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Epilogue—Unravelling Glycan Complexity☆

Weston B. Struwe

University of Oxford, Chemistry Department, Chemistry Research Laboratory, 12 Mansfield Road, Oxford Ox1 3TA, United Kingdom

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The *4th Beilstein Glyco-Bioinformatics Symposium* took place in Potsdam, Germany, and addressed several key issues facing the field of glycobiology. Presentations covered a range of disciplines from biology to computer science which provided a unique venue to discuss these challenges through an interdisciplinary approach. Researchers were offered an opportunity to not only present new research but also a unique environment to converse with other experts in the field and promote collaborations worldwide. The unique style of the Beilstein Symposia fosters a comfortable atmosphere which only furthers the exchange of ideas, knowledge and expertise to advance research in the glycosciences.

The 2015 meeting was entitled *Unravelling Glycan Complexity* and brought together chemists, biologists, bioinformaticians and computer scientists from 16 countries to promote the area of glyco-informatics. Presentations were innovative and highlighted key findings that emphasized the importance of glycan three-dimensional structure as it relates to interacting partners, appreciation for indistinct and dynamic genetic factors that contribute to systems glycobiology, understanding challenges and limitations in existing analytical methods and in oligosaccharide synthesis as well as demonstrations of the latest bioinformatics tools. Glycomics remains an important subject area among other—OMICS fields and its continued success is driven by pioneering and progressing research which was reflected in this year's meeting.

The Glyco-Bioinformatics Symposia focus on contemporary analytical challenges in glycoscience and aim to address important needs among researchers. This year, the stage was brilliantly set by the inaugural talk from Hans Vliegenthart who not only discussed the fine details of glycan structures but also how they relate to non-glycan moieties and the significance of glycoconjugate presentation. The importance of structure in a range of biological processes and the ability to dissect glycoconjugate structures, particularly by mass spectrometry, was further iterated in talks by Anne Dell, Joe Zaia, Cathy Costello, Peter Hufnagel and Kevin Pagel. Current capabilities, limitations and accurate data interpretation were emphasized as well as a comprehensive assessment of novel techniques, including ion mobility, new dissociation modes, high-resolution analysis and MS-imaging, providing an excellent outlook for enhanced methods. The discussions of glycan structure—function relationships continued through a series of talks examining carbohydrate interactions monitored by glycan/lectin microarrays and associated considerations in their design. Peter Seeberger discussed modern commercially available automated synthesis platforms and Todd Lowary described ''boutique'' arrays that accurately represent glycan structures used for diagnostics.

The use of shotgun glycan microarrays and the incorporation of existing metadata derived from genetic

E-mail address: weston.struwe@chem.ox.ac.uk

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and/or structural analyses, termed metadata-assisted glycan sequencing (MAGS), was presented by David Smith which aids to more accurately characterize glycan binders.

Glycan recognition in a range of biological systems from drug design to predicting glycan binding of bacterial proteins was presented, but interestingly underlying each talk was the application of innovative strategies to interrogate these interactions. The use of molecular dynamics to probe the effects of glycan conformation and protein desolvation in bacterial adhesion was presented by Stefanie Barbirz revealing how water can fine tune complex formation. The design and development of carbohydrate mimics for successfully targeting so-called ''undruggable target'' lectins was described by Beat Ernst and showed how high-affinity antagonists can be designed to inhibit difficult targets in a series of human diseases. The development and application of Metabolic Sia Engineering (MSE) from Rüdiger Horstkorte showed how cellular uptake and incorporation of synthetic precursors disrupts polysialylation which has potential for cancer treatment. Adam Godzik presented how homology modeling and understanding protein networks can be used to discover new glycan processing enzymes and carbohydrate binding models on bacterial cell surfaces. The application of surface plasma resonance imaging (SPRi) towards deciphering the molecular mechanisms between cell-surface glycosaminoglycans and target proteins was described by Sylvie Ricard-Blum. These interaction networks are curated in the MatrixDB database and focuses on extracellular matrix components. Jim Paulson presented the development and use of sialic acid coated liposomes with high-affinity to certain immune cells capable of stimulating target cells or delivery of chemo-therapeutic drugs.

Realizing glycan modifications and the interplay with proteomics/genomics is on the forefront of glycomics and several talks described these systems-based approaches. Lara Mahal explained how the use of lectin microarrays, data integration and microRNA network analysis of (glyco)gene expression may be used to predict regulation and interrogate the glycome. Work from Pauline Rudd illustrated how high-throughput glycan analysis in conjunction with genome-wide association studies can delineate genome—glycome relationships. The interplay of glycosylation and DNA transcription was further discussed by Gerry Hart in studies of O-GlcNAc modifications and the relationship with phosphorylation in diabetes.

Ultimately, the continued success of glycobiology hinges on these pioneering methods capable of interrogating glycan structure—function relationships in cellular processes but is also underpinned by inventive computational tools to fully grasp these complex datasets. Several talks explained the latest developments in software tools and databases tailored specifically for existing analytical methods. Nicki Packer compared existing genomics and proteomics tools currently available and how the glycomics community can improve and link existing databases.

The importance of developers working together with researchers to ensure the success of new tools was stressed as well as the merits of data sharing and cross-referencing datasets. Kiyoko Aoki-Kinoshita presented the Integrated Database Project of Japan as well as GlyTouCan, a glycan structure repository with unique accession numbers assigned to known glycan structures. Furthermore, the recent formation of GlycoRDF, a standardized ontology for storing glycan related data in RDF (Resource Description Framework) format was described which was also highlighted throughout the meeting. René Ranzinger expressed the need for a common infrastructure and also current problems in glyco-bioinformatics including what information ought to be stored, how to support software development and the existence of common support funds. Will York talked about implications in quantitative data analysis and the use of REQUIEM (RElative QUantitation Including Everything Meaningful) analysis for comparative analysis between samples. René Ranzinger, Will York and Carsten Kettner presented an update of the Minimal Information Required for a Glycomics Experiment (MIRAGE) Project designed to help facilitate the reproducibility of glycomics experiments through reporting guidelines in scientific journals and promote the implementation of congruent data formats to be adopted worldwide.

The Beilstein Glyco-Bioinformatics Symposium provokes discussions on current issues in glycoscience and challenges attendees how to tackle these needs among researchers with an emphasis on bioinformatics. The outlook for the development of dedicated repositories and tools to interrogate glycomics datasets has widely been realized by the glycomics community. This sentiment was recently echoed in the detailed 2012 report from the National Academy of Sciences entitled *Transforming Glycoscience: A Roadmap for the Future*. The Beilstein-Institut has been at the forefront of this effort having hosted the bi-annual Glyco-Bioinformatics Symposia since 2009. As by design the beautiful setting of the symposia helped stimulate discussions outside the oral and poster sessions, which without doubt cultivated new relationships that will spur continued growth in the field for years to come.

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