Summary

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The 5th Beilstein Glyco-Bioinformatic Symposium, entitled "Systems Glycomics" aimed at highlighting glycomic research and unique glycomic tools, and how it interacts or potentiallycan interact with other life science areas to solve emerging global and local research problems. It was held on the 13th–15th of June in Akademie Berlin-Schmöckwitz, Berlin, with more than 50 registered delegates representing 13 countries. The symposium was comprised of a mixture of comprehensive presentations about the subject, short poster ("flash") presentations (Richard Drake, Sergey Samsonov, John Hogan, Vinyaga Gnanapragassam, Issaku Yamada, Masaaki Matsubara, Oliver Grant, Kazuhiro Aoki, Sylvie Ricard-Blum, Bas Jansen, Kathirvel Alagesan, Niclas Karlsson and Tsuchiya Shinichiro)), and software presentations as well on Tuesday 13th (Markus Pioch; Issaku Yamada, Julien Mariethoz, Alessandra Gastaldello, Davide Alocci and Kiyoko Aoki-Kinoshita) and on Wednesday 14th (Oliver Grant, Yukie Akune, Miguel Rojas).

The poster session was held on Tuesday evening and the software demonstration session on Wednesday afternoon). The symposium also included an end-of-the-symposia panel discussion as well as plenty of time for unscheduled interactions and discussions during breaks for coffee and meals and at unscheduled evening and afternoons/evenings. The spirit of the Beilstein Symposium was maintained by the intimate interactions of senior and junior researchers in a confined location, not only for the conference but also for the accommodation. A limited number of participants and regulars as well as selected speakers provide continuity for the series as well as broadening the glycoscience topic that allows fruitful and interesting discussions throughout the days of the meeting.

The 2017 symposium's presentations covered topics of clinical application for glycoscience, model systems to investigate the role of glycans, new technologies to investigate glycoscience, novel data handling systems and software, development of molecular tools and arrays.

Talks

Nathan Lewis initiated the scientific discussion by highlighting the fact that a level of the single glycan disialylacto-N-tetraose amongst all human milk oligosaccharides determines the severity of necrotising enterocolitis in new-born. He then illustrated how Markov modelling can be used to engineer and understand the N-glycosylation regulation including both the role of glycosyltransferases and metabolic pathways.

Linda Hsieh-Wilson demonstrated the use of quantitative proteomics to identify O-GlcNAcylated proteins and their interactions and to display cellular interactions to understand how the dynamic O-GlcNAcylation is involved in cellular processes (HEK293T cells, brain network, normal versus disease conditions).

Nicolle Packer a summarized the current state-of-the-art of glycomic/glycoproteomic MS and concluded that the current technologies for glycomics and proteomics are truly on its way, while there is a lack of both coherent efforts to enable the interpretation of data and informatics tools to support the integration with other life science data bases on the one hand and the modelling of carbohydrate interaction on the other hand. In addition, there is still a lack of technologies for other type of complex carbohydrates.

René Ranziger presented the GRITS toolbox for glycomic MS and how it can be used for archiving annotating and analysis of data as well as associating metadata. The modular toolbox also allows the extension of the GRITS by other researchers plugins.

Ajit Varki informed about the history behind the SNFG nomenclature, the use of the nomenclature driven by the *Essentials of Glycobiology* and the work with the discussion group with NCBI to update, develop and maintain SNFG.

Serge Perez discussed the topic of how to expand the current nomenclature to include 3D representation. This includes the POLY-GLYCAN to generate oligosaccharide structures and the SweetUnityMol to visualise 3D glycans, still keeping features of SNGF in order to easily visualise glycan features.

Jim Paulson described the use of MS to determine the type of glycosylation (high mannose, complex, no-glycosylation) on individual sites on the HIV gp160, with the membrane bound protein characterised from model systems resemble the infectious type.

Weston Struwe followed up on the HIV spike by describing the gp120 consisting of mostly high-mannose, while gp41 have more complex glycans. The group has also characterised mannose binding lectins (Banlec and Griffithsin) for HIV immune targeting as well as the use of IM-MS for characterisation of glycan isomers

Gordon Lauc showed that in order to make sense of glycomic data, large clinical sets are required. He indicates that 80% of the glycosylation is heritable, but only a limited number of the loci that regulates IgG glycosylation is directly linked to glycosyltransferases. The introduction of a glycome age can be used for early detection of disease pre-symptomatically.

Kiyoki Aoki-Kinoshita described the use of the Celldesigner software to generate the glycosylation pathway in the *Neurospora* fungi. She used data from the SABIO-RK kinetic database to *in insilico* create various types and amounts of glycans for the wild-type and knockout strains of this fungal system. She also presented the Glycosmos, an international collaboration that provides a platform for repositories of glycans and glycoconjugates with links to other life science databases

Thisbe Lindhorst addressed the area of mimicking the interaction of the glycocalyx for carbohydrate interactions using synthetic ligands, in particular the type 1 fimbria FimH lectin. She also analysed the stereochemistry of lectin binding using photoswitchable glycomimetics.

Sabine Flitsch presented her efforts in generating IM-MS fragment libraries in order to characterise alpha/beta configuration of glycans and its application of determining the specificity of desialylating enzymes as well as the characterisation of natural glycosides which have been extended from amygdalin.

Larah Mahal described a lectin platform and miRNA proxy platform for the role of core fucosylation and FUT8 that is upregulated in melanoma metastasis. This affects the cleavage of adhesion molecule L1CAM and thus shaping cell migration.

Hiren Joshi introduced the term Glycotopiary which is a simple cell technology to address the glycosylation of O-linked, N-linked and heparan sulphate. Examples included the discovery of new O-mannosyl transferases and the engineering of adhesins that selectively binds muc7 and gp1ba, but not other mucins. The software tool Glycodomainviewer was presented as a way to capture and display sites of glycosylation on glycoproteins.

Ola Blixt presented the development and targeting of single chain antibodies to O-linked and advanced glycation end products, including the antibody scfv g2d11 that binds bis Tn antigen in gastric mucosa and scfv D1-B2 against AGE, staining atherosclerotic plaques and pancreatic cancer.

Erdmann Rapp has identified the lack of useful tools for the analysis of MS-deteced glycopeptides and introduced glyXtools^{MS} based on open ms c++. In practice, he and demonstrated its applicability on tandem data from IgG and fibrinogen.

Frédérique Lisacek introduced the glycomic tab on Expasy and associated modular software including Pepsweetener, calculator, Glynsight, Glycosite align, Glydin and Glyconnect.

Will York asked the question of how to navigate around the glyco-data and introduced a conceptual schema to visualise data based on RDF. His vision was a bioinformatics infrastructure based on the NIH R34 Grant, unifying the current resources in glyco-bioinformatics and databases.

Kerry Gilmore presented the automated glyco- assembly line, and the use of chemistry and reaction conditions to control stereochemistry to produce designed oligosaccharides.

Ten Feizi showed the development of an O-glycan array and demonstrated its usability to Rotavirus p(10) and p(19) interaction with porcine gastric mucin oligosaccharides and in particular the linear H type 1 structure.

Manfred Wuhrer discussed how to increase throughput for glycomics for and clinical relevance (colorectal cancer and MALDI imaging) and compared his findings applying different platforms (MALDI-MS, HILIC-HPLC and xCGE-LIF).

Gerald Hart updated us about the O-GlcNacylation and its involvement in nutrient regulation and transcriptional regulation, including O-GlcNAcylation of the tata binding protein (tbp), where the glycosylation of T114 impairs metabolic gene expression.

Matthew Campbell presented the development a repository, called Glycostore that stores analysis data from HLIC, PGC and CE analysis including retention times for N-glycans, O-glycans, glycolipids. In addition, he shows interconnections with other glycoresources using GlycoRDF ontology.

The talks were concluded by the presentation by Will York about the MIRAGE project , what it is, and how we should endorse the use of the guidelines. Finally, a panel talked about the

term “Systems Glycomics”. The panelists discussed both in terms how it can specifically identify the glycosylation as part of a systems biology approach as well as providing a “buzz word” that will help in providing attention to glycosylation for decision makers and funding agencies.