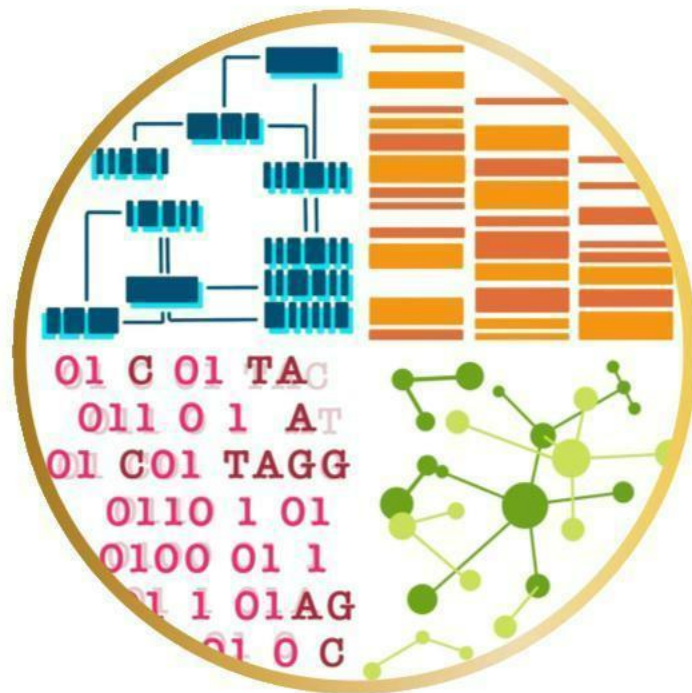


# Spring School

**MARCH 6-10, 2023**



## *From Omics to Systems Biology* **RESEARCH FOR FOOD, NUTRITION & HEALTH**



**DifE**

Funded by



Welcome to our Spring School “From Omics to Systems Biology - Research for Food, Nutrition & Health”.

This is a joint initiative of

- Leibniz Institute of Vegetable and Ornamental Crops (IGZ) e.V.,
- German Institute of Human Nutrition Potsdam-Rehbruecke (DIfE) and
- Leibniz Institute for Food Systems Biology at the Technical University of Munich (LSB).

Our Spring School will provide an insight into approaches, tools and methods in the field of omics technologies, bioinformatics, metabolic pathways and systems biology. In addition, it will also introduce topics of complementary skills including graphical abstract design, research ethics, and data management.

The joint learning experience of participants will also provide you with the opportunity for networking and exchange with young researchers from the participating institutes and with the invited experts.

## *Responsible Organizers*

### **IGZ**

Babette Regierer: [regierer@igzev.de](mailto:regierer@igzev.de)

Marina Korn: [korn@igzev.de](mailto:korn@igzev.de)

### **LSB**

Gisela Olias: [g.olias.leibniz-lsb@tum.de](mailto:g.olias.leibniz-lsb@tum.de)

Karin Sebald: [k.sebald.leibniz-lsb@tum.de](mailto:k.sebald.leibniz-lsb@tum.de)

### **DIfE**

Petra Wiedmer: [petra.wiedmer@dife.de](mailto:petra.wiedmer@dife.de)



### **Important things to bring to the Spring School:**

- A laptop
- Your poster with a graphical abstract of your current research project (as file and printed in A3 format)
- Curiosity and ambition to actively participate

## SCIENCE

Each day is dedicated to a scientific aspect in the spectrum from Omics Research to Systems Biology.

Keynote lectures covering each research aspect will provide an overview of the respective fields, current developments and future perspectives.

These introductions will always be followed by presentations that illustrate how these methods and techniques are applied in the different disciplines investigated in the organizing institutes. You are very much welcome to interact with the speakers and your fellows to discover new approaches for your own research, recognize interdisciplinary links and generate new research ideas.

## COMPLEMENTARY TRAINING

Each day will also introduce a topic relevant for doing research in daily practice, management and career development.

In this complementary training, we will address topics like graphical abstract design, research integrity, and data management. Special attention will be given to visualization of your research contents. We are looking forward already to the posters you will bring to the Spring School that have been prepared based on the principles of graphical abstract design. During the Spring School, you will have the opportunity to present your current field of research in a poster pitch (5 min).

**SPRINGSCHOOL  
FROM OMICS TO SYSTEMS BIOLOGY  
MARCH 6-10, 2023**

**MONDAY**

**06**

MAR

## **Omics**

Complementary: Science Communication

**TUESDAY**

**07**

MAR

## **Bioinformatics**

Complementary: Data Management

**WEDNESDAY**

**08**

MAR

## **Excursion**

DIfE & IGZ

**THURSDAY**

**09**

MAR

## **Network Analyses**

Complementary: Research Ethics

**FRIDAY**

**10**

MAR

## **Systems Biology**

Complementary: Evaluation of the Spring School

**SUN**  
Mar 5

**19:00** **Arrival and evening get-together in Potsdam**  
Restaurant: GenussWerkstatt


**MON**  
Mar 6

**09:00** **Welcome**   
Sabine Kunst (Joachim Herz Foundation)  
Veronika Somoza (LSB, online)

**09:30** **Introduction to Organizing Institutes** 

### **SESSION: OMICS**

**10:00** **How Potatoes Launched a new Era for Biology: the Learnings from Metabolomics for a Comprehensive Approach to Biological Systems (Keynote)**

Richard Trethewey (BASF) 

**11:00** **Break**

**11:30** **Analysis of Mass Spectrometry-based Untargeted Metabolomics Data - Open-source Tools for Programmers and Non-programmers**  
Andreas Dunkel (LSB)

**12:15** **Lipidomics and Cardiometabolic Health: Novel Biomarkers, Intervention Monitoring, and Improved Risk Assessment**  
Fabian Eichelmann (DIfE)

**13:00** **Lunch**

**14:00** **Principles of Proteomics and its Application in Crop Research**  
Katja Witzel (IGZ)

**14:45** **Break**

### **TRAINING: GRAPHICAL ABSTRACTS**

**15:15** **Good Visuals in Science Part II**  
Franziska Schwarz (SciVisto)

**16:00** **Hands-on Work**  
Participants & Franziska Schwarz (SciVisto)

**17:00** **Poster Presentation, Part 1**  
Participants

**18:00** **Get-together**  
DIfE



**~20:00** **End of 1st day**



This session takes place in the **conference center** (includes online talks)

TUE  
Mar 7

## SESSION: BIOINFORMATICS

- 09:00 **Unlocking the Secrets of Life: The Thrilling World of Bioinformatics (Keynote)**  
Erik Bongcam-Rudloff (SLU)
- 10:00 **Exploratory OMICS Data Analysis**  
Dirk Walther (MPI-MP)
- 10:45 **Break**
- 11:15 **Linear Methods Linking Omics Data with Phenotypic Results** Chen Meng (BayBioMS, online) 
- 12:00 **Tools for *in silico* Exploration of Single Cell Transcriptomics**  
Pascal Gottmann (DifE) 
- 12:45 **Lunch**

## TRAINING: DATA MANAGEMENT

- 14:00 **Introduction to Data Management**  
David Ambrosek (DifE)
- 15:00 **Introduction to Hands-on Training**  
Babette Regierer (IGZ) & David Ambrosek (DifE)
- 15:15 **Break**
- 15:45 **Hands-on Work: Compilation of Data Management Plan for own Research**  
Participants, Babette Regierer (IGZ) & David Ambrosek (DifE)
- 16:45 **Poster Presentation, Part 2**  
Participants
- 19:00 **Dinner**  
Restaurant: Peter Pane



This session takes place in the **conference center** (includes online talks)

# PROGRAM

SPRINGSCHOOL  
MARCH 6-10, 2023

**WED**  
Mar 8

**10:00**      **Visit DIfE**

**11:30**      ***Transfer to IGZ (bus)***

**12:00**      **Visit IGZ**

**13:30**      ***Lunch bag***  
***Transfer to Potsdam Main Station (bus)***


**Free Afternoon**

THU  
Mar 9

## **TRAINING: ETHICS, RESEARCH INTEGRITY, OPEN SCIENCE**

- 09:00** **Introduction: Responsible Research & Innovation – A Concept to Embed Research in the Society**  
Babette Regierer (IGZ)
- 09:15** **Research Integrity & Open Science**  
Susanne Hollmann (University of Potsdam)
- 10:15** **Gender & Diversity Dimension in Research**  
Babette Regierer (IGZ)
- 10:30** **Break**
- 11:00** **Poster Presentation, Part 3**  
Participants
- 13:00** **Lunch**

## **SESSION: NETWORK ANALYSES /METABOLIC PATHWAYS**

- 14:00** **Poster Presentation, Part 4**  
Participants
- 14:45** **Bringing Networks to Life in the Life Sciences (Keynote)**  
Baruch Barzel (Bar-Ilan University, online) 
- 15:45** **Break**
- 16:15** **Methodologies for the Construction and Analysis of Large-scale Molecular Interaction Maps**  
Matti Hoch (University of Rostock)
- 17:00** **Metabolic Changes in the Liver during NAFLD Progression**  
Nikolaus Berndt (Charité)
- 17:45** **Repurposing Biochemical Genetics in the -omics Era**  
Alisdair Fernie (MPI-MP)
- 19:00** **Dinner**  
Restaurant: Villa Toscana Rehbrücke



This session takes place in the **conference center** (includes online talks)



FRI  
Mar 10

## **SESSION: SYSTEMS BIOLOGY, MODELLING & MACHINE LEARNING**

- 08:00** **Molecular Modeling in the Era of AI (Keynote)**  
Antonella Di Pizio (LSB) 
- 09:00** **A Network-based Integrative Workflow to Identify and Prioritize Disease Signatures**  
Shailendra Gupta (University of Rostock) 
- 09:45** **Harnessing Machine Learning to Explore Bitterness of Compounds for Pharmacological Opportunities**   
Eitan Margulis (The Hebrew University of Jerusalem, online)
- 10:30** **Break**
- 10:45** **Cross-kingdom Principles how Interactome Networks Orchestrate Genetic Architecture and Infectious Disease Perturbations**   
Pascal Falter-Braun (Helmholtz Centre Munich, online)
- 11:45** **Evaluation of and Reflection on the Spring School**  
with Lunch Snack
- ~13:00** **Concluding Remarks and End of Spring School**



This session takes place in the **conference center** (includes online talks)

## **Richard Trethewey (BASF) – Keynote**

How Potatoes Launched a New Era for Biology: the Learnings from Metabolomics for a Comprehensive Approach to Biological Systems

With the development of the tools for plant genetic manipulation focus turned to the engineering of metabolic pathways to improve crop performance and enable the production of new sustainable products. Early attempts at manipulating metabolic pathways were almost always unsuccessful due to the limited ability to predict complex biochemical systems and the inability to rapidly measure important metabolic characteristics. Overcoming these challenges drove the development of metabolomics as a technology and scientific field. However, as metabolomic information became more widely available it only served to demonstrate that a holistic approach to systems biology is required to advance understanding.

## **Andreas Dunkel (LSB)**

Analysis of Mass Spectrometry-based Untargeted Metabolomics Data – Open-source Tools for Programmers and Non-programmers

Modern high-resolution mass spectrometry in hyphenation with gas or liquid chromatography enables the analysis and characterization of the complex composition of individual metabolites in biological systems. These approaches generate large amounts of complex and high-dimensional data requiring innovative and reproducible data analysis tools to deal with the typical tasks in a metabolomics workflow ranging from raw data processing via metabolite annotation to data analysis using statistics and network analysis. A wide range of open-source software tools providing freely available advanced processing and analysis approaches has been developed by the scientific community either in the form of extension packages for programming and statistics environments such as R or Python, as stand-alone software or as web-based solutions. The lecture will provide an overview of state-of-the-art tools targeting the various steps of the data processing workflow with users having different levels of programming experience in mind.

## **Fabian Eichelmann (DIfE)**

Lipidomics and Cardiometabolic Health: Novel Biomarkers, Intervention Monitoring, and Improved Risk Assessment

Lipidomics provides a comprehensive approach to studying the complex and diverse nature of lipids in biological systems, allowing for a deeper understanding of lipid metabolism and its role in metabolic health. In the context of population health, lipidomics can help identify novel biomarkers for cardiometabolic diseases, monitor the effects of dietary interventions, and improve risk assessment for at-risk individuals. Studying lipidomics is crucial in advancing our understanding of the underlying mechanisms of metabolic disorders and developing targeted therapeutic interventions.

## **Katja Witzel (IGZ)**

Principles of Proteomics and its Application in Crop Research

Proteins perform and control all processes in the cell, from gene regulation to physiology. Molecular activities from transcription to translation to metabolic networks result in the exponential amplification of compounds and capturing the dynamics of proteomes is a central key in understanding functional regulation. The lecture will introduce the principles of proteome research, present strategies for proteome analytical techniques and give examples on the application of proteomics in crop research.

## **Erik Bongcam-Rudloff (Swedish University of Agricultural Sciences) – Keynote**

Unlocking the Secrets of Life: The Thrilling World of Bioinformatics

Bioinformatics is a multidisciplinary research field within the Life Sciences. Analyses of genomic information and data mining of complete genome sequences is dependent on advanced computational tools including bioinformatics programs and databases. Bioinformatics develops tools for the analyses of these big data sets such as complete genome and metagenomics sequences, transcriptomes and epigenomes. Several -omics areas are dependent on deep knowledge in molecular genetics including genomics, transcriptomics and epigenomics. These -omics areas use molecular genetics to produce large amount of data that are then analyzed by bioinformatics tools.

In my talk, I will provide a brief introduction to the field of Bioinformatics, highlighting a few success stories. Additionally, I will discuss the new possibilities that Next Generation Technologies offer for research, as well as the technologies that will revolutionize our daily lives as we know them.

## **Dirk Walther (MPI-Molecular Plant Physiology)**

Exploratory OMICS Data Analysis

In this presentation, the importance of exploratory data analysis will be discussed and relevant approaches to data normalization and visualization will be presented.

## **Chen Meng (BayBioMS)**

Linear Methods Linking Omics Data with Phenotypic Results

This presentation explores computational methods that connect omics data with phenotypic outcomes, specifically the identification of biomarkers for predicting variables like drug sensitivity and clinical outcomes. Extracting relevant biomarkers from high dimensional omics data poses a challenge, leading to the development of various statistical methods. The focus of this talk is about linear regression-based methods, which are explained through intuitive examples to aid the audience's comprehension of the challenges posed by high-dimensional omics data. Solutions to these challenges include using penalties, which are not limited to linear regression, but have also been integrated into commonly used methods such as PCA, PLS, and PLS-DA. The presentation concludes with real-world examples that demonstrate the practical application of these methods in published research.

## **Pascal Gottmann (Dife)**

Tools for *in silico* Exploration of Single Cell Transcriptomics

Single cell RNA sequencing is a emerging technology, but new types of data offer us new opportunities for analysis. Working with a single cell RNA sequencing dataset from islets of Langerhans, I will introduce different methods that go beyond differential expression and demonstrate which new knowledge you might be able to get.

## **Baruch Barzel (Bar-Ilan University) – Keynote**

### Bringing Networks to Life in the Life Sciences

Network science has seen spectacular advances uncovering the underlying maps of social, biological and technological systems. Strikingly, we have discovered an array of recurring structural patterns that bridge these seemingly diverse systems, exposing a universality that crosses domains of inquiry. But can we translate these findings on network *structure* towards understanding, predicting and ultimately influencing their actual *dynamic* behavior? To demonstrate this, we will show how to (mathematically) revive a failed microbial network, bringing it back to life through a set of minimal therapeutic interventions.

## **Matti Hoch (University of Rostock)**

### Methodologies for the Construction and Analysis of Large-scale Molecular Interaction Maps

Diseases are often multifaceted and are triggered by spatial and temporal disturbances in multiple biological processes. Consequently, the involved molecules and cells form large-scale communication networks across multiple tissues. This complexity makes it difficult to identify targets, predict outcomes of drug interventions, and provide personalized treatment options. Computational models can help process information and search for patterns by combining existing knowledge on molecular interactions in biological processes with large-scale experimental or clinical data. In this context, so-called disease maps have been developed as publicly available platforms that integrate state-of-the-art network models into an intuitive interface to enable disease-specific *in silico* simulations and data analyses.

## **Nikolaus Berndt (Charité - Universitätsmedizin Berlin)**

### Metabolic Changes in the Liver during NAFLD Progression

Non-alcoholic fatty liver disease is the hepatic manifestation of metabolic syndrome ranging from steatosis to fibrosis, cirrhosis, and even hepatocellular carcinoma. The liver is a metabolically most active organ, responsible for the synthesis and degradation of carbohydrates, proteins, and lipids. We show how molecular resolved kinetic modeling of central liver metabolism together with proteomics data can be used to evaluate changes in the metabolic capacities of the liver during disease progression and how these changes can be used for the classification of patients and the evaluation of treatment options.

## **Alisdair Fernie (MPI-Molecular Plant Physiology)**

### Repurposing Biochemical Genetics in the -omics Era

Serendipitously, biochemical genetics shares a birth with genetics with both being co-discovered by Mendel, whilst until recently it was synonymous with electrophoretic separation of proteins and the screening thereby of genetic variance. The advantageous widespread adoption of post-genomic tools has however brought us to a golden age for biochemical genetics one that encompasses its component disciplines and much more. I will introduce this providing an example from my own groups research before listing a range of fragmented plant biochemical pathways which has recently been completed using analogous approaches.

# ABSTRACTS – SYSTEMS BIOLOGY, MODELLING & MACHINE LEARNING

SPRING SCHOOL  
MARCH 6–10, 2023

## **Antonella Di Pizio (LSB) – Keynote**

Molecular Modeling in the Era of AI

Advances in artificial intelligence are ushering in a new era in molecular modeling. In my talk, I will introduce molecular design, its use in the biological sciences, and the importance of analyzing molecular interactions from single molecules to cellular contexts. Case studies focusing on the molecular systems of taste and smell will be presented.

## **Shailendra Gupta (University of Rostock)**

A Network-based Integrative Workflow to Identify and Prioritize Disease Signatures

The understanding of underlying mechanisms of multifactorial diseases, including cancer, is complex as it is maintained by various nonlinear feedback and feedforward regulatory components. Using a case study on tumor metastasis, I present an integrative workflow that combines structural analyses of the network, integration of high throughput data, and mechanistic modelling to identify and prioritise diagnostic, prognostic, and therapeutic signatures.

## **Eitan Margulis (The Hebrew University of Jerusalem)**

Harnessing Machine Learning to Explore Bitterness of Compounds for Pharmacological Opportunities

The bitter taste is known for its physiological importance, however, it still presents challenges, especially for the food and pharma industries. We utilize Machine Learning methods to predict bitterness of compounds and their possible biological targets in order to explore their pharmacological opportunities as well as assist in bitterness masking of drugs.

## **Pascal Falter-Braun (Helmholtz Centre Munich)**

Cross-kingdom Principles how Interactome Networks Orchestrate Genetic Architecture and Infectious Disease Perturbations

Biochemical networks mediate the translation of genotypic and environmental information into cellular and organismal phenotypes. The goal of research at the Institute of Network Biology (INET) is to understand the principles and specifics of protein interaction network function, and how perturbations by microbes and genetic variation cause disease phenotypes and modulate disease risk. We pursue a systems biology approach that combines large-scale protein-protein interaction mapping, bioinformatics, and hypothesis-driven experiments to understand plant and human host network function and their modulation by genetics and microbial agents. I will present key technological approaches, and data that cover plant-pathogen network analysis and interactions of both SARS-CoV-2 and commensal bacterial microbes with the human host to illustrate specific insights and emerging common principles.

## **Franziska Schwarz (SciVisto) – Good Visuals in Science Part II**

Talk: In the second part of our workshop, we will review the process of putting together data and images for the creation of our outputs, either it is a presentation, a poster or a graphical abstract. Even social media formats are an option. We will talk about their different appearance and why they function the way they do, if done right. We will get a deeper insight on formatting them to our needs, layout designs and working with colors and contrast.

Hands-on Work: All participants will get a feedback to their own work as well. We will practice with more hands-on examples how to improve given abstracts by the guidelines presented and will compare notes on the keynote given that day and get insights to the process of graphic recording and will challenge everyone's active listening skills.

## **David Ambrosek (DifE) - Research Data Management**

We are going to approach research data management from a practical side. After answering the fundamental questions of who, when, how and why, with particular emphasis on the research data lifecycle, we will delve into some examples. Here you will have the chance to identify their strengths and weaknesses. The last segment you will have an opportunity to develop a plan of your own - perhaps in interactive rounds.

## **Babette Regierer (IGZ) - Ethics, Research Integrity, Open Science**

Responsible Research & Innovation (RRI) represents a new governance and values framework that encourages creativity and opportunities to make science more responsive towards societal needs and global challenges. Key aspects within this framework are research ethics and research integrity, open science, gender equality, public engagement, governance for structural changes and science education for capacity building in RRI.

## **Susanne Hollmann (University of Potsdam) – Research Integrity & Open Science**

The way we perform research should always follow the principles of good research practice. Implementing Open Science principles including transparency and reproducibility along the entire research life cycle is a mechanism to ensure reliable and trustworthy science.

## **Babette Regierer (IGZ) - Research Integrity and Gender & Diversity Dimension in Research**

The concept of Responsible Research & Innovation (RRI) provides guiding principles to ensure that research is ethically appropriate, not harmful for the environment and relevant to the society. Gender & diversity aspects are additional dimensions under the RRI concept and relevant to reflect on the expected outcomes of a research project, their relevance for different groups in the society, e.g. minority or vulnerable groups - and can also become an inspiration for unusual innovative solutions.





**Leibniz Institute of Vegetable and Ornamental Crops (IGZ)**  
The IGZ conducts basic plant research with the aim to advancing the understanding of plants and their interactions with the environment. It strives for excellence in designing sustainable management systems in horticulture and thus operates at the interface between plant biology and environmental sciences with the principles of plant utilization. IGZ has its focus on fundamental aspects of plant health and nutrition in horticulture, plant composition and quality, analysis of plant production systems, and the contribution of plants to food security and human nutrition.



**Leibniz Institute for Food Systems Biology at the Technical University of Munich (LSB)**  
The LSB comprises a new, unique research profile at the interface of Food Chemistry & Biology, Chemosensors & Technology, and Bioinformatics & Machine Learning. As this profile has grown far beyond the previous core discipline of classical Food Chemistry, the Institute spearheads the development of a Food Systems Biology. Its aim is to develop new approaches for the sustainable production of sufficient quantities of food whose biologically active effector molecule profiles are geared to health and nutritional needs, but also to the sensory preferences of consumers. To do so, the Institute explores the complex networks of sensorically relevant effector molecules along the entire food production chain with a focus on making their effects systemically understandable and predictable in the long term.



## German Institute of Human Nutrition Potsdam-Rehbruecke (DifE)

The DifE investigates the causes of nutrition-associated diseases in order to develop new strategies for prevention, treatment and nutritional recommendations. Its research interests include the causes and consequences of the metabolic syndrome, a combination of obesity, hypertension (high blood pressure), insulin resistance and lipid metabolism disorder, the role of nutrition for healthy aging and the biological bases of food choices and dietary behavior.



## Joachim Herz Foundation

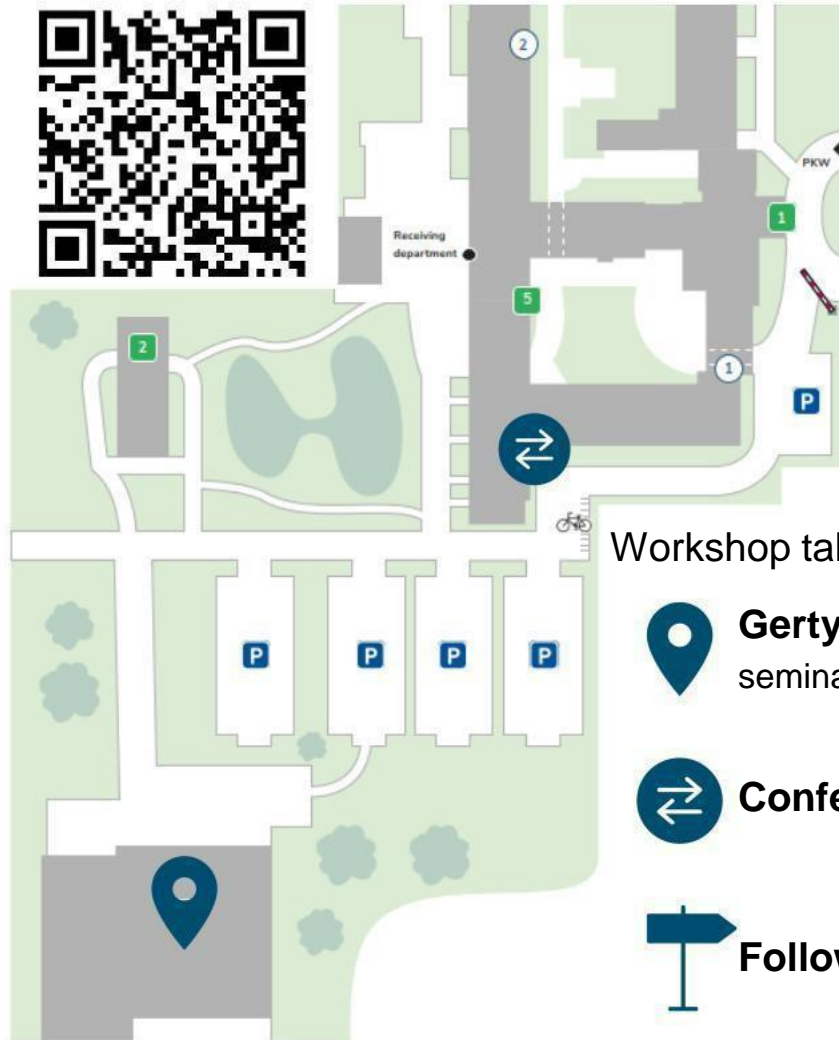
The Joachim Herz Foundation in Hamburg, Germany, promotes education, science, and research in economics and the natural sciences as well as the personal development of teens and young adults. In these areas the foundation also funds small, innovative third-party projects. Additional funding is granted to support research projects in the fields of medicine, law and engineering technology as well as projects promoting the exchange between Germany and the United States. The Joachim Herz Foundation was founded in 2008 after the death of German entrepreneur Joachim Herz. It is one of the largest private foundations in Germany.




## Address for your navigation (DIfE campus E):

Arthur-Scheunert-Allee 114-116

14558 Nuthetal / Germany




Workshop takes place in the


 **Gerty Cory Building (GCH)**  
seminar rooms in the basement


 **Conference Center**

 **Follow the signs**


## RESTAURANTS

 GenussWerkstatt  
Potsdam

 Peter Pane  
Potsdam

 Villa Toscana  
Rehbrücke

## ACCOMODATION

 the nui Amity | City- Hotel  
Potsdam