



BEILSTEIN SYMPOSIUM

# Omics Meets Structure – Deciphering the Glycome



## Beilstein Glyco-Bioinformatics Symposium 2025

July 1-3, 2025  
Dom Hotel Limburg  
Limburg (Lahn), Germany

## Beilstein-Institut and Open Science

The non-profit Beilstein-Institut is one of the most respected organizations in the communication and dissemination of high-quality information in chemistry. Since 1951, when the foundation was established by the Max Planck Society, we have been fulfilling our mission to support the scientific community by providing high-quality information that is essential for research.

Our role has evolved over the years: from the production of the Beilstein Handbook and Database, to being one of the first open access journal publishers in chemistry, to host of interdisciplinary symposia and webinars and supporter of open data initiatives. We believe that free access to scientific research results, giving everyone in the world an equal chance to participate in the exchange of experimental findings and data, is the best way to advance science.

**Open Science** is a new paradigm to scientific research. It is based on cooperation and creates new ways to disseminate information and broaden knowledge through digital technologies and new collaborative tools. It aims to make the primary outputs of publicly funded research results – publications (open access) and the research data (open data) – publicly accessible in digital format with no or minimal restriction.

The Beilstein-Institut supports open science and makes the results of its projects freely available to the scientific community, which is an essential contribution to the foundation's mission to advance the chemical and related sciences. All journal articles, conference proceedings, webinars and videos are open access to allow the worldwide, unhindered sharing and exchange of ideas. This allows scientists, students, educators and the public the opportunity to inform themselves of the latest developments in research and to build on these ideas to further advance scientific knowledge.

Our two diamond open access journals, the *Beilstein Journal of Organic Chemistry* and the *Beilstein Journal of Nanotechnology*, which we fully fund, have no fees for authors or readers. Both journals are produced and managed by the Beilstein Editorial Office team, who work together with a global scientific network of experts that are responsible for the peer review. In 2015, the Beilstein Journals were awarded the DOAJ Seal which recognizes the exceptionally high level of publishing standards and best practices adhering to these journals. In addition, as our journals are Plan S compliant, they meet all technical specifications and policy requirements as outlined by cOAlition S. This means publishing with our journals will ensure compliance with all major funding agency publishing mandates including NIH, NSF, UKRI, ERC, DFG, RCUK, European Commission and Wellcome Trust.

Both journals publish thematic issues on subjects of high contemporary interest; these are often edited by guest editors, further expanding our network and outreach.

Launched in April 2019, a further addition to our publishing platform is the Beilstein Archives. This is the preprint server for the Beilstein journals. During the manuscript submission process, authors have the option to request that the manuscript is posted as a preprint, which is the version of the manuscript before peer review. Our preprints are posted on average within two days, allowing authors to rapidly disseminate their research results and ensuring that they claim priority for their work. Currently, over 25% of our authors select the preprint option.

The Beilstein-Institut runs two data standards projects: STRENDA which is concerned with the reporting of enzymology data and MIRAGE which is working on guidelines for the reporting of glycomics experimental results. Both of which are now widely accepted and acknowledged by the scientific community.

The direct interaction and the exchange of thoughts and ideas between scientists are supported by a program of regularly hosted symposia. These international meetings are organized by the Beilstein-Institut and cover a variety of topics ranging from organic chemistry and biochemistry to nanotechnology and open science as well as interdisciplinary meetings on contemporary topics.

The Beilstein-Institut has been hosting symposia since 1988. Each meeting is always a unique event, and the lively and intense exchange of thoughts and ideas of the participants turn it into a memorable and lasting experience. The number of participants is usually limited to around 50 and the program is designed specifically to allow sufficient time for discussions. The talks also provide a framework and catalyse discussions which often go on into the night and have led to subsequent cooperation projects. The resulting exchange between researchers, at all stages of their careers, is the underlying goal of the meeting and gives the Beilstein Symposium their unique character.

Upcoming events in this year are:

**Beilstein Enzymology Symposium 2025**

*Natural and Synthetic Evolution of Synthesis*

September 9–12, 2025, Rüdesheim, Germany.

Scientific Program:

Pimchai Chaiyen, Tobias Erb and  
Carsten Kettner

[www.enzymology.beilstein-symposia.org](http://www.enzymology.beilstein-symposia.org)

**Beilstein Organic Chemistry Symposium 2025**

*Organic Semiconductor Materials:  
Challenges and Opportunities*

September 23–25, 2025, Frankfurt/Main,  
Germany

Scientific Program:

Stefan Bräse and Jessica Wade

<https://www.beilstein-institut.de/en/symposia/organic-semiconductor-materials-challenges-and-opportunities/>

**6<sup>th</sup> EnzymeML Workshop**

September 29–October 2, 2025, Rüdesheim,  
Germany

Scientific Program:

Jürgen Pleiss, Santiago Schnell and  
Carsten Kettner

<https://www.beilstein-institut.de/en/projects/strenda/meetings/6th-enzymeml-workshop/>

**Beilstein Organic Chemistry Symposium 2025**

*Technologies Shaping Future Directions in  
Synthesis*

October, 14–16, 2025, Limburg, Germany

Scientific Program:

Anna Slater and Luigi Vaccaro

<https://www.beilstein-institut.de/en/symposia/technologies-shaping-future-directions-in-synthesis/>

You will find regularly updated information about our symposia at [www.beilstein-symposia.org](http://www.beilstein-symposia.org).

# **Book of Abstracts**

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## Overview

Over the last decade the fields of glycobiology and glycochemistry in combination with in-silico applications have been augmented by a further field - glycomics. A major aim of glycomics research is to achieve a comprehensive identification and characterization of the repertoire of glycan structures present in an organism, cell or tissue at a defined time. In addition, glycans and glycoconjugates have been increasingly perceived by the proteomics and genomics communities as essential elements in physiological and pathological processes rather than as decorative elements of lipids and proteins.

Glycans are extremely complex and diverse in their structures and thus it has been necessary to develop a wide range of experimental techniques and instrumentation for their detection and analysis. With the advancement of techniques for the interactive and structural analysis of glycoconjugates their essential role in phenomena such as cell adherence, cell-cell interactions, molecular trafficking, biosynthetic quality control, signal transduction and host-pathogen recognition, became apparent. Much efforts have been spent into describing both the structure and binding of glycans and these investigations also resulted in the observation of patterns of glycosylation which change in dependence of the developmental status of the cells. This makes glycosylation patterns an important marker for the detection of diseases and cellular malfunction. However, exciting questions are still unanswered that include the way of “encoding” and control of these diverse patterns and structure-function relationships of the vast variety of glycan structures and patterns. First milestones have been reached towards deciphering the purpose of glycan structures by applying a combination of experimental and bioinformatics tools.

In addition, the continual improvement of analysis methods and computational techniques leads to glycan characterization and identification with increased depth, speed and efficiency but also generates ever increasing amounts of data of variable quality and completeness. In addition, the validation of glycan structure assignments is impeded by a common reporting procedure which does not allow for the comprehensive description of relevant experimental parameters, computational methods and underlying assumptions. This in turn makes the successful annotation of data from the literature as well as mining in databases an uncertain endeavor and furthermore hampers interpretation and reproduction of this data.

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With the support of the community-driven initiative, MIRAGE (Minimum Information Required for a Glycomics Experiment) much effort has been spent into changing the reporting culture and providing software tools for processing, annotating, storing and mining of data. Even though this is a long way to go to gain the acceptance by the community much progress has been made in the establishment of a global infrastructure that integrates the disparate glycan data from diverse sources.

This symposium aims to bring together scientists that “produce” the data with those scientists that “use” the data and make it available to the community. In particular, speakers of the symposia will contribute to unravel the complexity of glycans and deliver insights into the diverse physiological and structural manifestations of sugars by covering aspects such as: carbohydrates in diagnosis and therapy, bridging the gap between analysis and storage of glycan data, structure–function relationships of carbohydrates, carbohydrate–protein interaction and glycoarrays and software tools for analysis and data mining.

Enjoy the Symposium!

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## Scientific Committee

Nicholas M. Riley  
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Barcelona, Spain  
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Carsten Kettner  
Beilstein-Institut  
Frankfurt am Main, Germany  
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## Registration

All participants must be registered to have access to the conference area.

Participants can ask the organizers for a confirmation of the payment of the conference registration fee. Insurance of participants against accidents, sickness, cancellation, theft, property damage or loss is not covered. Participants are advised to take out adequate personal insurance (see also “Liability and Insurance”).

Participants are responsible for settling their hotel bills directly with the hotel on departure. The total price for participants staying at the Dom Hotel Limburg is 942,- EUR and includes both accommodation for four nights and the conference package that covers lunches, dinners and coffee breaks as well as admits access to the conference room.

**Participants not staying at the Dom Hotel Limburg are requested to register with the hotel for booking and paying the conference package, i.e. 438,- EUR per person.**

Extras, such as drinks, telephone calls etc. are not included in the price.

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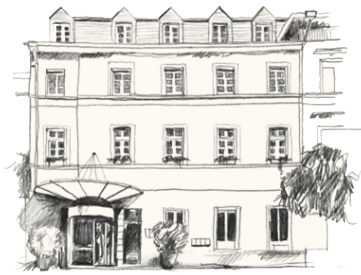
## Conference Venue

Both, the conference and lunches and dinners will take place at the conference hotel, i.e.:

Dom Hotel Limburg  
Grabenstraße 57  
D-65549 Limburg (Lahn)  
Germany

T +49 (0)6431-9010  
F +49 (0)6431-6856

[www.domhotellimburg.de](http://www.domhotellimburg.de)  
[info@domhotellimburg.de](mailto:info@domhotellimburg.de)



The hotel offers wireless internet access free of charge. The hotel accepts MasterCard, Visa and EC-Cash (Maestro-Cards).

## The Symposium

The symposium will be held from July 1 to 3, 2025, with the 30 June and the 4 July for travelling.

The setting and the limited number of participants (max. 60 persons) provide a very convivial atmosphere for the ready exchange of thoughts and ideas.

The scientific program will take place over three days and will

start at 9:00 am on Tuesday, the 1<sup>st</sup>, and

end in the late afternoon (ca. 5:30 pm) on Thursday, the 3<sup>rd</sup>.

If you wish to extend your stay, please contact the hotel directly.

For the **length of the individual talks**, please refer to the program. Speakers should allow sufficient time for discussion at the end of their talks (e.g. a 40 min slot includes 30 min talk + 10 min for questions). We will have an LCD projector connected to a Windows PC available.

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## **Presentations of Posters and Software**

### **Poster Exhibition:**

**Tuesday, Wednesday, and Thursday afternoon, during the coffee breaks**

#### **Location of the posters**

The poster exhibition will be placed close to the conference room. Your poster board will be marked with your poster number which is same in the abstract book.

#### **Poster mounting**

Please mount your poster on Monday, 30<sup>th</sup> from 6:00 pm or on Tuesday, 1<sup>st</sup> at the latest by 8:30 am. Your poster will be on display throughout the symposium.

**You are asked to remove all poster materials from the board after the coffee break on Thursday, 3<sup>rd</sup>** otherwise it will be taken down on time and disposed by the organizers. The organizers cannot take any responsibility for this material.

#### **Poster material**

The size of your poster board is 120 x 90 cm (height x width) and will be marked with your poster number. Hanging material for the poster boards will be provided on-site.

#### **Presentations**

The oral poster presentations will take place as indicated in the scientific program. The presentations should not exceed 3 min.

Please make sure that you have delivered your final presentation to the organizers in time.

We will have an LCD projector (XGA) connected to a Windows PC available.

### **Software Demonstration:**

**Tuesday, July 1, and Thursday, July 3 during the coffee breaks**

#### **Location**

The software demonstration will take place in a separate room (“Roter Salon”) close to the conference room. Each software presenter will have a separate table marked with your software demo number which will remain the same in the abstract book.

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**Material**

Please bring in your own device for the software demo. Please make sure in time that everything is running and login the wireless LAN for internet if necessary.

**Presentations**

The elevator pitch presentations will take place as indicated in the scientific program. The presentations should not exceed 3 min.

Please make sure that you have delivered your final presentation to the organizers in time.

We will have an LCD projector (XGA) connected to a Windows PC available.

**Liability and Insurance**

The Beilstein-Institut will not be liable for any accident, theft or damage to property, nor for any delays or modification in the program due to unforeseen circumstances.

Participants and accompanying persons are advised to arrange personal travel and health insurance.

**Scientific Program****Monday, June 30**

19.00 Welcome reception

19.30 Dinner

## Tuesday, July 1

09:00	Opening and Introductory Remarks	Carsten Kettner
	<i>Session Chair: Marthe T. C. Walvoort</i>	
09:20	How does Nature Make Glycosidic Bonds? Insight into the Catalytic Mechanisms of Glycosyltransferases	Carme Rovira
10:00	Atomistic and Molecular Studies of HS Biosynthesis Enzymes	Liang Wu
10:40	Software Lightning Talks <i>Chaired by René Ranzinger</i>	Presentations #1–5
11:00	<i>Coffee Break and Software Demo</i>	
11:45	Computational Modelling to Probe the Enzyme Organisation Needed for Specific Glycan Processing in the Mammalian Golgi	Dani Ungar
12:25	Structural and Mechanistic Studies of ER-based <i>N</i> -glycosylation Enzyme and Biotechnological Applications	Kaspar Locher
13:05	<i>Lunch</i>	
	<i>Session Chair: Nicholas M. Riley</i>	
14:15	Poster Lightning Talks #1	Poster #1–9
14:45	Protein <i>O</i> -mannosylation: Structure, Function and Disease	Adnan Halim
15:25	The Interplay Between Protein <i>O</i> -mannosylation and <i>N</i> -glycosylation	Sabine Strahl
16:05	Poster Lightning Talks #2	Poster #10–19
16:35	<i>Conference Photo, Coffee Break and Poster Session</i>	
17:05	Lipopolysaccharides: Fantastic “Structures” and where to Find them	Flaviana Di Lorenzo
17:45	Kdo Derivatives to Perturb LPS Biosynthesis	Marthe T. C. Walvoort

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18:25	Functional Diversity in Oligomerization of UDP-glucose Pyrophosphorylases	Jana I. Führung
19:05	<i>Close</i>	
19:30	<i>Dinner</i>	

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**Wednesday, July 2**

*Session Chair: Ben Schumann*

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09:00 *Opening*

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09:05 Seeing is Believing: Tools to Explore your Glycoproteomics Data      Nicholas M. Riley

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09:45 Organizing Glycan Data with Archetypes, Subsumption Relations and Motifs      Kiyoko Aoki-Kinoshita

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10:25 *Coffee Break and Poster Session*

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10:45 A Bunch of Protein-glycan Interactions: The Power of NMR and MD in the Analysis of Molecular Recognition Events      Roberta Marchetti

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11:25 GlyGen: Empowering Research through Active Data Sharing      René Ranzinger

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12:05 Glycan Microarrays: A Rich Data Source for Unravelling the Glycointeractome      Yan Liu

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12:45 *Lunch*

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13:30-  
18:00 *Excursion*

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19:30 *Dinner*

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### Thursday, July 3

09:00	<i>Opening</i>	
	<i>Session Chair: Guinevere S. M. Lageveen-Kammeijer</i>	
09:05	Towards High-throughput Mass Spectrometry Glycomics	Manfred Wuhrer
09:45	Chemical Labelling-assisted Glycoproteomics	Xing Chen
10:25	Systems Glycobiology Reveals new Cancer-promoting Glyco-enzymes in the Tumour Microenvironment	Morten Thaysen-Andersen
11:05	<i>Coffee Break and Software Session</i>	
11:40	Sugar Science: Unlocking Glycosylation in Medicine	Róisín O’Flaherty
12:20	Chemical Precision Tools to Dissect the <i>O</i> -GalNAc-Glycoproteome	Ben Schumann
13:00	<i>Lunch</i>	
	<i>Session Chair: Carme Rovira</i>	
14:00	Adaptation of H2N2 Influenza Viruses to Human Airway Receptors	James C. Paulson
14:40	Development of New Methodology to Identify Proteins Containing Glycans with $\alpha$ -2,8-linked Sialic Acids	Lisa Willis
15:20	New Approach to Study and Modulate Siglecs and their Glycan Ligands	Matthew Macauley
16:00	<i>Coffee Break and Poster session</i>	
16:30	Galectins and Glycoproteins: Regulation of their Molecular Interactions	Ana Ardá Freire
17:10	Conformational Mimicry: A Strategy for Selective Glycosidase Inhibition	Marta Artola
17:50	Microbial Glycosylation: Finding new Antimicrobial Targets and Building New Tools	Nichollas E. Scott
18:30	<i>Closing Remarks</i>	Carsten Kettner



19:30 *Dinner*

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## List of Posters

The poster presentation includes a short (3 min) oral presentation on Tuesday, July 1, and the poster sessions during the coffee breaks as indicated in the program. The posters will be displayed throughout the entire symposium from Tuesday, July 1, to Thursday, July 3.

#1	Exploring <i>O</i> -Glycobiomarker in Osteoarthritis: Lubricin Glycoforms in Plasma and Synovial Fluid.	Niclas G. Karlsson
#2	Integration of GAGomics into Multi-glycomics towards Systems Glycobiology	Marissa L. Maciej-Hulme
#3	Annotating Glycan Functions to Build Connectivity Across Datatypes	Michael Tiemeyer
#4	Identifying Sialyted Glycoproteins in the Kidney: Mapping the Glycosylation Targets of hST3Gal1	Warren W. Wakarchuk
#5	<i>Prevotella copri</i> Lipopolysaccharide: an Integrated Structural and <i>in-silico</i> Analysis	Luca De Simone Carone
#6	Unraveling the Molecular Mechanisms of a New Cellulose Oxidative Cleaving Enzyme	Mariana A. B. Morais
#7	The Mouse N-Glycome Atlas - High-resolution <i>N</i> -glycan Analysis of 23 Mouse Tissues	Johannes Stadlmann
#8	Deciphering the Glycome of Serine Rich Repeat Proteins	Dimitris Latousakis
#9	The Identification and Functional Prediction of Putative Polysaccharide Sulfotransferases	Ravina Mistry
#10	Glycosylation Remodeling Mediates the Degenerative Phenotype of <i>Nucleus pulposus</i> and <i>Annulus fibrosus</i> Cells Under pH and Osmotic Stress	Junqiao Lyu
#11	Computational Approaches for Analysis of Protein-glycosaminoglycan Interactions	Sergey A. Samsonov
#12	Glycoprofiling of Extracellular Vesicles by Lectin-based Methods	Muhammad Umair Khan
#13	A Key Player in Glycogen Metabolism: the Human Glycogen Debranching Enzyme	Christian Roth

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#14	Temporal <i>N</i> -glycoproteomic Differences Between COVID-19 Survivors and Non-Survivors at Hospital Admission and Beyond	Xue Yu
#15	Screening Anti-glycan Antibodies in Serum and Cerebrospinal Fluid Using Glycan Microarrays	Fabienne Weber
#16	Decoding Glycan Signatures: the Impact of Diet and Lifestyle on IgG and C3 <i>N</i> -glycosylation Patterns	Maksym Shmatkov
#17	Mapping Functionally Important Regions in Biotherapeutic Proteins through Combined Use of High-end Analytical Techniques and Molecular Modelling	Garoufallia Stavridou
#18	Effect of GMPPB Deficiency on Neuronal Development	Obinna Umeh
#19	Transforming Residue-Level Deep Learning into Scalable Protein-Level Classification of Carbohydrate Sulfotransferases	Dylan Young

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## List of Software Demonstrations

The software demonstrations includes a short (3 min) oral presentation on Tuesday, July 1, as well as the demo sessions during the coffee breaks as indicated in the program.

#1	I-GPA for Glycoproteomic Search Engines with HCD and CID Tandem MS Data	Heeyoun Hwang
#2	GlycoGenius: the Ultimate High-throughput 1 Glycan Composition Identification Tool	Guinevere S. M. Lageveen-Kammeijer
#3	Labile Annotation Tool	Kristian L. Karlic
#4	Glycomics Workbench: Harnessing the Power of AI for Deciphering the Glycocodes	Arun K. Datta
#5	Bruker GlycoScape - a Real-time, Database-free Glycoproteomic Analysis Tool	Gad Armony
#6	GlyGen and GlyTableMaker	René Ranzinger
#7	GlyCounter	Nicholas M. Riley

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# Abstracts

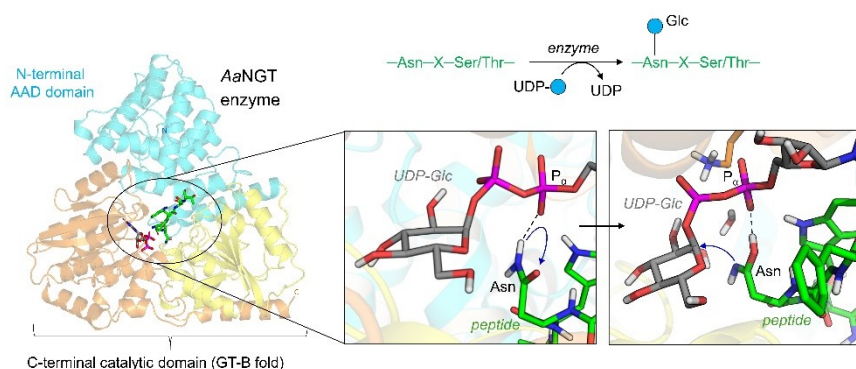
**Tuesday**

## How does Nature Make Glycosylic Bonds? Insight into the Catalytic Mechanisms of Glycosyltransferases

**09:20**
**Carme Rovira**

 Universitat de Barcelona  
 Department of Inorganic and Organic Chemistry  
 Barcelona, Spain

Glycosyltransferases (GTs) are the primary enzymes responsible for synthesizing glycosidic bonds in glycans and glycoconjugates. Over the past decades, extensive research has aimed to elucidate their catalytic mechanisms [1], which in turn supports the rational design of enzyme inhibitors. Most retaining GTs are thought to operate via the ‘front-face’ or  $S_{N1}$ -like mechanism [2], in which the catalytic base is the  $\beta$ -phosphate of the donor nucleotide rather than a protein residue.



In contrast, inverting GTs generally follow a  $S_{N2}$  mechanism involving a protein side chain as the catalytic base [3]. However, recent experimental and computational studies have shown that two inverting GTs involved in protein glycosylation deviate from this canonical mechanism: *O*-fucosyltransferase 1 (POFUT1) [4] and *N*-glycosyltransferase [5]. Remarkably, unlike typical inverting GTs - but akin to their retaining counterparts - these enzymes employ the phosphate groups of the donor nucleotide to promote catalysis.

Our findings, based on state-of-the-art *ab initio* quantum mechanics/molecular mechanics (QM/MM) simulations and informed by recent crystal structures, provide a detailed atomistic view of these noncanonical enzymatic strategies.

### References

- [1] L. L. Lairson et al., *Annu. Rev. Biochem.* **2008**, *77*, 521–555.
- [2] A. Ardèvol, C. Rovira, *J. Am. Chem. Soc.* **2015**, *137*, 7528–7547.
- [3] J. Darby et al. *ACS Catal.* **2020**, *10*, 8590–8596.
- [4] B. Piniello et al. *ACS Catal.* **2021**, *11*, 9926–9932.
- [5] B. Piniello et al. *Nat. Commun.* **2023**, *14*, 5785.
- [6] Y. Liu et al. *J. Am. Chem. Soc.* **2024**, *146*, 39, 26707–26718.

### **Computational codes:**

AMBER (<https://ambermd.org>), CPMD (<https://github.com/CPMD-code>),  
CP2K (<https://www.cp2k.org>), PLUMED (<https://www.plumed.org>)

Tuesday

## Atomistic and Molecular Studies of HS Biosynthesis Enzymes

10:00

Liang Wu

The Rosalind Franklin Institute  
Center for Proteomics and Metabolomics  
Didcot, United Kingdom

Biological carbohydrates are some of the most complex molecules in life, reflecting a sophisticated repertoire of enzymes responsible for generating and modulating their structures. Seminal efforts in glycobiology have resolved structures of many individual carbohydrate processing enzymes, revealing how each catalyzes precise biochemical transformations. Despite this, we still have limited understanding of how many complex oligo/polysaccharides are formed, highlighting an overall lack of knowledge regarding multi-enzyme biosynthesis pathways.

We are interested in the biosynthesis and regulation of the complex polysaccharide heparan sulfate (HS), which is produced by all animal species, and plays vital roles in extracellular processes including cell adhesion, cytokine signalling, and host-pathogen engagement. Mammalian HS biosynthesis is mediated by a host of different enzyme activities within the Golgi (polymerases, sulfotransferases, epimerases etc). Several pathogenic bacteria have also evolved capability to produce HS mimetics, likely aiding their evasion from host immune responses. Because of the biological importance of HS, there is intense interest in understanding the enzymes responsible for its construction, and how they work to generate functional structures.

Here, I present recent mechanistic studies of two HS biosynthesis enzymes:

1 - PmHS2 from *P. multocida*, a dual activity polymerase widely used for the chemoenzymatic production of HS mimetics. We build upon reported structures of PmHS2, generating new substrate and product complexes that provide insight into its bifunctional reaction cycle, including a potentially rare covalent glycosyltransfer mechanism.

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2 - NDST1, a dual activity deacetylase/sulfotransferase enzyme in the human HS biosynthesis pathway. NDST1 shows an unusual back-to-back arrangement of its catalytic domains, imposing strong constraints on functional interplay between its two catalytic domains. Aided by activity modulating nanobodies, we carried out biochemical and biophysical analysis of NDST1 activity, finding that non-catalytic binding likely operates alongside turnover to mediate domain cooperativity.

Collectively, our work provides further insights into the diverse substrate recognition, binding and processing mechanisms employed during enzymatic HS biosynthesis.

**Tuesday**

## **Computational Modelling to Probe the Enzyme Organisation Needed for Specific Glycan Processing in the Mammalian Golgi**

**11:45****Dani Ungar**University of York  
Department of Biology  
York, United Kingdom

The non-templated polymerisation process of *N*-glycosylation results in a highly heterogeneous population of glycan structures. To limit randomness, the glycan processing machinery is dynamically sorted into different Golgi cisternae using vesicle trafficking that is organised by the conserved oligomeric Golgi (COG) complex. However, this organisation cannot stop stochastic enzyme competition, making it difficult to devise precise biosynthetic rules and preventing us from controlling resulting glycan distributions.

We developed a computational model of *N*-glycan biosynthesis that relies on stochastic simulation of the competing enzymatic reactions to generate a heterogeneous computational glycan profile. The composition of the profile is dependent on the used parameters that represent effective enzymatic rates (an amalgamation of intrinsic enzyme activity, enzyme concentration and sugar nucleotide donor concentration) of the participating enzymes in each of the simulated Golgi cisternae. The simulated profile is then fitted to experimentally determined ones using Approximate Bayesian Computation to understand how the parameters and as a consequence enzyme organisation in the Golgi, change between different states of the biosynthetic system.

We present examples of applying the model to problems in both fundamental and applied glycobiology. Questions we can tackle range from the increased presence of Man5 glycans on therapeutic antibodies towards the end of the two-week bioreactor-based production period and the mechanism of site-specific glycosylation on the Fc region of immunoglobulin G (IgG) heavy chains.

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For both questions the glycan biosynthesis model was adapted to the typical glycan profile of IgGs that were produced in either an industrial cell line and setting (for the bioreactor question) or wild type and mutant cell lines in our laboratory.

We observe interesting behaviours for both galactosylation and the Mgat1 catalysed reaction that cannot be described without use of our modelling approach.

**Tuesday**

## **Structural and Mechanistic Studies of ER-based *N*-glycosylation Enzymes and Biotechnological Applications**

**12:25****Kaspar Locher**

Eidgenössische Technische Hochschule (ETH) Zürich  
Institute of Molecular Biology and Biophysics  
Zürich, Switzerland

In eukaryotes, protein *N*-glycosylation begins in the endoplasmic reticulum, where a series of membrane-associated or membrane-integral enzymes (ALG proteins) catalyze the biosynthesis of the dolichylpyrophosphate-linked oligosaccharide  $\text{GlcNAc}_2\text{Man}_9\text{Glc}_3$ . This glycan is recognized by oligosaccharyltransferase (OST) and transferred *en bloc* to acceptor proteins of the secretory pathway.

In the first part of the presentation, I will discuss structural studies of key enzymes of this pathway, for which we single particle cryo-electron microscopy. We combine our structural studies with synthetic approaches and functional investigations to elucidate the mechanism of the involved enzymes. Our results provide insight into how ALG enzymes facilitate the biosynthesis of the lipid-linked oligosaccharide (LLO) that is subsequently transferred by multimeric OST. I will also discuss glycan recognition by OST and inhibition of OST by small-molecule compounds.

In the second part of the presentation, I will discuss our progress in establishing a fully enzymatic pipeline that can assemble ER-based *N*-glycan intermediates and transfer them onto polypeptides, generating homogeneous *N*-glycopeptides. Defined *N*-glycan intermediates ranging from  $\text{GlcNAc}_2$  to  $\text{GlcNAc}_2\text{Man}_9\text{Glc}_3$  could be generated and transferred without the need for chemical synthesis. The transfer is catalyzed using purified oligosaccharyltransferases from protists. Our pipeline allowed us to stoichiometrically attach glycans to polypeptides containing multiple acceptor sequons, generating poly-glycosylated species.

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We tested the useability of our pipeline by generating glycopeptides of virus surface proteins containing high-mannose *N*-glycans, which may have applications in serum testing or for vaccine development. Our pipeline can be combined with glycan extension and modification enzymes to generate a wide range of homogeneous glycopeptides for diagnostic and therapeutic applications.

**Tuesday**

## **Protein *O*-mannosylation: Structure, Function and Disease**

**14:45****Adnan Halim**

University of Copenhagen  
Copenhagen Center for Glycomics (CCG)  
Department of Cellular and Molecular Medicine  
Copenhagen, Denmark

Mammalian *O*-linked mannose (*O*-Man) glycosylation has emerged from being regarded as a remnant of a yeast specific type of *O*-glycosylation to becoming perhaps the most complex type of *O*-glycosylation with three distinct pathways orchestrated by *POMT1/POMT2*, *TMTC1-4* and *TMEM260* gene families in the last few years. Extensive studies into alpha-dystroglycan and the first recognized *O*-Man pathway directed by *POMT1-POMT2* have had major impact on diagnosis and therapy of a large subgroup of muscular dystrophies. With the knowledge of new *O*-Man biosynthetic pathways selectively serving important cell-surface adhesion molecules and receptor proteins, new insight into basic cellular functions and congenital disorders of glycosylation (CDGs) is emerging. During this talk, analytical approaches (glycoengineering and glycorptomics) will be presented to highlight discoveries and structure-function relationships for specific protein substrates and enzymes.

The presentation will also cover recent progress and insight into *O*-Man dysfunction and disease.

Tuesday

## The Interplay Between Protein O-mannosylation and *N*-glycosylation

15:25

**Shahidul Alam, Sina Noor, Marcus Hoffmann, Markus Bartels, Christian Thiel, Erdmann Rapp and Sabine Strahl**

University of Heidelberg  
Centre for Organismal Studies (COS), Glycobiology  
Heidelberg, Germany

Protein *O*-mannosylation is an essential post-translational modification that critically influences glycoprotein function. In this study, we explore how defects in protein *O*-mannosylation—specifically in POMT-deficient cells— affect the maturation and function of integrin  $\beta 1$ . Our findings reveal that loss of POMT activity interconnects with the *N*-glycosylation pathway, resulting in the accumulation of high-mannose and hybrid-type *N*-glycans, accompanied by a marked reduction in complex *N*-glycan structures. This glycosylation imbalance correlates with a significant decrease in mature, cell surface-localized integrin  $\beta 1$ , impairing integrin-mediated adhesion and signaling. Mechanistically, we identify downregulation of the ER-resident mannosidase MAN1B1 in POMT-deficient cells as a contributing factor to defective integrin  $\beta 1$  processing and trafficking.

Importantly, overexpression of MAN1B1 partially restores integrin  $\beta 1$  maturation, underscoring a functional link between *O*-mannosylation and *N*-glycosylation pathways. These results provide new insights into the molecular crosstalk between glycosylation pathways and advance our understanding of the pathogenesis of POMT-related disorders.

**Tuesday**

## **Lipopolysaccharides: Fantastic “Structures” and where to Find them**

**17:05****Flaviana Di Lorenzo**

University of Naples Federic II  
Department of Chemical Sciences  
Naples, Italy

Gut microbiota is an essential actor in the modern concept of human health driving many host physiological and pathological processes, including immune system modulation [1]. Initial sensing of microbes by the host immune surveillance is mediated by the recognition of microbial-associated molecular patterns, such as lipopolysaccharides (LPSs), which are typically conserved among bacteria, i.e. they are shared by both commensal, mutualistic and pathogenic microbes inhabiting our intestines [1]. Due to its chemical structure, LPS is considered a potent elicitor of immune inflammatory reactions in mammals and is usually associated with perilous bacteria and detrimental outcomes for human health [2]. Nevertheless, LPS also decorates the membranes of harmless and beneficial Gram-negative bacteria composing our gut microbiota [2]. How LPS is tolerated and remains (apparently) silent in the gut is a major unsolved question representing a frontier in our understanding of innate immunity.

Deciphering the chemical structure and immunological properties of LPS from gut microbes, especially of those able to establish a neutral or beneficial relationship with the human host, is of paramount importance in biology, with tremendous repercussions for basic and clinical domains of biomedicine. In this frame, a detailed structure to function study focused on LPS from gut microbiota will give insights in the mechanisms at the basis of host-microbe crosstalk, both at the intestinal and systemic level. This will provide, in parallel, priceless information about how gut microbes modulate immune response through their LPSs, thus resulting in an unprecedented improvement of the knowledge of the immune system [1,2].

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Overall, the structural and functional information as well as the chemical tools that can be delivered by analyzing LPS from microbiota will result in advances beyond the state-of-the-art in the biomedical field, as they furnish a starting point (i) to create novel immune-therapeutics and (ii) to identify new biomarkers with diagnostic, prognostic, and/or predictive value in the frame of immune-mediated pathologies.

In this communication, I will show recent results about the chemical structure and immunological properties of LPS from some beneficial gut bacteria that revealed unique and interesting features. I will show the potential of these glycomolecules in the perspective of a future design of novel inflammation-silencing drugs as an alternative therapeutic approach for the treatment of immune inflammatory disorders.

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**Tuesday****17:45**

## **Kdo Derivatives to Perturb LPS Biosynthesis**

**Marthe T. C. Walvoort**University of Groningen  
Stratingh Institute of Chemistry  
Groningen, The Netherlands

All bacterial cells are enveloped in a dense layer of glycan structures, called the glycocalyx, which is important for bacterial cell integrity and cell-cell interactions and communication. Polysaccharides are a major component of this glycocalyx, and their structures are very different between bacterial species, including between pathogenic and probiotic bacteria.

Lipopolysaccharides (LPS) play an important role in the Gram-negative bacterial cell glycocalyx by maintaining cellular integrity and generally function as the first defense layer against environmental stress. 3-Deoxy-D-manno-oct-2-ulosonic acid (Kdo) is a highly conserved monosaccharide that resides in the inner core region of LPS and links the lipid A region to the extending polysaccharide chain through the hydroxyl group on its C-5 position.

In our research, we aim to perturb bacterial LPS biosynthesis by targeting Kdo. We generated chemically synthesized Kdo-analogs, and investigated their efficiency of incorporation using metabolic labeling in different pathogenic *E. coli* strains, with the goal to increase cell-permeability and bacterial susceptibility to antibiotics.

**Tuesday**

## Functional Diversity in Oligomerization of UDP-glucose Pyrophosphorylases

**18:25****Jana I. Führung**

Hannover Medical School  
Institute for Clinical Biochemistry  
Hannover, Germany

The enzyme UDP-glucose pyrophosphorylase (UGP) occupies a central role in carbohydrate metabolism and glycan synthesis in all kingdoms of life by providing UDP-glucose. This nucleotide sugar and its derivatives are not only essential for various vital processes in all eukaryotes, but also prerequisite for the synthesis of many important virulence-associated polysaccharides and glycoconjugates in bacterial, fungal and protozoan pathogens. As such, UGPs represent candidate anti-virulence drug targets. However, given the structural conservation of the enzymes' active site, it is important to identify and target species-specific structural and/or mechanistic features in order to avoid concomitant inhibition of the host UGP.

In studying the structure and function of UGPs from protozoan, bacterial and fungal pathogens as well as their human host, we have found that UGPs exist in various oligomeric states, which are in each case closely linked to the respective enzymatic mechanism. Specifically, our findings reveal that both tetrameric bacterial UGPs as well as octameric human UGP utilize intermolecular contacts, enabled by their particular oligomeric assembly, which stabilize the active site and thus promote enzymatic activity.

These insights not only improve our understanding of the catalytic mechanism of human UGP – an essential enzyme that, however, is also found to be upregulated in various human cancers – but can also facilitate the development of species-specific inhibitors of pathogen UGPs.

**Wednesday****09:05**

## Seeing is Believing: Tools to Explore your Glyproteomics Data

**Nicholas M. Riley**University of Washington  
Department of Chemistry  
Seattle, WA, United States of America

Glycopeptide tandem MS spectra are complex and often challenging to interpret, even with modern search engines that have significantly improved the ability to assign glycopeptide identifications. Here I will discuss several strategies our group is developing to improve our data analysis, including tools called GlyCounter and the Interactive Peptide Spectral Annotator (IPSA). First, GlyCounter is an open-source, freely available tool that extracts oxonium ion information from raw data files to provide a snapshot of glycoproteome content that can be valuable for subsequent method optimization and database searching. Second, our re-factored version of IPSA, which we call IPSA 2.0, addresses difficulties in efficient manual evaluation of glycopeptide tandem mass spectra.

IPSA 2.0 enables users to systematically inspect peptide-specific and glycan-specific fragment ions (such as B and Y), while also accommodating other modifications that might complicate the spectra. By comparing annotated peaks against experimental fragmentation patterns, researchers can quickly spot mismatches where a proposed assignment fails to match observed ions. Users can then modify the glycan composition or reassign the modification site until the ion coverage satisfies the spectral data. This level of fine-grained data curation significantly lowers the likelihood of misassignments that can arise from overlapping precursor masses, incomplete fragmentation, or uncertain modification sites. As I discuss these tools, I will highlight several examples of how they have helped our group refine the methods we use to interrogate the glycoproteome.

**Wednesday****09:45**

## **Organizing Glycan Data with Archetypes, Subsumption Relations and Motifs**

**Kiyoko F. Aoki-Kinoshita**

Soka University  
Glycan and Life Systems Integration Center  
Tokyo, Japan

There are over a quarter million registered entries in the international glycan repository GlyTouCan as of May, 2025, and this number continues to increase. However, not all of the glycans in GlyTouCan are consistent in terms of their ambiguity. As has been published previously, glycans can be registered as monosaccharide compositions or fully-defined glycans where all glycosidic linkage conformations are specified. Moreover, when the reducing end differs, the glycan ID also changes. Thus, when one handles glycans in their research, researchers need to be aware of these issues. In order to ease the accessibility of glycan data in GlyTouCan and GlyCosmos, we have been implementing methods for filtering glycans. Most recently, we have defined “glycan archetypes” as a key concept when handling glycans with differing reducing ends. We are also incorporating subsumption concepts in collaboration with GNOME, and searching/filtering of glycans are facilitated by the use of motifs. The latest developments to implement these concepts in GlyTouCan and GlyCosmos will be presented.

Wednesday

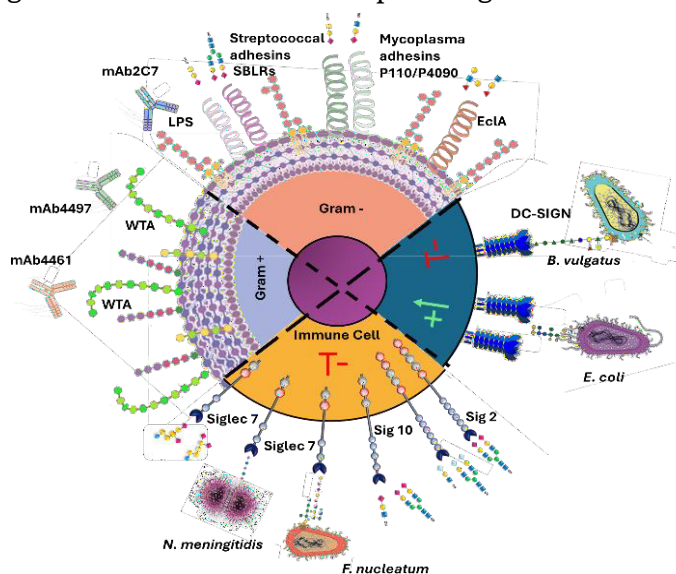
10:45

## A Bunch of Protein–glycan Interactions: The Power of NMR and MD in the Analysis of Molecular Recognition Events

Roberta Marchetti

University of Naples Federico II  
Department of Chemical Sciences  
Naples, Italy

Protein–glycan interactions play pivotal roles in numerous biological processes, ranging from cellular recognition to immune response modulation. Understanding the intricate details of these interactions is crucial for deciphering the molecular mechanisms underlying various physiological and pathological conditions. With the aim to fill this gap, in the last years, our research efforts were directed to the analysis of different systems of protein–glycan interactions by the means of synthetic, spectroscopic, biophysical and computational methods (Figure 1). To address the challenge of modelling complex bacterial glycans, we are currently developing, in collaboration with the group of Prof. Woods, University of Georgia, a GLYCAM-Web user-friendly interface, namely **BACT** (BACTERIAL Carbohydrates Tool), to easily generate 3D models of complex oligosaccharides.



Schematic representation of studied protein–glycan interactions.

By applying this combined and integrated approach, we dissected the molecular basis of the binding between host proteins, including Siglecs [1] and C-type lectins such as DC-SIGN [2], and both endogenous and exogenous glycans. In addition, we unveiled the recognition of complex glycans, typically exposed on host cells' surface, by microbial receptor proteins, such as streptococcal Siglec-like adhesins [3] and mycoplasma cytoadhesins [4].

Finally, we investigated the action of selected monoclonal antibodies against multidrug-resistant strains of *Neisseria gonorrhoeae*[5] and *Staphylococcus aureus* [6].

Overall, our outcomes contributed to the fields of structural glycobiology and molecular recognition studies.

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**Wednesday****11:25**

## **GlyGen: Empowering Research through Active Data Sharing**

**René Ranzinger**University of Georgia  
Complex Carbohydrate Research Center  
Athens, GA, United States of America

Understanding the roles of glycosylation in development and disease is often impeded by the complexity and heterogeneity of relevant biological data. GlyGen is a data integration initiative designed to democratize glycoscience research by providing a comprehensive, user-friendly platform that unifies diverse datasets—including glycan structures, glycosylation enzymes, glycoproteins, and associated genomic and proteomic information. To achieve this integration, GlyGen has established international collaborations with database providers from different domains (including but not limited to EBI, NCBI, PDB, and GlyTouCan) and data producers. Information from these resources and groups are standardized and cross-linked to allow queries across multiple domains. To facilitate easy access to this information, an intuitive, web browser-based interface (<https://glygen.org>) has been developed as well as interfaces for programmatic access using APIs or a SPARQL endpoint.

For each glycan and protein in the dataset, GlyGen provides a details page that displays information from the integrated resources in a concise representation. Individual details pages are interlinked with each other allowing easy data exploration across multiple domains. For example, users can browse from the webpage of a glycosylated protein to the glycan structures that have been described to be attached to this protein, and, from there, to other proteins that carry the same glycan. All information in GlyGen is transparently linked back to their original sources, allowing users to easily access and browse additional information in these resources as well. The GlyGen portal provides multiple different search interfaces for users to find glycans and proteins based on their properties or annotations.

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Beyond the data on glycans and proteins, GlyGen also provides multiple tools for example to study glycosylation pathways, investigate relationships between glycans based on incomplete structures or to map different ID namespace used for glycans or proteins. Additionally, the platform supports data generators by offering mechanisms to publicly share datasets with the broader research community and databases including GlyGen.

Our mission is to provide scientists with an easy way to access complex information that describes the biology of glycans and glycoproteins. To schedule an individual demo of GlyGen or to contribute data to GlyGen contact René Ranzinger ([rene@ccrc.uga.edu](mailto:rene@ccrc.uga.edu)).

**Wednesday****12:05**

## **Glycan Microarrays: a Rich Data Source for Unraveling the Glycointeractome**

**Yan Liu**

Imperial College London  
Glycosciences Laboratory, Department of Metabolism  
London, United Kingdom

The interactions of glycans with their binding partners, governed by an intricate 'glyco-code', influence many of the key biological processes in all living organisms. As prominent host cell surface molecules, glycans mediate cell adhesion and trigger cell signalling, and serve as attachment sites for microbes playing a critical role in colonization and infection. Glycan microarray technologies, first introduced in 2002 by Professor Ten Feizi and colleagues at Imperial College London (ICL), have revolutionized approaches to the molecular dissection of glycan-protein interactions over the past two decades. The data generated through various glycan microarray platforms on diverse glycan-binding proteins, viruses, and microbes continue to bridge the knowledge gap in glycan-mediated interactions within the complex interactome.

Since its establishment in 2012, the ICL Carbohydrate Microarray Facility has become a leading international resource, fostering collaborative research across the biomedical community. In this talk, I will provide an update on the technological advancements of the microarray systems within our Facility and highlight new discoveries from interdisciplinary collaborations that have provided insights into glycan interactions at the host-microbe and immune interfaces. These include intriguing findings related to glycan density, presentation, and assay conditions for microarray readouts, underscoring the importance of considering experimental metadata. In the AI era, discussions are underway to establish a curated glycan array data resource, crucial for predicting glycan-protein interactions and advancing our understanding of the glycointeractome -- a fundamental component in decoding broader biological networks.

**Thursday**

## **Towards High-throughput Mass Spectrometry Glycomics**

**09:05****Manfred Wuhrer**

Leiden University Medical Center  
Center for Proteomics and Metabolomics  
Leiden, The Netherlands

Glycans are implicated in most if not all major human diseases. They modulate cellular interaction, differentiation, pathogen entrance and immune activation. Hence, glycomics is an essential layer for comprehensively studying molecular processes of diseases. This talk will present high-sensitivity, high-throughput mass spectrometry workflows for glycomic and targeted glycoproteomic analysis of large clinical sample collections. The workflows rely in part on robotics for sample preparation, automated measurement, followed by data and curation relying on various spectral and analyte quality parameters processing using in house-developed software solutions.

During the past 10 years we have evolved these workflows and applied them for studying glycomic changes and signatures associated with major metabolic, inflammatory, infections and malignant diseases. This resulted in robust, replicated disease glycomic markers of various diseases including pancreatic cancer and fibrotic fatty liver disease. These glycomic markers can be determined from minute amounts of blood. For a number of diseases the blood glycomics markers have potential for screening of high-risk populations as well as for treatment monitoring.

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Thursday

09:45

## Chemical Labelling-assisted Glycoproteomics

**Xing Chen**<sup>1,2</sup><sup>1</sup>Peking University, College of Chemistry and Molecular Engineering<sup>2</sup>Beijing Normal University, College of Chemistry  
Beijing, China

Protein glycosylation, characterized by its structural complexity, diversity, and high heterogeneity, regulates various biological and physiological processes. Based on the glycosidic bond and glycan structure, the major types of protein glycosylation include *N*-linked glycosylation, mucin-type *O*-linked glycosylation, and *O*-GlcNAcylation. Comprehensive analysis of protein glycosylation is a prerequisite for understanding the biological function of protein glycosylation, but remains challenging. To address this challenge, we take advantage of chemical labeling of glycans with clickable unnatural sugars and develop an effective platform for comprehensive analysis of intact *N*-linked, *O*-linked, and *O*-GlcNAcylated glycopeptides in one sample from cell lysates and tissues. The chemical labeling-assisted glycoproteomics strategy is applied to generate large-scale datasets of protein glycosylation in various tissues of mice, demonstrating its potential in facilitating our understanding of glycobiology.

Thursday

## Systems Glycobiology Reveals new Cancer-promoting Glyco-enzymes in the Tumour Microenvironment

10:25

**Rebecca Kawahara<sup>1,2</sup>, Naaz Bansal<sup>1</sup>, Liisa Kautto<sup>1</sup>, Priya Dipta<sup>1</sup>, The Huong Chau<sup>1</sup>, Benoit Liquet-Weiland<sup>3,4</sup>, Seong Beom Ahn<sup>5</sup>, Kaith Stubbs<sup>6</sup>, and Morten Thaysen-Andersen<sup>1,2</sup>**

<sup>1</sup>Macquarie University, School of Natural Sciences, Sydney, NSW, Australia

<sup>2</sup>Nagoya University, Institute for Glyco-core Research (iGCORE), Aichi, Japan

<sup>3</sup>Macquarie University, School of Mathematical and Physical Sciences, Sydney, NSW, Australia

<sup>4</sup>Université de Pau et Pays d'Adour, Laboratoire de Mathématiques et de leurs Applications de PAU, CNRS, Pau, France

<sup>5</sup>Macquarie University, Medical School, Sydney, NSW, Australia

<sup>6</sup>The University of Western Australia, School of Molecular Sciences, Perth, WA, Australia

New therapeutic targets and non-invasive prognostic markers are needed to improve survival of colorectal cancer (CRC) patients. Towards this goal, we applied integrative systems glycobiology approaches to tumor tissues and PBMCs from CRC patients and matching controls as well as to CRC patient-derived cell lines to accurately map the changes in *N*-glycosylation accompanying CRC. Firstly, quantitative glycomics and glycoproteomics revealed that non-canonical paucimannosidic proteins from monocytic and cancer cell origins are prominent signatures in CRC tumor tissues, and that their expression associates with CRC progression. Guided by these novel relationships, we then showed that *N*-acetyl- $\beta$ -D-hexosaminidase subunit B (HEXB) facilitates paucimannosidic protein biosynthesis in CRC cells and is intimately involved in processes underpinning CRC metastasis (adhesion, migration, invasion, proliferation). Finally, HEXB activity was found to be elevated in PBMCs and plasma from patients with advanced CRC relative to matching controls while plasma HEXB activity correlated strongly with CRC patient survival.

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Our study demonstrates how integrated glycomics and glycoproteomics approaches can unveil new cancer drivers, opening exciting avenues for better prognostication, disease risk stratification and therapeutic interventions in CRC.

**Thursday**

## **Sugar Science: Unlocking Glycosylation in Medicine**

**11:40****Róisín O’Flaherty<sup>1,2,3</sup>**<sup>1</sup>Maynooth University, Department of Chemistry, Maynooth, Ireland<sup>2</sup>Maynooth University, Kathleen Lonsdale Institute for Human Health Research, Maynooth, Ireland<sup>3</sup>University of Galway, CÚRAM, SFI Research Centre for Medical Devices, Galway, Ireland

The human glycome describes the complete repertoire of glycans that are free or covalently linked to lipids, proteins or RNAs in the human body. Glycans control and define fundamental molecular, cellular, tissue, organ and systemic biological processes, direct physiological functions, provide nutrition and are involved in several human diseases, including cancer and autoimmune diseases [1]. Researchers can now routinely assess how the secreted and cell-surface glycomes reflect overall cellular status in health and disease. In fact, changes in glycosylation can modulate inflammatory responses, facilitate implantation and fertilisation, enhance antibody effector functions, or enable viral immune escape. This presentation focuses on the development of novel glycoanalytical technologies that provides crucial information on the alterations of glycosylation that: (a) impacts the safety and clinical efficacy of biotherapeutics [2, 3] (b) shapes the infant gut microbiome [4] and (c) can be exploited as a biomarker for patient stratification and personalized medicine [5, 6]. The presentation is also going to highlight a clinical translation success story for diagnosis and monitoring of Classical Galactosaemia [7]. New insights into the structure and function of the human glycome can now be applied to therapy development and could improve our ability to fine-tune immunological responses and inflammation, optimize the performance of therapeutic antibodies and boost immune responses to autoimmune diseases. These examples illustrate the potential of the emerging field of ‘glycomedicine’.

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**Thursday**

## Chemical Precision Tools to Dissect the *O*-GalNAc-Glycoproteome

**12:20****Benjamin Schumann**Imperial College London  
Francis Crick Institute, Department of Chemistry  
London, United Kingdom

Alterations in glycoprotein expression and composition are an undisputed corollary of cancer development. Consequently, some of the most important tumor biomarkers are heavily glycosylated. Understanding cancer-induced glycoproteome changes is paramount but hampered by experimental limitations. Protein glycosylation is mediated primed by the activities of >200 glycosyltransferases mainly located in the secretory pathway. Since these transferases are interdependent through compensation and competition, traditional methods of molecular cell biology fail to fully address the complexity of glycoprotein biosynthesis. Furthermore, workflows in mass spec-glycoproteome analysis are often restricted to isolated cell lines that do not adequately reflect the interaction between tumor and microenvironment. Thus, we lack strategies to understand 1) the protein substrate specificities of individual glycosyltransferases and 2) which glycoproteins are made by cancer cells in response to their microenvironment. We also 3) miss chemical probes to investigate and disrupt cancer-relevant glycosylation events.

Here, I describe chemical “Precision Tools” to interrogate the details of cellular protein glycosylation. We employ bump-and-hole (BH) engineering to render glycosyltransferases receptive to a chemically modified nucleotide-sugar substrate that carries a bioorthogonal tag and is not used by wildtype transferases. Engineering individual transferases allows differential profiling of their protein substrate specificities. We found that establishing cellular BH systems required an artificial biosynthetic pathway to deliver the corresponding nucleotide-sugar to the secretory pathway. We have also made inroads towards the discovery of inhibitors of important glycosylation enzymes. Thus, chemical Precision Tools allow us to profile protein glycosylation as a key player in cancer biology.

Thursday

## Adaptation of H2N2 Influenza Viruses to Human Airway Receptors

14:00

**James C. Paulson<sup>1</sup>, Chika Kikukchi<sup>1</sup>,  
Aristoteles Antonopoulos<sup>2</sup>, Shengyan Wang<sup>1</sup>,  
Assel Biyasheva<sup>3</sup>, Ankit Bharat<sup>3</sup>, Ryan McBride<sup>1</sup>,  
Anne Dell<sup>2</sup>, Robert Schleimer<sup>3</sup> and Stuart Haslam<sup>2</sup>**

<sup>1</sup>The Scripps Research Institute, Department of Immunology and Microbiology, La Jolla, CA, United States of America

<sup>2</sup>Imperial College, London, United Kingdom

<sup>3</sup>Northwestern Medical School, Chicago, IL, United States of America

Influenza A viruses contain two surface glycoproteins required for infection and transmission: hemagglutinin (HA) and neuraminidase (NA). HA mediates virus attachment to sialic acid-containing glycan receptors on the host cell surface, and NA known as the ‘receptor destroying’ enzyme, releases new viral particles from the cell by removing sialic acids that would *otherwise serve as receptors for the HA*. Human influenza pandemics occur when a new influenza strain from birds or swine acquires the ability to transmit in an immunologically naïve human population, causing severe disease worldwide.

Once in the human population, the virus mutates to evade the human immune response while maintaining its ability to transmit and infect. It is well documented that the HA of human influenza viruses bind to receptors with sialic acids linked  $\alpha$ 2-6 to galactose (human-type receptors), while the HA of avian viruses binds to receptors with sialic acids linked  $\alpha$ 2-3 to galactose (avian-type receptors). The longest circulating human influenza strain is the H3N2 virus, which entered the human population from an avian virus in the pandemic of 1968, and acquired the human-type receptor specificity needed for transmission in the human population. In recent years, the H3NA virus has evolved a strong preference for sialylated glycans with poly-LacNAc repeats or “extended glycans.” To better understand this change in receptor specificity in the context of natural receptors, we have analyzed the glycome of human airway epithelial cells.

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We have found that such extended receptors are indeed present and are more prominent in the trachea than in nasal epithelial cells. Using a synthetic glycan library representing the diversity of *N*-glycans in the airway glycome, we find that the extended glycan chains with at least 3 Gal $\beta$ 1-4GlcNAc repeats are required for binding the HA of recent H3N2 viruses. Surprisingly, this restricted receptor specificity causes the HA to preferentially bind to ciliated epithelial cells in contrast to HA from earlier strains, suggesting a shift in tropism to ciliated epithelial cells.

(Funded in part by NIH grant R01AI114730, and CEIRR contract 75N93021C00015).

Thursday

## Development of New Methodologies to Identify Proteins Containing Glycans with $\alpha$ -2,8-linked Sialic Acids

14:40

**Lisa Willis**

University of Alberta  
Department of Medical Microbiology and Immunology  
Edmonton, AB, Canada

Sialic acids (Sias) are critical contributors to human health and disease. However, the majority of research focused on the structure and biology of sialylated glycans has been limited to those containing  $\alpha$ 2,3- and  $\alpha$ 2,6-linked Sias (e.g. monoSia). Far less attention has been given to the  $\alpha$ 2,8-linked Sias, which form linear homopolymers that can be short (oligoSia) or long (polySia). This lack of insight into the biology of oligoSia and polySia stems from the fact that they are less abundant than monoSias and are also more labile, both of which makes them more challenging to study with conventional glyco-analytical tools. To address these issues, we have developed new methodology to study both short and long  $\alpha$ 2,8-linked Sias. We applied our new methodology to several components of human blood and identified dozens of new proteins. This work highlights the extensive distribution of  $\alpha$ 2,8-linked Sias and provides a starting place from which we can elucidate their biology.

Thursday

## New Approach to Study and Modulate Siglecs and their Glycan Ligands

15:20

**Matthew Macauley**University of Alberta  
Department of Chemistry  
Edmonton, AL, Canada

Siglecs are sialic acid-binding Immunoglobulin-type lectins that are expressed on the surface of immune cells and couple sialoglycan-ligand recognition to modulating immune cell signaling. Siglecs function through high multivalency on the cell surface, which enables them to leverage avidity. This can mean that studying Siglec-ligand interactions outside of their native context can be challenging. To solve this challenge, we developed new tools to study Siglecs (Rodrigues *et al.*, *Nat Comm*, 2020). These tools have been invaluable for us to uncover new critical interactions with sulfated carbohydrates (Jung *et al.*, *ACS Chem Bio*, 2021; Jung *et al.*, *ACS Chem Bio*, 2024). More recently, we have been profiling Siglec ligands on cancer cells at an unprecedented scale. Ongoing efforts are attempting to use bioinformatics methods to compare these ligands to RNAseq and proteomics datasets to elucidate what genes/proteins are required to be expressed to create ligands for individual Siglecs.

Recently, we have unveiled a second-generation platform wherein Siglec proteins are displayed on liposomes to mimic the high multivalency that Siglecs take on within their native environment (bioRxiv 2025.06.10.658684). Specifically, we engrafted a SpyTag onto a soluble Siglec and developed a method to site-specifically modify SpyCatcher with lipid. This enabled the creation of SpyCatcher on liposomes at a defined density and assembly of Siglec-liposomes. The modular assembly of Siglec-liposomes makes their multivalency tunable, enabling multiplexing of different Siglecs on the same liposome or on different liposomes with different fluorophores. Using Siglec-liposomes, we profiled Siglec ligands on many cell types, which reveals new insights into Siglec ligands. Importantly, Siglec-liposomes are compatible with *in vivo* studies, and we find that Siglec-7-liposomes bind to the brain vasculature in a mucin-dependent manner.

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Moreover, we find that Siglec-liposomes modulate T cell function, increasing T cell proliferation in a ST3Gal1-dependent and CD43-independent manner. Ongoing efforts to advance a better understanding of Siglecs ligands with our new Siglec biochemical tools will be discussed.

Thursday

## Galectins and Glycoproteins: Regulation of their Molecular Interactions

16:30

**Ana Freire Ardá**

CIC bioGUNE  
Department of Molecular Recognition & Host-pathogen Interactions  
Derio, Spain

Through recognition of specific glycoconjugates on the cell surface and in the extracellular matrix, Galectins, a family of evolutionarily conserved glycan-binding proteins, regulate a myriad of biological processes, many of which are associated with immune homeostasis. Their interaction with specific immune checkpoint regulators, such as TIM-3 or VISTA, has been shown to play a prominent role in pathological conditions, including cancer and autoimmunity.

Although these molecular recognition processes are known to be glycan mediated, the elements at the structural and molecular level that regulate them are not well understood.

Herein, by combining Nuclear Magnetic Resonance with other biophysical techniques and *in-silico* and biochemical approaches, we try to shed light into the different molecular mechanisms that Galectins use to interact with specific glycans and glycoproteins.

Thursday

## Harnessing Computational Approaches for the Rational Design of Conformationally Locked Glycosidase Inhibitors, Probes and Degraders

17.10

**Marta Artola**

Leiden University  
Department of Medical Biochemistry  
Leiden, The Netherlands

Glycosyl hydrolases (GHs), which catalyse the cleavage of glycosidic bonds in complex carbohydrates, operate through enzyme-specific conformational itineraries during catalysis. Understanding and accurately mimicking these conformational transitions is crucial for the rational development of selective inhibitors and chemical probes. Computational methods, particularly *ab initio* metadynamics, which provide detailed conformational free energy landscapes (FELs), have proven instrumental in mapping these dynamic catalytic pathways and guiding the design of structurally preorganised, mechanism-informed ligands.

For instance, covalent nanomolar inhibitors targeting  $\alpha$ -glucosidases have been designed using 1,6-*cis*-cyclic sulfate electrophiles, which emulate the  ${}^4C_1$  conformation of the initial Michaelis complex [1]. Similarly, introducing a nitrogen atom at the pseudo-anomeric position has enabled 1,6-*cis*-cyclic sulfamidates to act as selective competitive inhibitors for  $\alpha$ -galactosidases [2] and  $\alpha$ -glucosidases [3], depending on the specific configuration. Expanding on this approach, we recently synthesized 1,6-*trans*-cyclic sulfates and sulfamidates that adopt a flipped  ${}^1C_4$  chair conformation. Given the unique  ${}^3S_1$  (Michaelis complex)  $\rightarrow$   ${}^3H_4$  (transition state)  $\rightarrow$   ${}^1C_4$  (product) conformational pathway of inverting GH47- $\alpha$ -mannosidases, a mannose-configured 1,6-*trans*-cyclic sulfamidate specifically targets GH47- $\alpha$ -mannosidases by mimicking their  ${}^1C_4$  product conformation. This strategy has enabled the development of selective inhibitors for GH47- $\alpha$ -mannosidases through a “bump-and-hole” design approach [4].

In addition, we have shown that  $\beta$ -D-arabinofuranosyl cyclitol aziridines adopt a  ${}^3E$  conformation in the active site, which resembles the  ${}^1S_3$  initial Michaelis complex conformation, leading to the development of selective GBA2 activity-based probes, inhibitors, and potential covalent proteolysis targeting chimeras [5].

This presentation will highlight how molecular dynamics simulations, conformational mapping, and mechanism-based modelling have been integrated with chemical biology to enable the design of conformationally locked GH modulators. These tools are advancing both our fundamental understanding and our ability to develop therapeutic strategies for carbohydrate-processing disorders.

### References

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Thursday

## Understanding Microbial Glycosylation to Identify new Antimicrobial Targets

17.50

**Nichollas E. Scott**

University of Melbourne,  
Department of Microbiology and Immunology  
Melbourne, VIC, Australia

Protein glycosylation is an important but poorly understood aspect of microbial physiology. Over the last decade, significant strides have been made in characterizing bacterial glycosylation, with mass spectrometry (MS) emerging as an indispensable tool. While early studies focused on confirming the presence of glycosylation by repurposing eukaryotic glycoproteomic techniques, the unique characteristics of microbial glycosylation necessitate the development of fit-for-purpose microbial glycoproteomic approaches.

Focusing on bacterial *O*-linked glycosylation systems, our work seeks to improve our understanding of the substrates and functions of microbial glycosylation to enhance human health. By leveraging MS and enrichment tools in conjunction with bioinformatics undertaken within Msfragger [1], including the use of “open searching [2]” to identify unique glycan/carbohydrates, as well as the incorporation of bacterial-specific carbohydrate associated ions to improve peptide scoring, we have found that even highly diverse glycosylation systems are now tractable with glycoproteomics.

We demonstrate how these informatic tools can be used to assess and validate the creation of a new set of monoclonal antibodies to the bacterial-specific nonulosonic acid sugar Pseudaminic acid. Using this tool, we demonstrate that the *O*-linked glycosylation systems of *Campylobacter jejuni* and *Helicobacter pylori* extend beyond the previously reported Flagellin substrates, confirming multiple novel *O*-linked glycoproteins exist within these systems. Extending the application of this antibody to multi-drug-resistant bacteria such as *Acinetobacter baumannii*, we excitingly show these affinity tools not only allow glycoproteomic analysis but also provide new ways to track alterations in glycan structures between bacterial species and block lethal animal infections.

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Collectively, this work demonstrates that by expanding the microbial glycoproteomics toolkit, new insights into *O*-linked glycan biosynthesis pathways can be gained and that microbial glycosylation systems may be ideal targets for developing antimicrobial therapies.

### References

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# Poster Abstracts

**Tuesday****Poster  
#1**

## **Exploring O-Glycobiomarker in Osteoarthritis: Lubricin Glycoforms in Plasma and Synovial Fluid**

**Niclas G. Karlsson<sup>1</sup>, Ali Reza Afshari<sup>1</sup>, Vincent Chang<sup>2</sup>,  
Kristina A. Thomsson<sup>3</sup>, Jennifer Höglund<sup>3</sup>, Ellie Browne<sup>2</sup>,  
George Karadzhov<sup>2</sup>, Keira E. Mahoney<sup>2</sup>, Taryn M. Lucas<sup>2</sup>,  
Henrik Ryberg<sup>4</sup>, Kamlesh Gidwani<sup>5</sup>, Kim Petterson<sup>5</sup>,  
Ola Rolfson<sup>3</sup>, Lena I. Björkman<sup>3</sup>, Thomas Eisler<sup>6</sup>,  
Tannin A. Schmidt<sup>7</sup>, Gregory D. Jay<sup>8</sup> and Stacy A. Malaker<sup>2</sup>**

<sup>1</sup>Oslo Metropolitan University, Oslo, Norway

<sup>2</sup>Yale University, New Haven, CT, USA

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<sup>5</sup>University of Turku, Turku, Finland

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<sup>7</sup>University of Connecticut Health Centre, Farmington, CT, USA

<sup>8</sup>Brown University, Providence, RI, USA

Lubricin is a mucin-domain glycoprotein that is crucial for joint lubrication and synovial homeostasis. Given that arthropathies such as osteoarthritis (OA) and rheumatoid arthritis (RA) are concomitant with altered lubricin glycosylation in synovial fluid (SF), we investigated if glycoforms of lubricin also could be detected in OA patients' plasma, reflecting the health status of the OA joint.

We used a combined glycomic/glycoproteomic approach to characterize the glycosylation of lubricin in synovial fluid and plasma. An improved mucin-selective enrichment strategy which employs a catalytically inactive mucinase (StcE) conjugated to solid support allowed us to obtain glycoform specific glycoproteomic data from the low abundant lubricin present in OA patients plasma (<10 mg/ml). The combined glycomic and glycoproteomic data allowed us to design a sensitive lectin assay to screen for differences in plasma lubricin glycoforms from a biobank of late stage OA patients and controls (224 individuals).

Our data suggest that glycosylation of lubricin is different comparing SF with plasma. Moreover, the glycosylation of plasma lubricin is altered in OA patients compared to controls.

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We were also able to attribute the difference in SF and plasma lubricin glycosylation to the presence SF and plasma specific lubricin splice variants. Future efforts are being directed towards quantification of the glycosylation of the various splice forms present in plasma.

**Tuesday**

## **Integration of GAGomics into Multi-glycomics Towards Systems Glycobiology**

**Poster****#2****Marissa L. Maciej-Hulme and Niclas G. Karlsson**

Oslo Metropolitan University, Department of Pharmacy, Oslo, Norway

Sulphated glycosaminoglycans (GAGs) are a group of heterogenous linear, sulfated polysaccharides that play a role in many diseases including cancer, cardiovascular, and kidney diseases. The structural variety of GAGs has greatly challenged the development and utility of GAG analytics, particularly for native structures, leaving a significant gap in GAG technologies for clinical application. Mass spectrometry (MS)-based profiling with glycoinformatics offers a top-down approach that can retain variety in large data sets, providing an exploratory approach to clinical samples. Previously we have developed single GAGomics of sulphated oligosaccharides using human plasma, which retains the structural complexity of each individual GAG chain and generates a GAG ‘index’ (or GAG-ome) for each patient. Now our aim is to integrate GAGomics with other glycomics by developing a sequential purification workflow that enables multi-faceted analysis of GAG oligosaccharides, proteoglycan glycoproteomics, *N*-glycomics and *O*-glycomics from a single sample, followed by tailored glycoinformatics. Fractionation of glycans using this sequential preparative approach will enrich current multi-glycomics profiling of heterogenous samples or samples with limited material, whilst retaining biologically relevant GAG data for connection with other analyses. Finally, the creation of GAG-friendly, tailored glycoinformatics pipelines will enable: 1) integration of the additional class of glycans with existing frameworks, 2) data interrogation resulting in better exploration of glycosylation changes in biological data and 3) identify future challenges for the GAGomics field in the systems glycobiology space.

### References

Maciej-Hulme, ML. Kim, J, Roberts ET, *et al. BioRxiv. 2024*, DOI: 10.1101/2024.09.18.613784

**Tuesday****Poster  
#3**

## **Annotating Glycan Functions to Build Connectivity across Datatypes**

**René Ranzinger<sup>1</sup>, Raja Mazumder<sup>2</sup>, D. Natale<sup>3</sup>, K. Ross<sup>3</sup> and Michael Tiemeyer<sup>1</sup>**

<sup>1</sup>University of Georgia, Athens, GA, USA

<sup>2</sup>George Washington University, Washington DC, USA

<sup>3</sup>Georgetown University, Washington DC, USA

Dynamic changes in protein and lipid glycosylation impact protein homeostasis, membrane functions, development, inflammation, immunity, aging, neural function, pathogen interactions, and almost all aspects of human health from fertilization to death. However, current bioinformatic resources that capture disease and phenotype information focus primarily on the macromolecules represented within the central dogma of molecular biology (DNA, RNA, proteins). To gain a more complete understanding of human disease, there is a need to capture the functional impact of glycans and glycosylation on biological processes. Ideally, an ontology that would describe glycan functions could also connect with existing gene, protein, disease, and phenotype/function ontologies to explore mechanistic insights using terms and relationships that reflect the relative contributions made by different molecular entities. This presentation will explore the resources already available within the bioinformatic community for representing glycan functions, describe ab initio attempts to develop hierarchical descriptions of glycan functions, and demonstrate the adaptation of causal activity models for capturing glycan functions in important contexts. Several well-known examples of glycan functions will be used to demonstrate the promise and limitation of current models.

Tuesday

Poster  
#4

## Identifying Sialyted Glycoproteins in the Kidney: Mapping the Glycosylation Targets of hST3Gal1

Daryl Siapuatco<sup>1</sup>, Nicole Thompson<sup>1</sup>, Matthieu Lemaire<sup>2</sup>  
and Warren W. Wakarchuk<sup>1</sup>

University of Alberta, Edmonton, AB, Canada  
SickKids Research Institute, Toronto, ON, Canada

The human kidney is a complex organ which is very sensitive to damage from various diseases. It is also a tissue which carries a large number of proteins that have glycans terminated in sialic acid. When enzymes from pathogens like *Streptococcus* strip off the sialic acid, kidney function is compromised. However, we don't know which proteins are the ones impaired after the infection. Humans have 20 different sialyltransferases which add sialic acid to various cellular glycoconjugates and are specific for certain classes of receptor molecules. This work aims to map the glycosylation targets of one of these human sialyltransferases (hST3Gal1). Using a HUVEC cell line in which hST3Gal1 has been inactivated through CRISPR technology, the whole cell fractions of these cells will be treated with recombinant ST3Gal1 and a sialic acid donor conjugated to a biotin reporter molecule. Once the glycosylation targets have been labelled with the biotin conjugate, they will be enriched using streptavidin resin and identified through proteomics. This will provide glycoprotein targets for follow up research to determine which biological pathways are affected by the lack of terminal sialylation and how it results in loss of proper kidney function.

Tuesday

Poster  
#5

## ***Prevotella copri* Lipopolysaccharide: an Integrated Structural and *in-silico* Analysis**

**Luca De Simone Carone<sup>1,2</sup>, Roberta Cirella<sup>2</sup>,  
Francesca Olmeo<sup>2</sup>, Emanuela Andretta<sup>2</sup>,  
Valentina Mazziotti<sup>2</sup>, Marcello Mercogliano<sup>2</sup>,  
Antonio Molinaro<sup>2,3,4</sup> and Flaviana Di Lorenzo<sup>2,3,4</sup>**

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<sup>1</sup>Department of Biology

<sup>2</sup>Department of Chemical Sciences

<sup>3</sup>Task Force on Microbiome Studies

<sup>4</sup>CEINGE-Biotechnology Avanzate Franco Salvatore, Naples, Italy

The human gut microbiota plays a crucial role in maintaining host health through complex interactions involving digestion, metabolism, immunity, and disease resistance. Among the diverse bacterial taxa inhabiting the gut, the genus *Prevotella* has gained significant attention due to its variable roles in human health and disease. *P. copri*, a dominant species within this genus, has been linked to beneficial outcomes such as improved insulin sensitivity and reduced allergic responses. However, it has also been implicated in inflammatory conditions, underscoring its dual and ambiguous role [1]. Central to the interaction between Gram-negative bacteria like *Prevotella* and their host is the lipopolysaccharide (LPS), a glycolipid of the outer membrane, significantly influencing host immune responses [2,3].

Deciphering the precise structure of LPS from gut microbiota species like *P. copri* is essential to understand why certain bacteria exhibit this dual role in health and disease. Up to date, little is known about *P. copri* LPS composition and its function in host interactions. In this sense, we employed NMR and mass spectrometry techniques to investigate the full structure of the *P. copri* DSM 18205 LPS, discovering that it produces a lipooligosaccharide (LOS), i.e., an LPS devoid of the polysaccharide portion, with an unprecedented chemical structure. Furthermore, a bioinformatics approach was utilized to identify the operons in *P. copri* DSM 18205 genome. Gene functions were predicted through an integrative approach involving multiple bioinformatics tools.

Moreover, we constructed a functional protein association network for LPS biosynthesis using STRING, based on Gene Ontology (GO) terms. Overall, we were able to identify multiple regions encoding genes necessary for the biosynthesis of *P. copri* DSM 18205 LOS. Our findings provide a foundation for future research aimed at unravelling the complex interplay between this bacterium, its LOS and host health outcomes.

## References

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Tuesday

Poster  
#6

## Unraveling the Molecular Mechanisms of a new Cellulose Oxidative Cleaving Enzyme

**Mariana A.B. Morais<sup>1</sup>, Clelton A. Dos Santos<sup>1</sup>,  
Fernanda Mandelli<sup>1</sup>, Renan Y. Miyamoto<sup>1</sup>,  
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Douglas A.A. Paixão<sup>1</sup>, Joaquim M. Junior<sup>1</sup>,  
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Felippe M. Colombari<sup>1</sup>, Gustavo H. Gimenis<sup>1</sup>,  
Camila R. Santos<sup>1</sup>, Nicolas Terrapon<sup>3</sup>, Vincent Lombard<sup>3</sup>,  
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Cellulose is the most abundant plant polysaccharide and an essential biopolymer for the production of biorenewables, including biofuels and biochemicals. Due to its intrinsic recalcitrance, microbial communities have developed sophisticated molecular strategies to tackle cellulose depolymerization. Herein, we have investigated the microbial communities and their associated enzymatic systems for the breakdown and utilization of sugarcane-derived polysaccharides, employing metagenomic analysis of soil samples that have been covered with sugarcane bagasse for over 20 years. Among the recovered arsenal of carbohydrate-active enzymes (CAZymes), we identified a novel class of metalloenzymes capable of cellulose deconstruction through an unprecedented structural scaffold for oxidative carbohydrate cleavage.

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By combining X-ray crystallography and *in silico* modeling, we revealed that the enzyme, named CelOCE (Santos et al., 2025), features a copper-based catalytic center and a flat exposed surface that enables cellulose binding and promotes its oxidative cleavage, in agreement with the experimental results. These findings expand the current microbial enzymatic model for cellulose breakdown, offering new insights that may contribute to address global challenges in energy transition and to the development of a bio-based economy.

### Reference

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Acknowledgements: National Laboratory for Scientific Computing (LNCC/MCTI); São Paulo Research Foundation (FAPESP)

Tuesday

## The Mouse N-Glycome Atlas – High-resolution N-glycan Analysis of 23 Mouse Tissues

Poster  
#7

Johannes Helm<sup>1</sup>, Stefan Mereiter<sup>2</sup>, Tiago Oliveira<sup>2</sup>,  
Friedrich Altmann<sup>1</sup> and Johannes Stadlmann<sup>2</sup>

<sup>1</sup>University of Natural Resources and Life Sciences, Vienna, Austria

<sup>2</sup>Institute of Molecular Biotechnology of the Austrian Academy of  
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Over 50% of all human proteins are post-translationally modified by glycans, which alter their functions in fundamental biological processes. Mice (*mus musculus*) represent the most common mammalian model organism to study fundamental biological processes, including glycosylation. Because of isomeric variance, the comprehensive analysis of protein-linked N-glycans is a challenging task. Coupled with high-resolution mass-spectrometry, porous graphitic carbon (PGC)-LC is a powerful and widely used method for isomer-specific glycan analysis. Here we showcase a consistent and complete PGC-LC-MS/MS N-glycome dataset of 23 different mouse tissues, critically complementing existing glycan data-repositories. We used PGC-LC to chromatographically separate even closely related N-glycan isomers and an Orbitrap Exploris 480 mass-spectrometer for data-acquisition. Multivariate data analysis revealed tissue-specific N-glycome signatures, highlighted organ-intrinsic regulations of glycobiological pathways and confirmed prior glycobiological knowledge, as exemplified by the brain N-glycome. This dataset can be used for fundamental glycobiological research, glycan analytical benchmarking, the development of new mass-spectrometric data analysis tools, glycobiological pathway modelling and simulation, as well as for integrative systems biology.

**Tuesday**

## **Deciphering the Glycome of Serine Repeat Proteins**

**Poster  
#8****Dimitris Latousakis, Ryan Griffith, Nathalie Juge  
and Max Loraine**

Quadram Institute Bioscience, Norwich, United Kingdom

The discovery and characterisation of new glycosyltransferases (GTs) that perform novel reactions is crucial for advancing biochemical synthesis of carbohydrate molecules. Our research focuses on the bacterial accessory secretion system (aSec), a protein glycosylation pathway dedicated to the post-translational modification and subsequent secretion of serine-rich repeat proteins (SRRPs). The accessory secretion system, a specialized protein secretion system found in certain Gram-positive bacteria, plays a key role in bacterial virulence, adhesion, and adaptation by modifying proteins that interact with the host environment. We employ MALDI-TOF mass spectrometry, which provides detailed insights into the glycosylation patterns, to analyse the glycosylation of native and recombinant SRRPs. We also use computational analyses to study the glycosyltransferases involved in SRRP modification in each species. We have identified that glycosylation patterns can be strain-specific, and through our studies, we have discovered enzymes with high sequence similarity but differing substrate specificities. By comparing these enzymes, we have pinpointed amino acid residues that mediate donor specificity. This work has significant implications for the synthesis of tailored glycoproteins and the broader field of glycoscience.

**Tuesday****Poster****#9**

## The Identification and Functional Prediction of Putative Polysaccharide Sulfotransferases

**Ravina Mistry**University of Liverpool, School of Life Sciences, Liverpool,  
United Kingdom

The vast structural diversity of sulfated polysaccharides demands an equally diverse array of enzymes known as polysaccharide sulfotransferases (PSTs). PSTs are present across all kingdoms of life, including algae, fungi and archaea, and their sulfation pathways are relatively unexplored. Sulfated polysaccharides possess anti-inflammatory, anticoagulant and anti-cancer properties and have great therapeutic potential. Current identification of PSTs using Pfam has been predominantly focused on the identification of glycosaminoglycan (GAG) sulfotransferases because of their pivotal roles in cell communication, extracellular matrix formation and coagulation. As a result, our knowledge of non-GAG PSTs structure and function remains limited. The major sulfotransferase families, Sulfotransfer1 and Sulfotransfer2, display broad homology and should enable the capture of a wide assortment of sulfotransferases but are limited in non-GAG PST sequence annotation. In addition, sequence annotation is further restricted by the paucity of biochemical analyses of PSTs. There are now high-throughput and robust assays for sulfotransferases such as colorimetric PAPS (3'-phosphoadenosine 5'-phosphosulfate) coupled assays, Europium-based fluorescent probes for ratiometric PAP (3'-phosphoadenosine-5'-phosphate) detection, and NMR methods for activity and product analysis. These techniques provide real-time and direct measurements to enhance the functional annotation and subsequent analysis of sulfated polysaccharides across the tree of life to improve putative PST identification and characterisation of function. Improved annotation and biochemical analysis of PST sequences will enhance the utility of PSTs across biomedical and biotechnological sectors.

**Tuesday**

## **Glycosylation Remodeling Mediates the Degenerative Phenotype of *Nucleus Pulposus* and *Annulus Fibrosus* Cells under pH and Osmotic Stress**

**Poster****Junquiao Lyu****#10**

University of Galway, CÚRAM Research Ireland Center for Medical Devices, Galway, Ireland

Post-translational modifications (PTMs) are chemical alterations that occur in proteins after protein translation. These modifications frequently affect protein function by regulating protein stability, localisation, and interaction with other molecules. Glycosylation is a pivotal PTM process in which carbohydrates are enzymatically attached to proteins and lipids. It plays a critical role in protein folding, stability, subcellular localisation, and glycoprotein functionality. Protein glycosylation has emerged as a major area of research interest because of its diverse roles in cellular activities and its growing recognition as a pivotal factor in inflammation and disease. In our previous studies on intervertebral disc degeneration (IVDD) glycome in human intervertebral disc degeneration, we have comprehensively examined the *N*-glycome of the human disc with spatial and temporal resolution. The regulation of glycosylation in IVDD is closely associated with inflammatory pathways.

However, our current understanding of the specific structure-function relationships and the role of specific glycans in IVDD remains incomplete. This underscores the potential of glycosylation as a target for IVDD treatment by regulating cytokine levels. Moreover, there is an absence of an *in vitro* IVDD glycosylation model to study glycosylation profiles. This is based on prior IVDD glycosylation data obtained from patients with IVDD. To address this need, we developed the Response Surface Methodology and corresponding experimental approaches to optimise the IVDD glycosylation model.

This model incorporates parameters such as the pH and osmolarity of the medium, with the objective of enabling the quantification of high-throughput lectin staining data (ConA, AAL, and SNA).

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The IVDD model was then subjected to *in vitro* analysis to identify the key factors influencing its performance. Furthermore, RNA-seq was performed to compare glycosylation genes in human IVDD samples. The results of this study demonstrated that different pH values can influence ConA and AAL levels in intervertebral disc cells. In this study, we developed an *in vitro* glycosylation model for IVDD using a cross-modelling approach. This model provides a suitable *in vitro* framework for a cell-free approach to construct interventional glycosylation for IVDD treatment.

Furthermore, we observed the metabolic and cellular phenotypes of the optimised IVDD using an *in vitro* glycosylation model.

**Tuesday****Poster****#11**

## **Computational Approaches for Analysis of Protein-glycosaminoglycan Interactions**

**Sergey A. Samsonov and Marta Pagielska**

University of Gdańsk, Faculty of Chemistry, Gdańsk, Poland

Glycosaminoglycans (GAGs), linear anionic periodic polysaccharides made up of repetitive disaccharide units, play crucial roles in various biologically relevant processes within the extracellular matrix (ECM) encompassing cell development, proliferation, signaling, coagulation and angiogenesis. GAGs perform their functions through their interactions with specific protein partners, rendering them attractive targets for regenerative medicine. However, while the molecular mechanisms governing protein-GAG interactions remain unclear, classical experimental structure determination techniques face significant challenges when dealing with protein-GAG complexes. This is due to GAGs' unique properties, including their extensive length, flexibility, periodicity, symmetry, multipose binding and the high heterogeneity of their sulfation patterns constituting the “sulfation code.”

Hence, theoretical approaches are particularly promising in deciphering the code for understanding the structure-function relationship of these complex molecules. In our research, we develop and apply computational workflows based on molecular docking, molecular dynamics and free energy calculation approaches to systematically analyze GAG-containing systems. Here, we present an analysis of GAG interactions with cathepsins, a family of proteases whose activity is known to be modulated by GAGs. Despite the biological relevance of these interactions, the structural details of cathepsin-GAG complexes remain largely undefined due to the scarcity of experimental structures. To bridge this knowledge gap, we are developing a web-based database focused on the systematic computational analysis of GAG interactions with cathepsins. This effort covers all 11 members of the cathepsin family and 6 major classes of GAGs, resulting in over 300 unique complexes.

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The database incorporates advanced *in silico* techniques, including all-atom and coarse-grained molecular dynamics simulations, as well as replica exchange molecular dynamics, amounting to more than 5,000 simulations in total.

The resulting data will provide a comparative framework for computational studies of biomolecular interactions and may support the rational development of novel strategies in GAG-driven drug design.

**Tuesday****Poster  
#12**

## **Glycoprofiling of Extracellular Vesicles by Lectin-based Methods**

**Muhammad Umair Khan, Lucia Pažitná,  
Patrícia Dudoňová and Jaroslav Katrlík**

Slovak Academy of Sciences, Institute of Chemistry, Bratislava, Slovakia

Extracellular vesicles (EVs), including exosomes, are small, membrane-bound particles released by cells in both healthy and diseased states. They play a vital role in cell communication, immune response, gene regulation, metabolism, and wound healing. Their surface glycosylation patterns influence biological recognition [1,2]. In this study, we will work on a comprehensive glycoprofiling of EVs/exosomes based on affinity lectin-using techniques such as surface plasmon resonance (SPR), a sensitive, label-free optical technique that enables real-time analysis of biomolecular interactions, and lectin-based microarray, a high-throughput method with fluorescent labelling. We are focused on bladder cancer-related EVs. EVs/exosomes will be isolated via ultracentrifugation and characterized using Nanoparticle Tracking Analysis (NTA) to confirm size distribution and concentration while preserving native glycan integrity. For glycan analysis, we will test several strategies, such as the direct immobilization of EVs on sensorchip and microarray biochip substrates, the immobilization of EVs using antibody-functionalized chips, and lectin-coated chips to identify distinct glycan motifs.

This approach aims to capture dynamic glycan-protein interactions while maintaining exosome structural fidelity in several ways, to select the most suitable, and to use the data obtained from them for further processing using bioinformatics tools. As is well known, many diseases, including various cancers, are associated with altered glycosylation patterns that influence disease progression [1]. By comparing EVs glycan profiles between healthy and diseased individuals, this study seeks to identify disease-specific glycosignatures with potential diagnostic utility. The SPR-based platform offers significant advantages for glycoprofiling, including high sensitivity and the ability to monitor interactions without labeling, while the microarray platform enables high-throughput analysis.

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The findings may contribute to the development of non-invasive biomarkers of bladder cancer and targeted therapies, with broader implications for precision medicine in cancer and other disorders.

**Acknowledgements:** This work was supported by the grants APP0620 and ANSO-CR-PP-2021-01. Funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V04-00772.

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**Tuesday****Poster****#13**

## **A Key Player in Glycogen Metabolism: the Human Glycogen Debranching Enzyme**

**Christian Roth, Ruben Ananian and Zineb Chaabi**

Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Glycogen is a highly branched glucose polymer that is one of the most important energy storage in all kingdoms of live expect plants. Glycogen homeostasis is critical for human health and various disorders are related to malfunctions of enzymes in glycogen turnover. The debranching step is critical for continuous fast energy release from glyco-gen. Two catalytic functions are required for debranching, first a transfer of the remaining three to four glucose residues from the branch, followed by the hydrolysis of the 1-6 link-age of the last glucose of the branch. Human GDE (HsGDE) combines both functions in one multidomain enzyme. The N-terminal transferase domain and the C-terminal gluco-sidase domain is connected by two domains of unknown function. Kinetic data show that both domains act independently but the fusion enhances the affinity and speed of the reaction. How the different domains contribute to the overall function and regulation of HsGDE is not understood. To gain insight into the function of the domain arrangement on activity, regulation and stability of HsGDE, we use biophysical methods for example cryo-EM to unravel the structural details of HsGDE, the role of the structural elements in glycogen turnover as well as the general importance of HsGDE for glycogen homeostasis.

Tuesday

## Temporal *N*-Glycoproteomic Differences between COVID-19 Survivors and Non-survivors at Hospital Admission and Beyond

Poster

Xue Yu

#14

Utrecht University, Utrecht, The Netherlands

The COVID-19 pandemic has had a profound and lasting impact on global health, prompting continued investigation into its underlying biological mechanisms. In this study, we aimed to develop a robust quantitative *N*-glycoproteomics approach for complex plasma samples and to characterize the altered glycosylation profiles associated with COVID-19 severity.

We analyzed plasma samples from 16 survivors and 15 non-survivors, collected at three distinct time points following hospital admission. Using data-dependent acquisition (DDA) mass spectrometry, combined with a spectral library and the “match between runs strategy, we quantified 397 unique glycopeptides and 68 glycoforms, derived from 50 proteins across 86 glycosylation sites.

By assessing both cross-sectional differences and longitudinal changes, we identified several site-specific glycosylation alterations that may serve as potential biomarkers of disease severity. The most notable site-specific change was observed at C1QA N146, where glycoform N4H5F1S1 was elevated in survivors, while N4H5S1 was elevated in non-survivors. Additionally, we identified distinct glycosylation patterns in immunoglobulins between the two groups. At the first time point, non-survivors showed increased high-mannose structures at IgA N144 and enhanced bisection at IgG 3/4. Over time, non-survivors also exhibited increased bisection at IgA2 N320 and decreased bisection at IgM N46.

These findings indicate widespread dysregulation of glycosylation in the plasma of non-survivors, reflecting systemic disturbances in protein processing and immune signaling during severe COVID-19.

**Tuesday****Poster  
#15**

## **Screening Anti-glycan Antibodies in Serum and Cerebrospinal Fluid Using Glycan Microarrays**

**Fabienne Weber<sup>1,2</sup>, Julia Flammer<sup>3,4,5</sup>, Carola Geiler<sup>1</sup>,  
Sabine Schädelin<sup>5,6,7</sup>, Julinton Sianturi<sup>1,2</sup>, Jens Kuhle<sup>4</sup>,  
Anne-Katrin Pröbstel<sup>3,4,5,7</sup> and Peter H. Seeberger<sup>1,2</sup>**

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<sup>3</sup>Department of Neurology

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<sup>6</sup>Neurology, Multiple Sclerosis Center

<sup>7</sup>University Hospital Bonn, Bonn, Germany

Glycan microarrays allow researchers to screen many samples in a high-throughput manner using very small amounts of material. Carbohydrates play a pivotal role in various biological processes; however, the role of anti-glycan antibodies in neurological and neurodegenerative diseases remains largely unexplored. In addition, autoantibodies are involved in the development of autoimmune diseases, such as multiple sclerosis. The role that carbohydrate-targeting antibodies play in disease outbreak and progression is often unknown.

Using glycan microarrays containing 38 defined synthetic glycans, we elucidated glycan binding patterns in the sera and cerebrospinal fluid (CSF) of patients with different neurological diseases. The array contained synthetic glycans of pathogenic and mammalian origin that were preselected from a larger array, as well as control structures. We tested matched samples from 338 patients on the array. The assay was validated with a small set of samples

The choice of materials and secondary antibodies, as well as careful alignment of the samples and selection of the control samples, were crucial. We screened the immunoglobulins IgG, IgA, and IgM, revealing distinct binding patterns toward various selected glycans. These results may provide more insight into the role of carbohydrates and anti-glycan antibodies in the development of neurological diseases

Tuesday

## Decoding Glycan Signatures: the Impact of Diet and Lifestyle on IgG and C3 *N*-glycosylation Patterns

Poster  
#16

**Maksym Shmatkov<sup>1</sup>, Antonio Starčević<sup>1</sup>,  
Valentina Borko<sup>2</sup>, Olga Gornik<sup>2</sup>, Jurica Žučko<sup>1</sup> and  
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<sup>1</sup>Faculty of Food Technology and Biotechnology

<sup>2</sup>Faculty of Pharmacy and Biochemistry

IgG and C3 proteins are central components of the immune system, whose glycosylation influences their immune functions and is altered in inflammatory and metabolic diseases. Besides, different dietary components and lifestyle factors may have pro- or anti-inflammatory effects on the body. Therefore, we investigated the *N*-glycosylation of IgG and C3 proteins in the context of diet and lifestyle in a population of Croatian adults. The glycan profile of each participant was determined using high-throughput LC-MS, and obtained data was compressed using non-negative matrix factorization. After that, Kendall's tau metrics were calculated to find correlations between glycan profiles and lifestyle factors.

Correlation analysis revealed that one of the compressed IgG components, which primarily represented glycans associated with inflammatory diseases, has shown weak correlations with BMI, high consumption of salty snacks, chocolate, muesli and salami, in addition to high levels of serum HbA1c, glucose and uric acid. For the C3 glycosylation, the NMF component, represented by glycans, associated with type 1 diabetes, has shown weak correlations with high body weight, white wine consumption, elevated levels of serum uric acid, VLDL, triglycerides and glucose.

In addition, we trained a model to predict the age of the participants based on their IgG glycan profile, and compared the prediction errors to the lifestyle factors, considering that the glycome changes with age.

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We found that the model tended to overestimate the age of people with high consumption of salty snacks and underestimate it if they frequently used olive oil.

The correlation between certain factors or elevated serum parameters with proinflammatory or diabetogenic glycans supports their potential as markers of environmental influences on an organism. This insight could enhance individualized healthcare approaches and support the investigation of metabolic pathways involved in the development of different diseases.

Tuesday

## Mapping Functionally Important Regions in Biotherapeutic Proteins through Combined Use of High-end Analytical Techniques and Molecular Modelling

Poster  
#17**Garoufallia Stavrdiou<sup>1</sup>, Tim Rudd<sup>2</sup>, Paul Mateitschuk<sup>1</sup> and Paul Dalby<sup>2</sup>**<sup>1</sup>Medicines and Healthcare products Regulatory Agency, London, UK<sup>2</sup>University College London, Department of Biochemical Engineering, London, UK

Exploring the structural nuances of glycosylation is a complicated endeavour, requiring the combination of different techniques for accurate results. The second most common type of glycosylation, *O*-linked glycosylation (hereafter *O*-glycosylation), has been largely overlooked due to its inherent structural complexity and convoluted biosynthetic mechanism. However, with advances in biophysical techniques, such as the Orbitrap Eclipse mass spectrometer, and robust molecular dynamics (MD) simulations, studying *O*-glycosylation accurately is now more easily achievable. In the pursuit of this goal, the use of an appropriate model protein that presents a singular glycosylation site (glycosite) allows one to research the impact of different glycan structures on the conformational stability of the protein. Hence, the granulocyte colony-stimulating factor (GCSF) with its reported glycosite at threonine 134 is a fitting model protein. Conveniently, glycosylated GCSF (Lenograstim; Granocyte) is available commercially and by enzymatic cleavage the type of glycan attached to T134 was determined and confirmed via mass spectrometry.

In my research, I am focusing on the structural effects of *O*-glycans on GCSF, so that a consensus about the utility of *O*-glycans on protein biotherapeutics can be reached. Thus, mass spectra of lenograstim are presented, revealing the type of *O*-glycan core that is ‘decorating’ Lenograstim. In parallel, MD simulations in GROMACS reveal how glycans potentially impact global conformational stability based on the monosaccharides they are comprised of, which were built in Charmm-GUI. By attaching glycans to different glycosites, the effects of glycan macroheterogeneity are also explored.

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This way, a comprehensive and multi-faceted analysis of *O*-glycosylation is delivered, and the possible effects of *O*-glycan micro-and macroheterogeneity in GCSF are studied.

**Tuesday****Poster  
#18**

## **Effect of GMPPB Deficiency on Neuronal Development**

**M. Schurig<sup>1</sup>, Obinna Umeh<sup>2</sup>, H. Henze<sup>3</sup>, J. Jung<sup>3</sup>,  
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<sup>4</sup>Brandenburg Technische Universität Cottbus-Senftenberg, Senftenberg, Germany

Guanosine diphosphate-mannose pyrophosphorylase B (GMPPB) catalyzes the conversion of mannose-1-phosphate and GTP to GDP-mannose, which is required as a mannose donor for the biosynthesis of glycan structures necessary for proper cellular functions. Mutations in GMPPB have been associated with various neuromuscular disorders such as muscular dystrophy and myasthenic syndromes. Here, we report that GMPPB protein abundance increases during brain development, which is accompanied by an increase in overall protein mannosylation. To model the human disorder in mice, we generated heterozygous GMPPB KO mice using CRISPR/Cas9. While we were able to obtain homozygous KO mice from heterozygous matings at the blastocyst stage, homozygous KO embryos were absent beyond embryonic day E8.5, suggesting that the homozygous loss of GMPPB results in early embryonic lethality. Since patients with GMPPB loss-of-function manifest with neuronal disorders, we investigated the role of GMPPB in vitro. Thereby, we found that the siRNA-mediated knockdown of *Gmppb* impaired the neuron-like differentiation of N2A cells. Taken together, our data highlight the essential role of GMPPB during development and differentiation, especially in neuronal cell types.

Tuesday

## Transforming Residue-level Deep Learning into Scalable Protein-level Classification of Carbohydrate Sulfotransferases

Poster

**Dylan Young, David Fernig, Ed Yates and Igor Barsukov**

#19

University of Liverpool, School of Life Sciences, Liverpool,  
United Kingdom

The accelerated accumulation of genomic data has created a pressing need for a robust and reliable means of identifying putative carbohydrate-binding proteins at scale. While recent deep learning approaches, such as *DeepGlycanSite*, have shown strong performance in predicting carbohydrate-binding residues, they are not explicitly designed for whole-protein classification. Moreover, with their emphasis on identifying positive-binding residues, these models are typically not trained on proteins lacking such features, complicating their adaptation to such binary classification. To address this limitation, while still leveraging the impressive residue-level accuracy of existing deep learning algorithms, a suite of machine learning classifiers was developed, capable of interpreting residue-level probability signals from *DeepGlycanSite* to generate accurate, protein-level predictions of true carbohydrate-binding activity. These models were trained on a curated dataset of sulfotransferases—a superfamily of enzymes characterised by their transfer of sulfonyl groups from donor molecules to acceptor substrates, thereby modulating activity, solubility, and biological function of a wide range of targets, from xenobiotics and hormones to polysaccharides. While sulfotransferases can typically be identified by conserved catalytic motifs, distinguishing those with carbohydrate-specific activity remains a challenge, largely due to the variable and often non-conserved nature of their substrate recognition regions.

This classifier suite significantly outperformed all heuristic scoring methods tested, offering a robust and generalisable framework for identifying novel carbohydrate-active sulfotransferases, and demonstrates the potential for repurposing existing deep learning models for reliable protein-level classification.

# Software Abstracts

Tuesday

## I-GPA for Glycoproteomic Search Engines with HCD and CID Tandem MS Data

Software

Heeyoun Hwang

#1

Korea Basis Science Institute, Digital OMICS Research Center, Cheongju, Republic of Korea

Human glycoproteins exhibit enormous heterogeneity at each *N*-glycosite, but few studies have attempted to globally characterize the site-specific structural features. We have developed Integrated GlycoProteome Analyzer (I-GPA) including mapping system for complex *N*-glycoproteomes, which combines methods for tandem mass spectrometry with a database search and algorithmic suite. Using an *N*-glycopeptide database that we constructed, we created novel scoring algorithms with decoy glycopeptides, where 95 *N*-glycopeptides from standard  $\alpha$ 1-acid glycoprotein were identified with 0% false positives, giving the same results as manual validation. Additionally automated labeled or label-free quantitation method was developed that utilizes the combined intensity of top three isotope peaks at three highest MS spectral points. The efficiency of I-GPA was demonstrated by automatically identifying 619 site-specific *N*-glycopeptides with  $FDR \leq 1\%$ , and simultaneously quantifying 598 *N*-glycopeptides, from human plasma samples that are known to contain highly glycosylated proteins.

Fucosylation of glycoproteins plays an important role for structural stability and function of *N*-linked glycoproteins. Here, we report for the first time the classification of *N*-glycopeptides as core- and outer-fucosylated types using tandem mass spectrometry (MS/MS) and machine learning algorithms such as the deep neural network (DNN) and support vector machine (SVM). The best performing model had an accuracy of more than 99% against manual characterization and area under the curve values greater than 0.99, which were calculated by probability scores from target and decoy datasets. Finally, this model was applied to classify fucosylated *N*-glycoproteins from human plasma. Thus, the machine learning methods can be combined with MS/MS to distinguish between different isoforms of fucosylated *N*-glycopeptides.

Tuesday

Software  
#2

## GlycoGenius: the Ultimate High-throughput Glycan Composition Identification Tool

Hector F. Loponte<sup>1,2,3</sup>, Jing Zheng<sup>1</sup>, Yajie Ding<sup>1</sup>,  
Isadora A. Oliveria<sup>2</sup>, Kristoffer Basse<sup>1</sup>,  
Adriane R. Todeschini<sup>2,3</sup>, Peter L. Horvatovich<sup>1</sup> and  
Guinevere S. M. Lageveen-Kammeijer<sup>1</sup>

<sup>1</sup>University of Groningen, Groningen Research Institute of Pharmacy,  
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Federal University of Rio de Janeiro, Brazil

<sup>2</sup>Carlos Chagas Filho Biophysics' Institute

<sup>3</sup>Paulo de Góes Microbiology Institute

Mass spectrometry (MS) remains the gold standard for glycan analysis, yet its data complexity hampers progress in glycobiology. Existing tools lack full automation, requiring manual intervention and limiting research efficiency. To address this, we introduce *GlycoGenius* (GG), an open-source program for automated and streamlined glycomics data analysis. With an intuitive interface, GG minimizes manual effort through advanced algorithms, automated search space construction, glycan identification, scoring, quantification, and MS2 annotation across *N*- and *O*-glycans, glycosaminoglycans, glycopeptides and more. It enables in-depth visualization and analysis of spectra, chromatograms/electropherograms, and isotopic envelope profiles—all within a unified interface. Furthermore, GG supports most major operating systems, and integrates with MetaboAnalyst or general scripting languages (e.g. R, MATLAB, python) for advanced statistical analyses.

Performance evaluations show that GG outperforms manual analysis and competing tools. It identifies more *N*-glycans, including novel structures, and detects all *O*-glycans found by other software in significantly less time. Manual verification confirmed GG's high annotation accuracy. These results demonstrate that GG not only matches but surpasses existing tools, identifying glycans missed even by expert manual data interpretation, while greatly reducing data processing time.

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GG streamlines glycomics workflows, and enhances biological interpretation and detection of disease-associated glycosylation changes, thus empowering researchers to focus on biological insights rather than data processing and, ultimately, accelerating discoveries in glycan profiling and advancing biomedical research and therapeutic development.

For more information: <https://www.biorxiv.org/content/10.1101/2025.03.10.642485v1>

**Tuesday**

## Labile Annotation Tool

**Software****Kristian I. Karlic****#3**

The University of Melbourne, Department of Microbiology and Immunology, Melbourne, VIC, Australia

The generation of high-quality peptide spectrum annotations is critical for ensuring data quality and the assignment of novel modifications. While existing tools provide basic spectrum annotation, they often lack the flexibility and specificity required for complex spectral annotation, particularly those involving multiple labile modifications. This limitation makes large-scale analyses of extensively modified peptides prohibitively labor-intensive and inefficient, hindering detailed investigations of such datasets.

Here, we present a highly customizable interactive “Labile Annotation Tool”, that integrates peptide fragmentation associated ion types (a/b/c'/x/y/z') with user-defined custom ion series associated with labile modifications and diagnostic ions. This tool supports bulk analysis of peptide spectra and allows high-throughput export of publication-ready mass spectrum visualizations from peptide-spectrum matches generated by popular software tools such as MSFragger and MaxQuant. A distinctive feature of this tool is its capability to allow the comparison of identical modification assignments which possess differences in product ions and ion intensities. This simplifies comparisons of spectra to reveal distinct patterns associated with isobaric glycans derived from bacterial protein glycosylation events. Additionally, by implementing spectra rescoring incorporating labile fragment ions this dramatically improve the scoring of extensively modified peptide spectra more accurately reflecting the assignable features.

Combined, the Labile Annotation Tool streamlines the annotation of complex peptide fragmentation patterns and enabling rapid, high-throughput extraction of publication-ready spectra through an intuitive and user-friendly interface

Tuesday

## Glycomics Workbench: Harnessing the Power of AI for Deciphering the Glycodes

Software

#4

**Arun Datta<sup>1</sup>, Nitin Sukhija<sup>2</sup> and Kimberly Bruch<sup>3</sup>**<sup>1</sup>National University San Diego, CA, USA<sup>2</sup>Slippery Rock University of Pennsylvania, Slippery Rock, PA, USA<sup>3</sup>University of San Diego, SD Supercomputer Center, San Diego, CA, USA

Glycans, more specifically, glycodes [1], which are complex carbohydrate structures consisting of ten monosaccharides in humans, encode information for various biological processes, including cell-cell interactions, extracellular signals, and cell differentiation. Aberration in the structures of these glycodes have been observed in various pathological conditions including cancer. As our understanding of glycoscience grows, researchers increasingly recognize the significance of glycodes in development and diseases, therefore, attracting attention from biotech/pharma companies aiming for biomarker discovery and developing carbohydrate-based drugs. However, deciphering glycodes presents unique challenges. Glycomics, the structure-function study of glycodes, are difficult to perform compared to other ‘omics’ fields. Unlike the linear flow of information in the Central Dogma, Glycomics require detailed and meticulous analysis of glycosyltransferases, and glycosidases that orchestrate the assembly and modification of glycans, resulting in diverse glycodes.

Glycan-based drug discovery faces limitations due to the complexity and intricate nature of glycans—varying in size, branching patterns, and modifications, thus, posing hurdles for analysis and current detection technologies. Moreover, manual curation for generating information for learning and conducting research on a glycode’s structure and function is time consuming. Recent developments in the machine learning technologies, particularly GenAI, has created an unprecedented opportunity that can tremendously help in such analysis and better understanding the complexity involved. GenAI can also accelerate glycode analysis by automating tasks that once required weeks or even months of manual curation. Similar machine learning technologies, such as, AlphaFold and Rosetta, can be exploited to create artificial enzymes for chemoenzymatic synthesis of glycodes for therapeutic purposes. Glycomics Workbench is designed to achieve these goals.

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This CI- supported portal [2] is under development with ‘Molecule page’ defining every glycan related molecule. This presentation will include showing its features including the demonstration of the web-based Molecule page for ST6Gal I [3] as an example.

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Tuesday

## Bruker GlycoScape™ – A Real-time, Database-free Glycoproteomics Analysis Tool

Software

Gad Armony

#5

Bruker, Leidendorp, The Netherlands

GlycoScape is a real-time glycoproteomics application built on the Bruker ProteoScape (BPS) platform. GlycoScape identifies both peptide- and glycan-moieties of the glycopeptide using the “Myriad” algorithm. Each spectrum is first queried for the presence of oxonium ions: if present, the spectrum is searched for the *N*-glycan core fragmentation pattern. With the pattern found, the peptide- and glycan-moiety masses are calculated, and two derived spectra are generated: a peptide spectrum which is identified using a proteomics database search engine (ProLuCID), and a glycan spectrum which is identified by the Myriad glycan ID engine. Both identification results are then merged into glycopeptide identifications. Myriad glycan ID uses a unique approach where it generates all possible glycan compositions of the defined sugar building blocks that match the glycan-moiety mass, considering literally a “myriad of possibilities”.

The generated glycan compositions are then ranked according to the supporting fragmentation evidence in the spectrum. Myriad considers multiple isotope offsets for each glycan mass which helps resolve common mistakes like 2 dHex vs 1 NeuAc. Myriad’s database-free approach allows GlycoScape to identify novel glycan-moieties that are missing from currently existing glycan databases. Furthermore, novel glycans lacking the full *N*-glycan core can readily be identified since Myriad accepts partial *N*-glycan core fragmentation patterns. Another strength of the database-free approach is that users can define the sugar building blocks it should use. Any user-defined building blocks can be defined for the generation of glycan compositions, including multiple types of sialic acids (e.g. Neu5Ac and Neu5Gc); phosphorylated, derivatized, or labeled sugars. Leveraging these strengths, GlycoScape has been shown to successfully identify the correct type of sialic acid across different species, as well as to discover a novel truncated glycan, H1N2F1S1 in samples of patients with a rare congenital disorder of glycosylation - ALG1 CDG.

**Tuesday****Software****#6****GlyGen and GlyTableMaker****René Ranzinger**

University of Georgia, Athens, GA, United States of America

For René's software abstract, please refer to his abstract in the speakers' program.

**Tuesday****GlyCounter****Software****Nicholas Riley****#7**

University of Washington, Seattle, WA, United States of America

For Nick's software abstract, please refer to his abstract in the speakers' program.

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## Biographies

### **Kiyoko F. Aoki-Kinoshita**

became involved in glycoinformatics when she joined the Bioinformatics Center in Kyoto University in 2003. She developed several machine learning methods for modeling glycan recognition patterns by glycan-binding proteins. She started her own laboratory at Soka University in 2006 where she has been developing RINGS (<http://www.rings.t.soka.ac.jp>), which is a freely-available Web resource of data mining tools for glycan analysis. She has been developing the international glycan repository, GlyTouCan (<http://www.glytoucan.org>), for assigning unique accession numbers to all glycan structures and monosaccharide compositions (Aoki-Kinoshita, et al., NAR, 2021). Moreover, as of April, 2017, she has been PI of a project developing the GlyCosmos Portal (<https://glycosmos.org>), which aims to integrate glycomics data with other omics fields (Yamada, et al., Nat. Methods, 2020). GlyCosmos is a member of the GlySpace Alliance, which aims to provide an international collaboration between GlyGen and Glycomics@ExpASY, to openly maintain and share glycan-related data under the FAIR guidelines. Lastly, she is also responsible for developing the TOHSA Knowledgebase as a part of the Human Glycome Atlas (HGA) Project, which started in April 2023 as a Large-scale Academic Frontier Promotion Project of the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan

### **Ana Ardá Freire**

is Ikerbasque Research Associate Professor and Principal Investigator at the Chemical Glycobiology Lab in CIC bioGUNE Research Centre (Bilbao, Spain). Her research focuses on the study of molecular recognition phenomena, in particular on disclosing the molecular basis of glycan-mediated biological events related to immune regulation and host-pathogen interactions.

Ana studied Chemistry at University of A Coruña (Spain), from where she got her PhD degree in the field of Natural Products Chemistry in 2006. After that, she moved to The Netherlands to join the Bioorganic chemistry group of Prof H. Kamerling at the Bijvoet Center for Biological Research (Utrecht), where she began her ongoing journey to understand the biological relevance of glycans from a structural and chemical perspective. She then moved to Madrid, to the Center for Biological Research (CIB-CSIC) to join the group of Prof. Jiménez-Barbero, where she focused on the use of NMR tools and strategies to understand and characterize glycan structural features and their molecular recognition processes by protein receptors.

In 2014, she moved together with the group of Prof. Jiménez-Barbero to CIC bioGUNE Research Center in Bilbao (Spain). In 2015 she was awarded with the tenure-track-like Ramón y Cajal Fellow from the Spanish Ministry of Science, in 2022 she was promoted to Ikerbasque Research Associate, and in 2025 to Associate Professor. At CIC bioGUNE she is involved in different projects where, by employing a combination of different chemical, biophysical and biomolecular techniques and through different collaborations, she tries to understand from a molecular perspective, how glycans bind to specific protein receptors, mainly lectins and antibodies, in biologically relevant processes, mostly related to host-pathogen interactions and immune response.

### **Marta Artola**

completed her Ph.D. studies in 2014 at the MedChemLab at Universidad Complutense de Madrid (UCM) in Spain, where she worked on the validation of the FtsZ protein as a new therapeutic target for antibacterial drug discovery. During this period, she visited Prof. Sieber's Lab at Technische Universität München (TUM) in Germany to study the antibacterial activity of her compounds. Later, she joined Prof. Baran's Lab at The Scripps Research Institute in San Diego, where she was involved in the total synthesis of Ingenol photoaffinity probes. In 2015, Marta moved to Leiden University (The Netherlands) as a postdoctoral researcher under the supervision of Prof. Herman Overkleeft.

During her postdoc, she developed conformational inhibitors and activity-based probes for various glycosidases. In 2019, she was appointed as an assistant professor in the Medical Biochemistry Department at the Leiden Institute of Chemistry, where she leads her independent research group. Her group combines organic chemistry, chemical biology, and biochemistry to develop inhibitor libraries, protein degraders, and activity-based probes for carbohydrate processing enzymes, aiming to address unmet medical needs in target validation, diagnostics, and drug discovery. Recently, she was awarded a prestigious ERC Starting Grant focused on developing a novel targeted protein degradation strategy for the therapeutic regulation of Golgi proteins.

### **Xing Chen**

received his bachelor's degree in chemistry from Tsinghua University in 2002. He then completed his Ph.D. in chemistry with Professors Carolyn Bertozzi and Alex Zettl at University of California, Berkeley in 2007. After completion of the postdoctoral research at Harvard Medical School in the lab of Professor Timothy Springer, Dr. Chen started as an Assistant Professor of Chemistry at Peking University in 2010 and was promoted to Professor with

tenure in 2016. He is currently also Vice President of Beijing Normal University. Some of his recent awards include Hui Yongzheng Award for Outstanding Achievements in Glycoscience (2023), ACS Horace S. Isbell Award (2021), Xplore Prize (2010), and Tan Kah Kee Young Scientist Award (2020). His current research interest focuses on chemical glycobiology.

### **Flaviana Di Lorenzo**

is currently Associate Professor of Organic Chemistry at the University of Naples Federico II and CEINGE Institute of Advanced Biotechnology in Naples. She is the Principal Investigator of a 5-year *ERC Starting Grant* project and leads a research group of seven members, including three postdoctoral researchers (a chemist, a cell biologist, and a neurobiologist) and four PhD students (two chemists and two biologists), working at the intersection of organic chemistry, NMR spectroscopy, mass spectrometry, and (glyco)immunology.

Her research focuses on the structural characterization of bacterial glycans and glycolipids and their role in immune modulation, with applications in microbiome research and biomedical sciences. She has played a key role in developing chemistry-based approaches for microbial glycan profiling in biological samples, bridging fundamental research with biomedical applications. Her scientific excellence and leadership have been recognized with the prestigious 2024 Nowotny Award, granted by the International Endotoxin and Innate Immunity Society (IEIIS) for her outstanding contributions to the study of bacterial lipopolysaccharides (LPS) that shows potential for further scientific development.

Prof. Di Lorenzo has published over 80 peer-reviewed articles, including high-impact papers in *Chemical Reviews*, *Angewandte Chemie*, and *Nature Communications*. She has also contributed to six international book chapters and secured multiple competitive research grants, including from the Italian Ministry of University and Research (MUR), Italian Ministry of Foreign Affairs, the National Institutes of Health (NIH), European Commission etc.

Prof. Di Lorenzo has extensive international collaborations, with research stays and joint projects at Osaka University (Japan), the University of Münster (Germany), and EMBL Heidelberg (Germany), NIH Bethesda (USA), and many others. In particular, she is Special appointed professor at Osaka University with which she has a solid connection since 2015.

### **Jana I. Führung**

studied biochemistry at Leibniz University Hannover. Already during her diploma thesis at Hannover Medical School in the lab of Prof. Rita Gerardy-Schahn, she started investigating structure-function relationships of UDP-glucose pyrophosphorylases (UGPs) from protozoan parasites and their human host.

She deepened these investigations during her doctoral studies, for which she was awarded her doctorate in 2012. During her post-doc phase, she expanded her research on sugar-activating enzymes to CMP-sialic acid synthetase (CMAS) from pathogenic bacteria and their human host. In 2017, she started a dual employment at Hannover Medical School and Fraunhofer Institute for Toxicology and Experimental Medicine, where she was involved in establishing and managing a German-Australian research consortium (iCAIR<sup>®</sup>) and gained practical experience in translational preclinical research. In 2020, she returned full-time to Hannover Medical School to focus on her own fundamental research, which is currently focused on exploring and exploiting UGPs from pathogenic bacteria and fungi towards their utilization as anti-virulence drug targets.

### **Adnan Halim**

is a biochemist specialized in mass spectrometry-based glycoproteomics. He obtained his Ph.D. degree from Gothenburg University, Sweden, in 2012, where he developed methods based on hydrazide chemistry for enrichment of N- and O-linked glycopeptides from human tissues. This approach led him to the discovery of O-GalNAc linkage to tyrosine residues on amyloid-beta peptides from human cerebrospinal fluid. In 2012, Adnan was recruited to Copenhagen Center for Glycomics (CCG) where he pursued his postdoctoral training and interest in mass spectrometry, protein glycosylations and precise genome editing. At CCG, Adnan focused on the elusive O-linked mannose modification in eukaryotes and made major breakthroughs in this field through the discovery of cadherin/plexin O-mannosylations and the TMTC1-4 glycosyltransferases (GT105). More recently, his team uncovered a third biosynthetic pathway based on TMEM260 which is responsible for initiating O-Man glycosylation on plexin receptors. Adnan was promoted to associate professor/group leader at CCG in 2016. Using a combination of techniques, including CRISPR/Cas9 engineering in cell lines and advanced mass spectrometry, his team is currently exploring the functions and regulations of O-Man glycosylations in mammalian systems.

### **Carsten Kettner**

studied biology at the University of Bonn and obtained his diploma at the University of Göttingen. In 1999, he was awarded his PhD for his work on the biophysical comprehension of the yeast vacuolar ATPase using the patch-clamp techniques in the group of Adam Bertl at the University of Karlsruhe. As a post-doctoral student he continued both the studies on the biophysical properties of the pump and the investigation of the kinetics and regulation of the plasma membrane potassium channel (TOK1).

In 2000 he joined the Beilstein-Institut. Here, he is responsible for the organization of the Beilstein symposia and for the administration and project management of funded research projects.

In 2007 he was awarded his certificate of competence as project manager for his studies and thesis from the Studiengemeinschaft Darmstadt (a certified service provider). Since 2004 he coordinates the work of the STRENDA commission and promotes guidelines for reporting enzyme data along with the commissioners ([www.strenda.org](http://www.strenda.org)). These reporting standards have been adopted by, today, over 65 biochemical journals for their instructions for authors and are incorporated in the electronic data validation and storage tool, STRENDA DB. Since 2011, Carsten co-ordinates the MIRAGE project which aims at establishing uniform reporting and representation of glycomics data in publications and which became an essential hub for the development of glycomics infrastructure ([www.beilstein-mirage.org](http://www.beilstein-mirage.org)). In 2014, Carsten was appointed the head of the funding and conferences department which is also in charge of the foundation's public relationships. Carsten is very interested in any aspects of open science and open access and thus he is actively engaged in a number of initiatives that are dedicated to make scientific data open and accessible to the wider public including NFDI4Chem, Force11 and RDA (Chemical Data, FAIRsharing).

## **Yan Liu**

is an Associate Professor in Glycosciences at Imperial College London. With over two decades of expertise in glycan array technologies, she has a profound interest in understanding the roles of glycans in mediating interactions with their binding partners across diverse biological settings. She co-established, with Prof. Ten Feizi FRS, the ICL Carbohydrate Microarray Facility, now a renowned global resource. Her current research focuses on deciphering glycan-mediated interactions at the host-microbiome interface across respiratory, digestive, skin, and reproductive systems. She has a growing interest in developing novel glycan-based molecular tools for studying glycan involvement disease-associated microenvironments in autoimmune disorders, cancer, and neurological diseases, through interdisciplinary collaborations. Dr. Liu leads a team dedicated to maintaining a vibrant Carbohydrate Microarray Facility for the broad scientific community. She is a partner leader of the Horizon Europe-funded 'GLYCOTwinning' Network, the recently launched 'AUREUS' MSCA Doctoral Training Network, and the UK 'FluTrialMAP' research consortia. Actively engaged in the MIRAGE initiative and GlyGen glycan microarray data repository, she advocates for global standards in glycan microarray data reporting and sharing, aligning with FAIR principles to advance glycan-mediated molecular interactions in the AI era.

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## **Kaspar Locher**

studied Chemistry / Biochemistry at ETH Zurich. He obtained a PhD in Biochemistry in 1998 from the University of Basel working with Jurg Rosenbusch.

From 1999–2003, Locher pursued postdoctoral studies with Douglas Rees at Caltech, where he determined the first X-ray structure of an ABC transporter. In 2003, Locher was appointed Assistant Professor of Molecular Membrane Biology at ETH Zurich. In 2013, he was promoted to Full Professor. Locher's research expertise is the structural and mechanistic investigation of integral membrane proteins. One research focus is on active transport of lipids and drugs mediated by ATP-driven or secondary active transporters. Another focus is on protein glycosylation processes catalyzed by membrane-associated glycosyltransferases. To obtain mechanistic insight, high resolution structure determination is combined with *in vitro* and cellular functional studies and biophysical techniques.

In 2006, the Locher group determined the first structure of a multidrug ABC transporter. In 2011, the group reported the first structure of an oligosaccharyltransferase, a membrane-integral enzyme with a key role in protein *N*-glycosylation. In the past few years, the group has used single particle cryo-EM to determine structures of various human multidrug and lipid ABC transporters (ABCB1, ABCB4, ABCG1, and ABCG2) and of eukaryotic oligosaccharyltransferase complexes. The group also specializes in the generation of conformational antibodies, which support structural and mechanistic work. Locher received the FEBS Letters Young Investigator Award and is an elected member of EMBO and of the German National Academy of Sciences (Leopoldina).

## **Matthew Macauley**

is the Lemieux Chair of Carbohydrate Chemistry and a Professor within the Department of Chemistry at the University of Alberta. The Macauley lab leverages chemical and biochemical approaches to study a family of sialic acid-binding lectins, called Siglecs, which help control immune cells. Key areas of interest towards understanding Siglecs as cell surface receptors are: (i) the types of carbohydrate structures (glycans) that Siglecs recognize; (ii) how Siglecs control immune cells; (iii) and how these insights can be leveraged to skew immune cells.

## **Roberta Marchetti**

is an associate professor of Organic Chemistry since 2020 at the Department of Chemical Sciences, University of Naples “Federico II”. She got her Bachelor’ degree in Chemistry in 2007 and then the Master’ in Chemical Sciences in 2009. In 2013 she received a PhD in

Chemical Sciences from the University of Naples Federico II. She is specialized in organic chemistry, with a particular focus on the isolation, purification and characterization of bacterial glycolipids. Her research interests are mainly focused on the comprehension of glycoconjugate–protein interactions through the application of NMR spectroscopy and computational methods.

In the laboratory directed by Prof. Dr. Jesús Jiménez-Barbero, Centro de Investigaciones Biológicas, CSIC, Madrid, she has extended her knowledge of advanced NMR and computational techniques for the characterization of molecular interactions events. In 2016, she became a researcher (Rtd-A) at the Department of Chemical Sciences of the University of Naples Federico II, and in 2019 she won the competition for assistant professor (Rtd-B). Promising results of her research activity were the subject of several publications in peer-reviewed journals and allowed her to be awarded of an ERC starting grant 2019 with the “GLYCOSWITCH” project. She is currently the coordinator of the MSCA-Doctoral Network “AUREUS”.

### **Róisín O’Flaherty**

earned her BSc in Chemistry at Maynooth University and a PhD in Glycochemistry at Maynooth University, Ireland in 2012. She travelled to Australia to do a Research Fellowship in Glycochemistry at the Bio21 Institute, Melbourne University. In 2013–2015, she then worked as a Process Engineer in Intel in Leixlip, Ireland and then subsequently joined the National Institute for Bioprocessing Research and Training (NIBRT) in 2015, Ireland as a Senior Post-Doctoral Researcher utilizing her expertise in automation in the field of Glycoscience. In 2019, she was appointed Research Manager in the Cell Technology Group at NIBRT and worked on post-translational modifications in mammalian cell cultures before relocating to join Maynooth University as an Assistant Professor in the Department of Chemistry in 2020. She is responsible for the creation of some of the world’s most advanced automated glycoanalytical technologies, including one clinically validated and INAB accredited method for Classical Galactosemia in conjunction with the Mater Hospital. She heads up two labs at MU, one on glycoanalytical technology development and a mammalian cell culture lab. Her research focus is in the optimisation, purification and glycan characterization of complex biological matrices (e.g. blood serum, milk, and biopharmaceuticals (e.g. mAbs, erythropoiesis-stimulating agents, mainly expressed in CHO) towards understanding complex glycan processing pathway alterations during disease states. In 2025, she was appointed as a CURAM investigator focussing on harnessing glycosylation as a tool for (in)fertility.

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**James C. Paulson**

is currently Cecil and Ida Green Professor and Chair of Molecular Medicine at The Scripps Research Institute in La Jolla, CA. Prof. Paulson obtained his PhD (Biochemistry) in 1974 from the University of Illinois at Champaign-Urbana and did post-doctoral work at Duke University Medical Centre, in Durham, North Carolina from 1974–78. From 1978–1990 was promoted from Assist. Prof. to Prof. and Vice-Chair in the Department of Biological Chemistry at the UCLA School of Medicine. From 1990–1999 he served as Vice President and Member Board of Directors of Cytel Corporation, La Jolla, CA. From 1999-present, he has been Professor at The Scripps Research Institute, where he served as acting President & CEO from 2014–2015. He led the worldwide Consortium for Functional Glycomics from 2002–2012 and is a member of numerous academic and biopharma scientific advisory boards. His current research interests include elucidating the roles of glycan binding receptors in the regulation of immune cell signaling and in the suppression of unwanted immune responses and in the role of receptor specificity in the emergence of new human influenza pandemic viruses from avian influenza progenitors. He has published nearly 400 research articles, and his work has been recognized by many awards and honors, including the Claude S. Hudson Award, ACS (2023); Avadhesh Surolia Award for Excellence in Glycobiology (2022); Tamio Yamakawa Award, JCSG (2023); President's Innovator Award, SfG (2022); American Association for the Advancement of Science (AAAS) Fellow (2016); ACS Melville Wolfrom Award (2016); and Society for Glycobiology Karl Meyer Award -SfG (2009).

**René Ranzinger**

studied computer science at the universities of applied sciences Zittau/Görlitz (2002) and Darmstadt (2004) and moved to Dr. Willi von der Lieth's group at the German Cancer Research Center (2005–2009) to work on glycomics databases and mass spectrometric data interpretation software. In 2009 he moved Bruker Daltonics GmbH & Co. KG in Bremen to work on a glycomics module for the Proteinscape software. He received his PhD from the University of Heidelberg in 2010 and joined the Complex Carbohydrate Research Center (CCRC) at the University of Georgia (Athens, Georgia, USA) as a postdoctoral fellow to worked with Will York on Glycobioinformatics tools, databases and standards. In 2013 he became assistant research scientist at the CCRC and 2022 associate research scientist. Dr. Ranzinger's work focuses on the development of tools and databases to support Glycosciences research. He has been involved in the development of multiple freely available glycomics databases and knowledgebases including GlyGen, GlyTouCan and the Glycan Array Data Repository. Another interest is the development of software tools for the interpretation of mass spectrometric data. During his PhD he was involved in the development of GlycoWorkbench and GlycoPeakfinder. Starting 2011 he developed GRITS Toolbox at the CCRC.

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As part of different international working groups Dr. Ranzinger was working on the development of ontologies for glycomics data standardization and the definition of glycomics data reporting guidelines.

### **Nicholas M. Riley**

received his PhD in bioanalytical chemistry in 2018 for his graduate work in Dr. Josh Coon's group at UW-Madison, where he worked on mass spectrometry instrumentation and proteomics methodology. He focused on methods involving electron transfer dissociation, which introduced him to glycoproteomics. He went on to a post-doctoral position with Dr. Carolyn Bertozzi at Stanford University, where he worked on new chemical biology, mass spec, and informatic tools to characterize mucin-domain glycoproteins and cell-type specific secretomes. Since starting in Seattle in September 2023, his group uses state-of-the-art mass spectrometry and chemical glycobiology to investigate glycoproteome regulation in cancer progression and metastasis.

### **Carme Rovira**

is ICREA Research Professor at the University of Barcelona. She holds a PhD from UB and has carried out research stays in USA (University of North Carolina and Southern Illinois University), Germany (Max-Planck-Institut für Festkörperforschung) and UK (University of York). She works in the modeling of catalytic mechanisms in enzymes using computer simulation, with a focus on carbohydrate-active enzymes. She has received awards from the Catalonia government (2003), the Barcelona City Council (2016) and the European Carbohydrate Organization (2019). She received an ERC SyG in 2020 and is also President of the Computational Chemistry group of the Spanish Royal Society of Chemistry (RSEQ).

### **Benjamin Schumann**

trained in carbohydrate chemistry with Peter Seeberger at the Max Planck Institute in Potsdam, and in chemical glycobiology with Carolyn Bertozzi at Stanford. He joined the Francis Crick Institute and Imperial College London in 2018 as a Group Leader of the Chemical Glycobiology Lab. His group is using synthetic tools to probe, understand and manipulate glycans particularly in the secretory pathway of mammalian cells. A breakthrough technology in the lab features the use of engineered glycosyltransferases and biosynthetic enzymes to generate “precision tools” for individual enzymes, glycan sub-types and cells.

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Ben has received multiple awards including a Chemical Biology Horizon Prize (2021), the Dextra (2023) and Heatley (2024) Awards by the RSC and a Biochemical Society Early Career Research Award (2024). He is an EMBO Young Investigator and recipient of an ERC Starting Grant. In August 2025, he will be appointed as a Full (W3) Professor in Biochemistry at the Technical University Dresden.

### **Nicholas E. Scott**

is a world leader in the study of microbial glycosylation systems. He received his PhD from the University of Sydney (2012) on the development of approaches to enrich and analyze bacterial protein modifications. He undertook postdoctoral training in Canada (University of Alberta 2011-12 & University of British Columbia 2012–15), applying quantitative proteomics to systems biology studies, then returned to Australia (University of Melbourne, 2016–17) to develop approaches to track how protein modifications govern host-pathogen interactions. A/Prof Scott established his lab in late 2017 at the University of Melbourne, where his team focuses on developing tools and methods for dissecting bacterial glycosylation systems. A/Prof Scott has published >130 manuscripts in leading microbiology journals such as *PLoS Pathogens* and *Molecular Microbiology*, as well as respected proteomics journals including *Molecular & Cellular Proteomics*, *The Journal of Biological Chemistry*, and *Journal of Proteome Research*. The quality and regard for Dr Scott's work has led to awards across the fields of proteomics, microbiology, and glycobiology, including the Australasian Proteomics Society (APS) Early Career Awards (2016, 2017), the International Glycoconjugate Organization Young Glycoscientist Award (2019), the Australian Society for Microbiology Frank Fenner Award (2021), as well as Mid-Career Awards from the Australian Glycoscience Society (2024) & the APS (2025). A/Prof Scott's collaborative work has also resulted in team awards, including the 2024 Horizon Team Award from the Royal Society of Chemistry, and in 2021 he was named one of the 40 under 40 Rising Stars in Proteomics & Metabolomics by the *Journal of Proteome Research*.

### **Sabine Strahl**

is Professor and Director of the Department of Glycobiology at the Centre for Organismal Studies (COS), Heidelberg University. Her academic career began with a Ph.D. at the University of Regensburg, where she investigated the molecular mechanisms of protein O-mannosylation—a topic that remains central to her research. After postdoctoral work at UCLA, she returned to Germany and joined COS Heidelberg in 2004. Prof. Strahl's laboratory was the first to identify the O-mannosyltransferase PMT1 in yeast, and her group continues to explore the role of O-mannosylation in both fungi and mammals, with particular focus on its implications for congenital disorders of glycosylation (CDG).

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As the spokesperson for the DFG Research Unit FOR2509, she actively fosters collaboration within the glycobiology community. Her current research investigates the interplay between *O*-mannosylation and *N*-glycosylation pathways and their relevance to human disease, which she looks forward to presenting at this conference.

### **Morten Thaysen-Andersen**

obtained a PhD in Protein Chemistry in 2009 from Univ Southern Denmark and thereafter relocated to Australia to complete two fellowships awarded by the Danish Research Agency and Australian Research Council. Enabled by a Cancer Institute NSW fellowship (2014–17), he then established the Analytical Glycoimmunology lab at Macquarie Univ, Sydney, Australia. He is currently a tenured ARC Future Fellow (2022–26) at Macquarie Univ and was recently recruited to the Institute for Glyco-Core Research (Nagoya Univ, Japan) as Visiting Professor to establish a satellite lab in clinical glycoproteomics (2022–27). Andersen's research team develops and applies MS-based glycoproteomics methods for the comprehensive profiling of the heterogenous glycoproteome, which opens new avenues to decode the role of glycoproteins in complex biological processes. His current research program in glycoimmunology focuses on the innate immune system and immune disorders including inflammation (sepsis), host-pathogen interactions and cancer.

### **Dani Ungar**

Following a chemistry undergraduate degree in Budapest (Hungary) and PhD in biochemistry with Nobel Laureate Hartmut Michel at the MPI of Biophysics (Germany) I embarked on a postdoc at Princeton (USA) working with Gerry Waters and Fred Hughson to study membrane trafficking and protein sorting in the mammalian Golgi apparatus. It was at Princeton that I started to work on the conserved oligomeric Golgi (COG) vesicle tethering complex. I started using our knowledge of COG and its mutants to perturb enzyme sorting and thereby glycosylation homeostasis in the Golgi after starting my group at the University of York (UK). Recently my group has taken a multidisciplinary approach to understanding how glycan processing in the Golgi enables different functional glyco states of cells and glycoproteins. In collaboration with industrial partners we use a combination of molecular cell biology, analytical chemistry and computational modelling to understand the drivers of glycan processing that provide functional outputs of the glycosylation machinery.

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**Marthe T. C. Walvoort**

obtained her PhD degree in 2012 (*cum laude*) at Leiden University (the Netherlands) on the organic chemistry of carbohydrates. This was followed by a postdoctoral period in the glycobiology group of Prof. Barbara Imperiali at Massachusetts Institute of Technology (Boston, USA). In the end of 2015, Walvoort joined the University of Groningen as Assistant Professor and Rosalind Franklin fellow in the Chemical Biology division at the Stratingh Institute for Chemistry, and she was promoted to Associated Professor in Chemical Glycobiology in 2021.

In her research, Walvoort combines her expertise in organic (carbohydrate) chemistry and biochemistry to unravel the impact of sugars in health and disease. Current research topics include bacterial adhesin glycosylation and its impact on infection, the role of lipopolysaccharides in antibiotic susceptibility, and understanding the health effects of exopolysaccharides from probiotics.

For more info, check the group's website: [www.walvoortlab.com](http://www.walvoortlab.com).

**Lisa Willis**

received her B.Sc. in Biochemistry from the University of Victoria and Ph.D. in Molecular and Cellular Biology in the lab of Dr. Chris Whitfield at the University of Guelph. She did her postdoctoral fellowship with Dr. Mark Nitz in the Department of Chemistry at the University of Toronto, where she received the prestigious Banting Postdoctoral Fellowship. In 2019, she started as an Assistant Professor in the Department of Biological Sciences at the University of Alberta, where she is also an Adjunct Professor in the Department of Medical Microbiology and Immunology.

**Liang Wu**

studied Medicinal Chemistry at UCL, followed by a PhD at Cambridge looking at the interactions between proteins and noncoding RNAs. He moved to York in 2013 for a postdoc with Gideon Davies, to study the structure/function of sugar processing enzymes (particularly those involved in heparan sulfate (HS) degradation), and to develop novel chemical probes to track and inhibit these enzymes.

In 2020, he joined the Rosalind Franklin Institute, a UK national institute to develop physical sciences technologies for life sciences, under a Wellcome Trust Sir Henry Dale fellowship. His group investigates the structural basis of human HS biosynthesis, combining classical techniques such as X-ray crystallography and cryo-EM, with new imaging tools such as electron tomography, to dissect the organization of enzymes within cells.

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**Manfred Wuhrer**

is Prof. for Proteomics and Glycomics at the Leiden University Medical Center in the Netherlands. His research focuses on the development of mass spectrometric methods for glycomics and glycoproteomics, and their application in clinical research and biotechnology. Clinical applications cover the fields of rheumatoid arthritis, inflammatory bowel disease, colorectal cancer, pancreatic cancer, longevity, as well as various infectious diseases. Manfred studied Biochemistry at Regensburg University and obtained his PhD in 1999 at Giessen University, Germany. He joined the Leiden University Medical Center as a researcher in 2003. From 2013 to 2015 he was at the Vrije Universiteit Amsterdam as Professor for Analytics of Biomolecular Interactions. In 2015 he started his current role at the LUMC as Prof. and Head of the Center for Proteomics and Metabolomics. From 2016 to 2022 he has been chair of the Dutch Society for Mass Spectrometry (<https://www.nvms.nl/>).

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