197) is released. It contains improvements in the Graphical User Interface and in SBML. [Link to the service: https://www.denbi.de/services/373-copasi-creating-and-solving-mathematical-models-of-biological-processes](https://www.denbi.de/services/373-copasi-creating-and-solving-mathematical-models-of-biological-processes)
-  **SeqAN3** - the modern C++ library for sequence analysis. SeqAn3 is major redesign of SeqAn and has fundamental changes throughout the codebase. The new version has been launched in September 2018. [Link to the tool: https://www.denbi.de/services/370-seqan-a-c-library-for-the-analysis-of-sequences](https://www.denbi.de/services/370-seqan-a-c-library-for-the-analysis-of-sequences)
-  **SABIO-RK.** A new paper is published: SABIO-RK: an updated resource for manually curated biochemical reaction kinetics. <https://doi.org/10.1093/nar/gkx1065>
[Link to the database: https://www.denbi.de/services/374-sabio-rk-a-database-for-biochemical-reactions-and-their-kinetic-properties](https://www.denbi.de/services/374-sabio-rk-a-database-for-biochemical-reactions-and-their-kinetic-properties)
-  **BacDive.** A new publication appeared: BacDive in 2019: bacterial phenotypic data for high-throughput biodiversity analysis <https://doi.org/10.1093/nar/gky879>
[Link to the database: https://www.denbi.de/services/347-bacdive-the-bacterial-diversity-metadatabase-focuses-providing-organism-linked-information-covering-the-multifarious-aspects-of-bacterial-biodiversity](https://www.denbi.de/services/347-bacdive-the-bacterial-diversity-metadatabase-focuses-providing-organism-linked-information-covering-the-multifarious-aspects-of-bacterial-biodiversity)
-  **UseGalaxy.eu.** A easy to understand article has been released in German: Selbst ist der Forscher: Big-Data-Analysen leicht gemacht <https://www.laborpraxis.vogel.de/selbst-ist-der-forscher-big-data-analysen-leicht-gemacht-a-768506/>
[Link to service: https://www.denbi.de/services/357-usegalaxy-eu-freiburg-galaxy-server](https://www.denbi.de/services/357-usegalaxy-eu-freiburg-galaxy-server)
-  **SILVA.** A new item has been added: WASABI - SILVA's new spicy feature to inspect your alignments and trees in the SILVA ACT Tool. Click on the WASBI button in the job manager to start the interactive WASABI webapp. [Link to service: https://www.denbi.de/services/343-silva-a-comprehensive-on-line-resource-for-quality-checked-and-aligned-ribosomal-rna-sequence-data](https://www.denbi.de/services/343-silva-a-comprehensive-on-line-resource-for-quality-checked-and-aligned-ribosomal-rna-sequence-data)


THE de.NBI SCIENTIFIC ADVISORY BOARD AND PLENARY MEETING

This year's meeting of the de.NBI Scientific Advisory Board (SAB) will take place on 29 -30 November 2018 at the Seminaris CampusHotel in Berlin. The first day is dedicated to the plenary meeting with a report by the coordinator. The subsequent lectures will feature benefits and visions of selected de.NBI research fields namely human, plant and microbial bioinformatics as well as the superordinate topics service, training and data management. Furthermore, the recent developments in the de.NBI cloud and in workflow engines will be presented. The cooperation with ELIXIR and concepts for a sustainable continuation of the network are considered during the third session. The day will be concluded by a poster session, where all de.NBI projects present their progress since summer 2017.

Deutsches Netzwerk für Bioinformatik-Infrastruktur

3rd SAB Meeting and Plenary Meeting

29-30 November 2018, Berlin



On the second day, the de.NBI Plenary Meeting 2018 takes place. Service center coordinators will report on activities initiated to meet the reviewers' recommendations that were formulated at the midterm evaluation last year. The second session constitutes the ELIXIR-DE plenary meeting featuring the new ELIXIR program 2019-2023 and a discussion of next steps to improve the collaboration with ELIXIR.

Looking forward to meeting the consortium at the end of the month in Berlin!

ATTRACTING THE NEXT GENERATION OF BIOINFORMATICS STUDENTS

by Ivo Große, Steffen Neumann, Uwe Scholz

This year the **BioBYTE** summer school 2018 took place from 16 - 20 July 2018 at the MLU Halle and the de.NBI partners from the Leibniz Institutes IPK and IPB participated in teaching and organization. The target audience were curious pupils who want to discover the natural sciences and bioinformatics of the future. In total, 18 pupils from all over Germany and in their final two years before taking the A-level (Abitur) came to Halle for this all-week summer school.

The week started with the registration and a short introduction of the institutes and the team of the summer school, and Ivo Große motivated the fascination of bioinformatics. The participants were also able to visit the high-performance computer in the MLU computer center, which is used for various tasks in the life sciences data analysis.

The topic of the remaining day was "The World of Molecules - Computer Chemistry". The students built a variety of molecules with a Molecule Building Set, i.e. the toy-like models for bonds and atoms. Only then they switched to the PC pool in order to visualize these molecules on the workstations, and were tasked to find an antibiotic against *Listeria monocytogenes* with protein ligand docking. The students were thrilled that they were able to follow the first steps of drug development themselves. The evening program consisted of a guided tour through the treasure chamber of the Martin Luther University Halle.

Researchers from the German Crop BioGreenformatics Network (GCBN) at Leibniz Institute of Plant Genetics and Crop Plant Research in Gatersleben (IPK) demonstrated the field of bioinformatics in plant research, and the latest possibilities for DNA sequencing. The pupils also got to see the heart of the institute - the federal ex-situ-gene bank. Here, too, huge amounts of data are collected on the genetic diversity of our cultivated plants and their wild relatives. Finally Dr. Astrid Junker presented the topic of digital plant phenotyping. These systems record various parameters without damaging the plants. Sensors and camera systems of different wavelengths provide information on the growth of the plants. These parameters provide new insights into the genotype-phenotype-environment-interaction of cultivated plants.

The de.NBI team from the Center for Integrative Bioinformatics (CIBI) at the Leibniz Institute of Plant Biochemistry (IPB) in Halle introduced metabolomics, the investigation of metabolism. Supervised by biochemists, the students were then able to do practical laboratory work and extract metabolites from various plants, such as tomato, potato, paprika, physalis and bitter-sweet nightshade. The guided tour of the IPB included a visit to one of the mass spectrometers at the institute. They even had to solve a criminal mystery story, and find out whether a sample from a red stain was from blood or ketchup by computational data analysis of the mass spectrometry data.

The week also included introductions to machine learning, sequence assembly and sequence analysis tasks. On the last day, there was the closing event, and two girls won the special BioBYTE Online Quiz, answering all 17 questions correctly. Congratulations to Helene and Nikola!

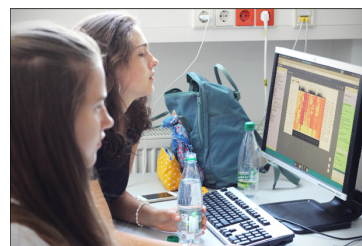
The BioBYTE Summer School provided the spark for enthusiasm for computer science in biology and accompanied the participants over the course days and hopefully beyond. In addition to gaining first insights into the world of bioinformatics, an important goal of the summer school was to inspire and motivate pupils to become interested in bioinformatics and to keep an eye on it, when choosing their profession and studies. The summer school provided a good mixture of "Hands on Science" - getting active oneself to try things out in the group and gain insights into ongoing research. We would like to thank all the participants and the local teams for their efforts, and acknowledge all financial and logistic

supporters of the BioBYTE Summer School from industry and research, including the IPK, IPB and de.NBI.



Figure 1: Research starts in the lab, where the participants extract metabolites from the samples. (Photo: IPB)

Figure 2: The next generation of bioinformaticians then process and analyze the data, to generate or validate biological insights. (Photo: MLU)



Further information at: <https://biobyte.uni-halle.de/>

1ST de.NBI CLOUD USER MEETING

With 47 participants, the first de.NBI Cloud User Meeting took place in a three-day event in Bielefeld, 29-31 October 2018.

In a use case session, early adopters presented their cloud applications. The talks focused on Virus-X, Snakemake, Spark-based bioinformatics tools, Nextflow, eggNOG-mapper and PhenoMeNal. The second and third day featured hands-on sessions for learning new technologies and best practices in the cloud. Workshops dealt with introductions to OpenStack and Nextflow. Service oriented workshops like Kubernetes instructed scientists to work with the cloud but were also useful to science gateway developers to build software which runs the actual cloud projects.

And finally, the attendees had the chance to meet cloud experts and talk to them about their problems and ideas, which provided valuable feedback that will help us to shape the future of the de.NBI Cloud.

Read more about the event at: <https://cloud.denbi.de/1st-de-nbi-cloud-user-meeting>

de.NBI SUMMER SCHOOL 2018 - RIDING THE DATA LIFE CYCLE

The de.NBI Summer School 2018, 2018 took place 03 - 07 September at BRICS in summery Braunschweig. The training event was organized by the Service Centers BioData, GCBN and de.NBI-SysBio. In addition, GFBio – The German Federation of Biological Data – was co-organizer of the summer school.

During the course week, 18 participants were instructed about the importance of proper research data management in general, and a practical toolbox for the acquisition, curation, documentation, archiving and publication of research data following the FAIR (Findable, Accessible, Interoperable and Re-usable) data principles.

The summer school covered different interesting lectures and hands-on sessions by de.NBI speakers and renowned European experts in the field, e.g. Erik Schultes (Leiden University / GO FAIR) and Carole Goble (University of Manchester).

de.NBI will follow up its successful summer school training program with a summer school on Data Science in Gatersleben planned for September 2019.



Read more about the event at: <https://www.denbi.de/training-archive-sorted-according-by-date/122-de-nbi-summer-school-2018-riding-the-data-life-cycle>





de.NBI @ CONFERENCES

Over the past three months the network has been presented at several conferences:

European Conference on Computational Biology 2018




From 8-12 September 2018 the Hellenic Society for Computational Biology and Bioinformatics organized the 17th European Conference on Computational Biology (ECCB) in association with ELIXIR. The ECCB 2018 took place in the historic city of Athens in Greece. It is the main computational biology event in Europe and welcomed scientists working in a variety of disciplines, including bioinformatics, computational biology, biology, medicine, and systems biology. The de.NBI Administration Office presented the training program, the network's activities, the de.NBI cloud and ELIXIR Germany at its poster at the Stavros Niarchos Foundation Cultural Center. Furthermore, de.NBI Partners taught workshops on



-  From an application to a fully integrated workflow – Comprehensive software engineering with SeqAn (by CIBI partners from FU Berlin)
-  Computational Mass Spectrometry with OpenMS – From Algorithms to Integrated Workflows (by CIBI partners from Tübingen University)
-  Modern and scalable tools for efficient analysis of very large metagenomic datasets (by BiGi partners from Bielefeld University and Giessen University)
-  Galaxy workshop (by RBC partners from Freiburg University)

German Conference on Bioinformatics 2018

The de.NBI initiative supported the scientific program of the GCB 2019, 25-28 September in Vienna. The GCB (German Conference on Bioinformatics) is an annual conference devoted to all areas of bioinformatics. For the first time ever, it was held outside of Germany, organized this year by the Austrian Bioinformatics Platform. Two de.NBI keynote lectures were presented by Lincoln Stein (The Pan-Cancer Analysis of Whole Genomes) and Christoph Sensen (Circulating Nucleic Acids as Markers for Chronic and Infectious Diseases). Lincoln Stein is program director, informatics and bio-computing, at the Ontario Institute for Cancer Research, where he is responsible for the management and analysis of large integrative cancer research projects including the International Cancer Genome Consortium. Christoph Sensen is professor at the Institute for Computational Biotechnology at TU Graz and working on the creation of 4D (spatial and temporal) systems for genome annotation and the visualization of genomic knowledge. In addition, de.NBI Partners taught three workshops at the conference:

-  Getting Started with the de.NBI Cloud (by BiGi partners from Bielefeld University and Giessen University)
-  Label-free quantification with OpenMS (by CIBI Partners from Tübingen University)
-  SeqAn3 – a modern C++ library for efficient sequence analysis (by CIBI partners from FU Berlin)

Please note the following date: The GCB 2019 (Precision Medicine - where Bioinformatics & Medical Informatics meet) will take place from September 16-19, 2019 in Heidelberg. Link: <https://gcb2019.de/>


de.NBI@e:Med Meeting 2018, 24-26 September 2018 in Berlin

The de.NBI network and the cloud were presented by Peter Belmann at the e:Med Meeting 2018, 24-26 September 2018 in Berlin. At the booth, he discussed different scenarios and use cases of the cloud with companies and scientists.

Further information at: <https://www.sys-med.de/de/meeting/emed-meeting-2018/>

de.NBI Workshops at upcoming conferences

de.NBI partners will be busy in teaching a variety of workshops or tutorials at conferences until the end of this year:

-  **European Galaxy Days 2018, Freiburg, 19-20 November 2018**
 - RNA-Seq data analysis in Galaxy: lessons learned and what next?
 - Single Cell in Galaxy, from pre-processing to analysis

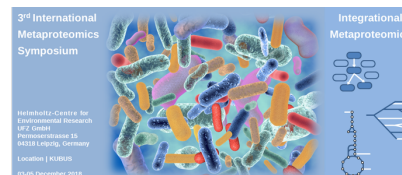
Further information at: <https://www.denbi.de/training/72-european-galaxy-days-2018>





de.NBI supported conferences

de.NBI will support the following conferences co-organized by de.NBI partners:

-  **3rd International Metaproteome Symposium, 03-05 December 2018 in Leipzig.** The conference features the topic “Microbiome Research and Integrating Metaproteomics into a Multi-Omics Pipeline”. This symposium is co-organized by Dirk Benndorf, University Magdeburg, and keynotes are supported by de.NBI. The symposium will be a great opportunity to broaden the discussion on the integration of datasets in different areas of microbial ecology and learn from other people's experience on different systems. [General information and registration at: https://www.ufz.de/index.php?en=44235](https://www.ufz.de/index.php?en=44235)



-  **European Bioconductor Meeting 2018, 06-07 December 2018 in Munich.** Bioconductor is an R package that provides tools for the analysis and comprehension of high-throughput genomic data. The meeting is for biologists, bioinformaticians, statisticians, programmers and software engineers. It aims to foster the exchange of technical expertise while keeping contributors up to speed with the latest developments in Bioconductor. This year's meeting is co-organized by Wolfgang Huber, EMBL Heidelberg and features two key note lectures supported by de.NBI. [General information and registration at: https://bioconductor.github.io/EuroBioc2018/](https://bioconductor.github.io/EuroBioc2018/)

-  **15th Gatersleben Research Conference on Applied Bioinformatics in Crops, 18-20 March 2019 at the Leibniz Institute of Plant Genetics and Crop Plant Research (IPK) in Gatersleben.** This conference will be of interest to Life Scientists, Bioinformaticians, Computer Scientists, Systems Biologists, Synthetic Biologists and others working or interested in the developing area of Applied Bioinformatics for crops. The meeting will provide an excellent environment and a range of opportunities to present and discuss methods, theoretical approaches, and their practical applications. Topics: • Image-Based Data Analyses and Data Visualization, • Distributed Computing, • Tools and Infrastructures, • Systems Biology and Modeling, • Biodiversity and Information Systems, • Breeding Informatics. Two keynote lectures will be invited by de.NBI.


















[General information and registration at: https://meetings.ipk-gatersleben.de/grc2019-abc/](https://meetings.ipk-gatersleben.de/grc2019-abc/)





UPCOMING EVENTS

The calendar lists the de.NBI training courses scheduled in the next months and events. All offers are accessible via the de.NBI web page. A number of training events are in the pipeline but not yet scheduled. Please consult the de.NBI training program for the actual dates.

Overview of upcoming de.NBI events



Date	Event	City	Organizer
 11 Nov 2018	Omics data analysis with R for Beginners – Lipidomicsforum 2018	Dortmund	BioInfra.Prot/LIFS
 11 Nov 2018	Hands-On Workshop on Lipidomics Software & Pipelines – Lipidomicsforum 2018	Dortmund	BioInfra.Prot/LIFS
 13 Nov 2018	Polyomics data integration and analysis	Bielefeld	BiGi
 15 Nov 2018	GTN CoFest on Training Material	online	RBC
 19 Nov 2018	Differential analysis of quantitative proteomics data using R	Bochum	BioInfra.Prot
 19 Nov 2018	Planathon on FAIR Data Management	Kassel	SIG 2, SIG 4, CAU
 19-20 Nov 2018	European Galaxy Days 2018	Freiburg	RBC, ELIXIR
 29-30 Nov 2018	de.NBI SAB Meeting and Plenary Meeting 2018	Berlin	CAU
 03 Dec 2018	4th BioImage Analysis Workshop using ImageJ/Fiji, ilastik and KNIME	Heidelberg	HD-HuB
 03-05 Dec-2018	3rd International Metaproteome Symposium	Leipzig	BiGi and UFZ
 06-07 Dec 2018	European Bioconductor Meeting 2018	Munich	HD-HuB, others
 06-07 Dec-2018	4th Systems Biology Developers Foundry (FAIRDOM/de.NBI)	Frankfurt	de.NBI-Sys-Bio, RBC
 06-07 Dec-2018	Galaxy RNA-seq data analysis workshop	Freiburg	RBC
 06-07 Dec-2018	DNA Methylation: Design to Discovery	Saarbrücken	HD-HuB
 23 Jan 2019	17. CCU Meeting	Gatersleben	CAU, GCBN

Date	Event	City	Organizer
 25 Feb-01 Mar 2019	7th Galaxy workshop on HTS data analysis	Freiburg	RBC
 19 Mar 2019	Tools for Systems biology modeling and data exchange: CO-PASI, CellNetAnalyzer, SABIO-RK, FAIRDOMHub/SEEK	Heidelberg	de.NBI-SysBio
 20-22 Mar 2019	Spring School "Computational Biology Starter"	Gatersleben	GCBN
 09 April 2019	18. CCU Meeting	Heidelberg	CAU, de.NBI-SysBio
 01-06 July 2019	Galaxy Community Conference 2019 (GCC2019)	Freiburg	RBC
 15-19 July 2019	Combine 2019 Conference	Heidelberg	de.NBI-SysBio

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

IMPRESSUM

RESPONSIBLE FOR CONTENTS

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SUBSCRIPTION

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