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Minutes of

The 11th

MIRAGE

WIBVGE Meeting

25th & 26th August, 2020

Online Meeting

22 December, 2020

Dr. Carsten Kettner

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These minutes summarize the conclusions, decisions and results from the 11th MIRAGE meeting which was hosted as an online meeting August 25th and 26th from 12 – 4 PM (CEST) on each day. The meeting has been divided into two half-day sessions due to the fact that this meeting was a global one with participants from about 20 time zones.

Any further information about the MIRAGE project is available at the project website, i.e. <https://www.beilstein-mirage.org>

The Agenda

At the Limburg MIRAGE meeting, June 2019, we agreed on a comprehensive task list. Thus, in a first approximation, status reports and content-related discussions will make the major part of our program.

25 August

Duration (est'd)	Topics
15 min	Opening and Overview Carsten Kettner
15 min	Overview GlyGen project René Ranzinger
15 min	Overview GlyCosmos Kiyoko Aoki-Kinoshita
15 min	Overview Glycan Array Database Ten Feizi, Yan Liu
	Guidelines
30 min	NMR Guidelines – finalization and approval Maria Angeles Canales, Jim Paulson
30 min	Glycan Binding Protein Array Guidelines – first draft Jim Paulson, Lara Mahal
15 min	Glycan Array Guidelines – update Ten Feizi
15 min	Tasklist

26 August

Duration (est'd)	Topics
10 min	Come together and Opening Carsten Kettner
30 min	INTACT Glycoproteins Guidelines Weston Struwe
15 min	Glycopeptide Analysis Guidelines – first draft Julien Mariethoz, Frédérique Lisacek
15 min	CE Guidelines – next steps Joe Zaia, Manfred Wuhler, Erdmann Rapp
15 min	Other Guidelines (from the ToDoList)
30 min	Data exchange format – mzIdentML Joe Zaia, Josh Klein
30 min	General: Guideline adoption by journals Nicki Packer, Daniel Kolarich, Jim Paulson, Ten Feizi, .et al. Suggestion (PR): Essential in Glycobiology – paragraph on MIRAGE in appropriate chapter? Q: Glycomics landscape (see MIRAGE website) – any projects to add
30 min	Tasklist until next meeting

List of Participants (as of August 2020)



Yukie Akune, Imperial College London, UK

Kiyoko Aoki-Kinoshita, Soka University,
Tokyo, Japan

Maria Angeles Canales, Universidad
Complutense de Madrid, Spain

Matthew Campbell, Griffith University, Gold
Coast, Australia

Catherine Costello, Boston University, Boston,
MA, USA

Ten Feizi, Imperial College London, UK

Jesús Jiminéz-Barbero, CIC bioGUNE, Derio,
Spain

Genivieve Kammeijer, Leiden University, The
Netherlands

Niclas Karlsson, Gothenburg University,
Sweden

Carsten Kettner, Beilstein-Institut

Kay-Hooi Khoo, Academia Sinica, Taipei,
Taiwan

Josh Klein, Boston University, Boston, MA,
USA

Daniel Kolarich, MPI of Colloids and
Interfaces, Potsdam, Germany

Yan Liu, Imperial College London, UK

Lara K. Mahal, University of Alberta,
Edmonton, Canada

Julien Mariethoz, SIB Geneva, Switzerland

Nicolle Packer, Macquarie University, Sydney,
Australia

Angelina Palma, University of Lisbon, Portugal

James Paulson, The Scripps Institute, La Jolla,
CA, USA

René Ranzinger, University of Georgia, Athens,
USA

Erdmann Rapp, MPI for Dynamics of Complex
Technical Systems, Magdeburg, Germany

Pauline Rudd, NIBRT, Dublin, Ireland

Lisete Silva, Imperial College London, UK

Weston Struwe, University of Oxford, UK

Hiroaki Tateno, NAIST, Ibaraki, Japan

Manfred Wuhler, Leiden University, The
Netherlands

Joseph Zaia, Boston University, Boston, MA,
USA

Status and Progress

Overview

Since the last meeting held in Limburg in June 2019, the MIRAGE project has made reasonable progress and many of the tasks negotiated have been started and developed by the MIRAGE members in charge.

After the technical introduction in GoToMeeting and Stackfield, the brief short self-introduction of all participants and a short personal view of each participant how they coped with the pandemic, CK gave an overview of the status and tasks agreed on the previous meeting. He started with those tasks he is responsible for:

- MIRAGE @ Wikipedia: Together with FL, MIRAGE has been added to a “Disambiguation” page on WikiPedia as there are many terms and pages annotated with MIRAGE, and the disambiguation page provides a structured list of all MIRAGE entries.
- MIRAGE website: the websites have been updated, dead links were removed, the MIRAGE landscape picture has been placed on the landing page, etc.
- MIRAGE Flyer: ready for shipping to the members of the Commission, will be done very soon.

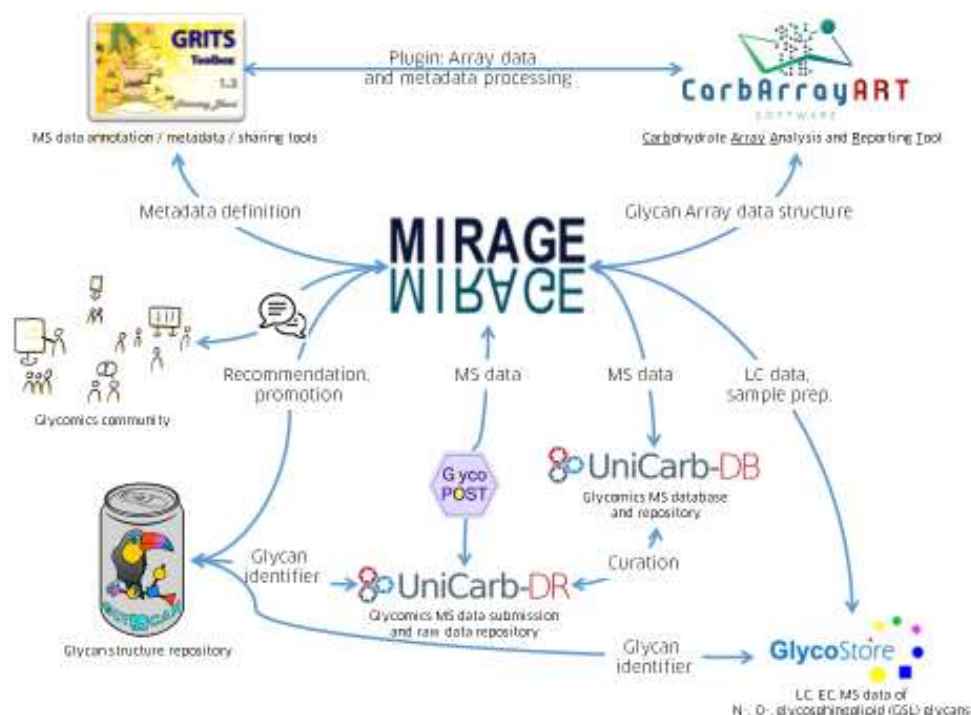


Figure. The MIRAGE landscape.

As we have had several invited guests in the meeting, CK gave a short overview of the MIRAGE landscape that considers the MIRAGE project a hub or platform for discussing and promoting exchange formats, standards and networking for repositories, databases and software tools.

In a retrospective, it has not been anticipated that MIRAGE would take this direction but the outcome fits very well with the statement from 2006 that “the scientific community agreed to establish a worldwide linked electronic infrastructure for the storage and analysis of carbohydrate structure data. As a prerequisite, standardized protocols were proposed for the exchange and the publication of experimental data and metadata” (Packer et al., 2008; PMID:18095367).

List of recommending repositories

CK reported that he is in contact with Nature’s Scientific Data that is in charge of maintaining a list of recommended repositories that is applicable for all Nature journals when authors submit manuscripts on experimental data which need to be deposited in a defined repository. The people in charge at *Scientific Data* were very helpful in sorting out how and whether GlyCosmos could be included on this list. However, an essential prerequisite for these repositories is that data stored are assigned an unambiguous identifier which is – not yet – the case for GlyCosmos.

Promotion with Journals

A long list of journals has been generated that are planned to be contacted with regards to suggesting them to recommend the MIRAGE guidelines in their instructions for authors. This list comprises the following journals: *PNAS*, *Nature*, *JBC*, *Science*, *Angewandte*, *JACS*, *Analytical Chemistry*, *Glycoconjugate J.*, *Cell*, *Pathogen*, *eLife*, *MCP*, and *Mol. Omics*.

Some contacts were successful, those with others are still pending.

- *Nature* – tight contact with TF and JP. It’s pretty likely that the MIRAGE Glean Array Guidelines will be adopted by Nature’s Reporting Guidelines.
- *PLOS* – very interested but not sure on the way of implementation.
- *Glycoconjugate J.* - recommends the MIRAGE Guidelines which are also applied during the review process.
- *MCP* – along with the MIRAGE Commission, MCP has developed the so called ‘Athens Guidelines which are checklists rather than real reporting guidelines that also acquire quantitative data in a tabular form. It has been discussed whether the Athens Guidelines could be adapted by adding a column in which the authors could enter these data and which could be used as supporting information.

- *RSC MolOmic Journal* – fruitful discussion within the editorial board with much positive feedback but no decision made yet.
- *BJOC* – the guest editors missed the MIRAGE Guidelines in the instructions for authors of BJOC. It was suggested to change this situation.

Guidelines

NMR Guidelines

Angeles Canales, Jesús Jiménez-Barbero and JP presented the final draft of the NMR Guidelines. Problem with this draft was that it would include data for two different reports: on glycan binding and glycan identification. The Commission decided to split the guidelines into two, review the titles and the introductory paragraphs, create a new or take an old dataset as an example as show case and template. The guidelines should be applied by other NMR groups to show that they are applicable in practice. After NMR data have been published, the guidelines can be published in a journal referring on the proof of concept.

Lectin Array Experiments Reporting Guidelines

After a conference call with Lara Mahal and Hiroaki Tateno the idea has emerged to use the Glycan array Guidelines as a template. In addition, in order to address the more general nature and being more consistent with the aims of the Glycan reagents specificity Guidelines it was suggested to rename this task into “*Glycan binding protein array Guidelines*”.

Glycan Binding Protein Array Guidelines

The draft presented by JP, LM and HT was accepted by the Commission. However, it was requested to align the structure of these guidelines to the structure of the others. It has been questioned (WS) how vendors could be engaged to provide their pieces of metadata required for a comprehensive reporting. As there is a solution available yet, this question remained open. In addition, it has been mentioned that there is no software support as the data analysis is mostly carried out manually.

Next steps are circulating the guidelines within HT's and LM's group for review, create and publish sample datasets, publication of the guidelines and referring to datasets that are published in compliance with the guidelines, assigning a DOI and registration with FAIRSharing.org, publication on the MIRAGE website.

LC Guidelines

The LC Guidelines have been made public on the project's website in March 2019 and published in Glycobiology on 26 March, 2019 (Volume 29, Issue 5, May 2019, Pages 349–354, <https://doi.org/10.1093/glycob/cwz009>).

Examples for experimental results applying LC for the analysis of glycans can be found on the MIRAGE website ("Examples").

In accordance with the Glycan microarray guidelines the generation of both a template and a completed example has been suggested.

Glycan Array Guidelines - Update

Initiated by their discussion with Nature on the adoption of the Glycan Array Guidelines by Nature, TF and YL suggested a slight update of these guidelines: raw datasets are recommended to be deposited in public repositories such as Synapse, Zenodo, Figshare etc. and assigned a DOI to become findable and accessible. In addition, these guidelines are aimed at to be applied by other groups producing glycan array data which need to be contacted by TF and YL. It is expected that from the other groups feedback the conclusion could be drawn that the existing guidelines are applicable or need some modification. One modification has been suggested, i.e. an additional field in the template asking for the DOI of the raw dataset.

INTACT Glycoproteins Guidelines

WS presented the first draft of these guidelines which have been appreciated by the Commission. In addition, he proposed the deposition of raw data in the standard MS repositories such as PRIDE, provided the submission process allows this type of data. Further improvements and modifications were demanded and another review round has been initiated. The individual tasks are listed in the tasklist below.

Glycopeptide Analysis Guidelines – first draft

On behalf of F. Lisacek, J. Mariethoz presented the first draft of the Glycopeptide Analysis Guidelines which has been reviewed by Xiaoning Wang and his group. In addition, JM presented an example of a template that includes data for the parameters defined in the guidelines. However, in addition to these more data have been entered such as species and species ID, disease and disease ID, protein database version, and PTMs. Although, this additional data was appreciated by the Commission as such a data set would be made more comprehensive, and as most of these data can be obtained automatically from other databases, a lively discussion started in which doubts were expressed whether this template would be helpful to make the Guidelines applicable. It

has been suggested to approach the HUPO study group for review of both. Furthermore, FL and JM are asked for making the Guidelines applicable for both single glycoproteins and glycoprotein mixtures. More to be found in the tasklist below.

CE Guidelines

With the demission of Franklin Leach due to other commitments JZ took over, again and he will proceed with the manuscript on the basis of a recent version. M. Wuhrer, G. Kammeijer and E. Rapp are willing to help. They agreed to first review this version and work on the recent version of a publication which may include existing data to create an example to demonstrate the data structure and to support the submission of this manuscript. The suggestion to submit this manuscript to *Glycobiology* was agreed. More in the task list.

Glycan reagents specificity Guidelines

JP reported the results of his studies on the relevance of such guidelines. From audio meetings he draws the conclusion that such guidelines seem to be very hard to specify as this field appears very diverse and may interfere with potential guidelines for reporting lectin specificity experiments. Thus, JP suggested to refocus on the aims initially in mind and to rename this task into “*Glycan binding protein specificity*” guidelines which also may include antibodies. He has identified a number of scientists interested in this topic including Lara Mahal.

Glycopeptide Analysis Guidelines

FL reported that the representation of glycopeptides is by far more diverse than initially anticipated and thus she has underestimated the efforts required to be able to present a first draft. For example, there are uncertainties on the representation of glycan compositions attached with peptides. There were a number of suggestions that are intended to support FL in rethinking this task including questions how the data have been obtained. In addition, the draft of a data generation workflow (comparable with that from the glycan microarrays) is considered an option to create a scaffold for future guidelines. Finally, it was suggested to first have a generic guideline document followed by a subsequent document that defines formats and orders of the composition of glycopeptides.

Ontologies and Metadata

The MIRAGE MS guidelines are currently used in UniCarb-DR and GlycoPOST as Excel files, for which a template was created at the MIRAGE meeting in Sapporo. However, a separate bioinformatics group meeting is needed to finalize the ontologies and controlled vocabularies to use in these systems. In particular, an exchange format for glycoconjugates is greatly needed as technologies to characterize glycoconjugates are increasingly being developed in the community. The HELM format is one representation that could be of interest for the community; the developers of HELM are in fact currently developing a way to incorporate glycans into their representation format.

Data exchange format mzIdentML

J. Zaia and J. Klein are working on a modification of mzIdentML, i.e. PSI data exchange format for protein MS data. For this purpose, mzIdentML will be extended by glycoconjugate-metadata. First work has been carried out, contact with software tool manufacturers has been established with request for comments and tests, but without feedback so far. With HUPO-PSI it has been agreed that the glycol-modifications proposed will be included as soon as the HUPO inter review process has been successfully completed. This status has been achieved; PSI will integrate the glycan-related metadata in mzIdentML. However, additional careful review is still required.

Tasklist

Task	Responsibility (lead)	Status
NMR Guidelines		
Split into two, revise the titles, provide short introductory paragraphs	A. Canales, J. Paulson	DONE
Example as show case and template		
Make NMR community aware and encourage to apply the guidelines for their reports		
Publication of the guidelines with reference to publications in accord to the guidelines		

Task	Responsibility (lead)	Status
Publication of the guidelines on the MIRAGE webpage, assign DOI and FAIRSharing.org ID	C. Kettner	DONE
Glycan Binding Protein Array Guidelines		
circulating the guidelines within HT's and LM's group for review,	H. Tateno, L. Mahal	
create and publish sample datasets,	H. Tateno, L. Mahal and others	
publication of the guidelines and referring to datasets that are published in compliance with the guidelines,	H. Tateno, L. Mahal	
assigning a DOI and registration with FAIRSharing.org, publication on the MIRAGE website	C. Kettner	
Glycan Array Guidelines – Update		
Contact other groups producing glycan array datasets, encourage to apply the guidelines	T. Feizi, Y. Liu	
Are modifications required?		
Add DOI field that refers to the dataset stored in a public repository		
INTACT Glycoproteins Guidelines		
Review guidelines	All	
In addition, contact John Klauson (U Alberta)	W. Struwe	
Check means to include fragmented INTACT proteins, contact Joe Gold from Robinson Group	W. Struwe	
Contact K. Aoki-Kinoshita to sort out whether these guidelines can become part of the GlycoPOST MIRAGE document	W. Struwe	
Create templates for various scenarios, i.e. binding, identification. Could be helpful for review process	W. Struwe	
Think of modularization of guidelines and referencing to other guidelines after the first review round	W. Struwe	

Task	Responsibility (lead)	Status
Glycopeptide Analysis Guidelines		
Contact HUPO study group (via Nicki) to review these guidelines	F. Lisacek, N. Packer	
Organization of a separate online meeting on this topic	C. Kettner	
Guidelines need to work for both single glycoproteins and glycoprotein mixtures	F. Lisacek, J. Mariethoz	
CE Guidelines		
Review of the current draft version	J. Zaia	In progress
Create an example file (structured table with real data included)	J. Zaia	
Review of draft version of the manuscript, submission to <i>Glycobiology</i> (?)	J. Zaia	
Assign with DOI, register with FAIRSharing.org, publish on MIRAGE website	C. Kettner	
LC Guidelines		M. Campbell
Provide template and completed example		
MIRAGE Website		
Updates required, redefinition of aims to be postponed.	C. Kettner	In progress
MIRAGE Flyer and promotion material		
Ship to members of the Commission for distribution	C. Kettner	
Update PPTX slide		
Update poster		
Update MIRAGE Wikipedia page		
Promotion with journals		
JPR to adopt Guidelines	J. Paulson	In progress
Nature	J. Paulson, T. Feizi	
Letter template to Commission (requires modifications for the corresponding needs)	J. Paulson, T. Feizi	
PLOS (One and other)	F. Lisacek	
Mol. Omics (in particular special issue)	N. Packer	

Task	Responsibility (lead)	Status
JACS (L. Kiessling) via Jesús Jiménez-Barbero	A. Canales	In progress
JBC (via Gerry Hart)	C. Kettner	In progress
ACS Chemistry Central Science via C. Bertozzi	J. Paulson	
Recommended Repository		
Contact Scientific Data to make them aware of at least three repositories for glycan data, i.e. GlyTouCan, Unicarb-DR, Glyco-POST	C. Kettner	DONE (for GlycoPOST and GlyTouCan)
Ontologies and Metadata		
Drafts for glycan arrays, MS, LC, and Sample Prep Strategy either for one-in-all or for separate ontologies	M. Campbell F. Lisacek R. Ranziner K. Aoki-Kinoshita N. Karlsson	In progress