



MIRAGE Commission @ work

Minutes of

The 12th **MIRAGE** Meeting

WIBVGE

22nd June, 2021

Online Meeting

December 17, 2021

Dr. Carsten Kettner

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These minutes summarize the conclusions, decisions and results from the 12th MIRAGE meeting which was hosted as an online meeting June 22 from 1 – 4 pm (CEST). With respect to the Joint Warren and Beilstein Symposium on Glycoscience held the other days this meeting has been restricted to one half day. It is very remarkable that this meeting saw participants from the Commission 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>

Thanks to JZ for his notes that helped me very well to compile this protocol.

The Agenda

At our online meeting in August 2020, 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.

22 June

	Topics
1.00	Welcome and opening
1.15	Consensus on agenda – suggestions for additional topics <ul style="list-style-type: none">• Overview report
2.00	Guidelines <ul style="list-style-type: none">• Reports and status of the guideline developments
3.00	Break (if requested)
3.15	Outreach and promotion <ul style="list-style-type: none">• Journals• Ontologies and metadata
3.45	General <ul style="list-style-type: none">• Suggestions from the group• Task list 2021/22• Next meeting?
4.00	Conclusions

List of Participants

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

Genivieve Kammeijer, Leiden University, The
Netherlands

Niclas Karlsson, Gothenburg University,
Sweden

Carsten Kettner, Beilstein-Institut

Kay-Hooi Khoo, Academia Sinica, Taipei,
Taiwan

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

Yan Liu, Imperial College London, UK

Akul Mehta, National Center for Functional
Glycomics, Boston, USA

Nicolle Packer, Macquarie University, Sydney,
Australia

James Paulson, ThKirchmarikalssene 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

Weston Struwe, University of Oxford, UK

Hiroaki Tateno, NAIST, Ibaraki, Japan

Manfred Wuhrer, Leiden University, The
Netherlands

Joseph Zaia, Boston University, Boston, MA,
USA

Status and Progress

Overview

Since the last meeting held online in August 2020, 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 into the online platforms used for this meeting, the brief short self-introduction of all participants and achieving consensus on the agenda, CK

gave an overview of the status and tasks agreed on the previous meeting. He started with those tasks he is responsible for:

- 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.

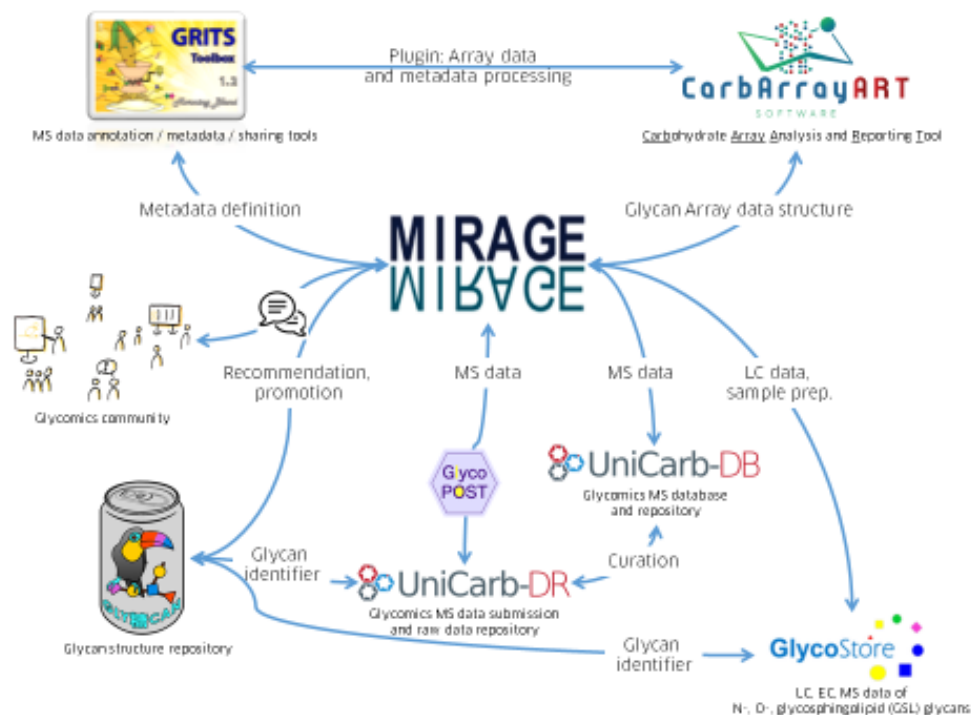


Figure. The MIRAGE landscape.

As we have had several invited guests in the meeting, of whom it could not be expected to be aware of the MIRAGE project website CK gave a short overview of the of both the website and 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.

The participants found this landscape very impressive and suggested to extend it with the glycoproteomics guidelines and connections to protein databases. However, as these guidelines haven't been finished so far they will be included in this image as soon as they will be available. FL raised the concern on how to include glycoproteins related sources in this image at this time and thus, this issue will be discussed in time.

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. However, due to some personal changes at Scientific Data this discussion has stopped.

In addition, another journal, *Molecular Omics*, requested advice from some members of the MIRAGE Commission (including KAK, FL, and DK) on how to include requirements of glycan data repositories on their webpage (<https://www.rsc.org/journals-books-databases/about-journals/molecular-omics/#data-exp>) and asked for additional guidance for the glycomics field. After an intense internal discussion and in order to provide a full picture of databases, repositories and guidelines available, we decided to set up a separate page within the MIRAGE websites which is available at <https://www.beilstein-institut.de/en/projects/mirage/recommendations/>.

NP mentioned that she's received feedback from the proteomics community that advised not to re-invent the wheel by creating new databases but use the existing ones. DK mentioned that GlycoPOST and Pride could be used. The projects GlyGen and Glyconnect are working on this.

MIRAGE @FAIRSharing.org

CK presented the list MIRAGE standards registered with FAIRSharing.org. As this record is an important means for visibility and proof of impact it has been suggested to permanently update the records with the corresponding databases and repositories.

MIRAGE flyers

The MIRAGE flyers are finalized and printed but not sent out due to the pandemic situation. CK (and many others) have been forced into remote working, and there were only a few chances to get back to the offices. In addition, sending out to the members of the commission would have been difficult as they haven't been able to receive the flyers either. Flyers will be sent out as soon as possible, and the Commission confirmed that they are still "valid".

n

Promotion with Journals

Still a long list of journals is awaiting 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 Gcan 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.
- *RSC MolOmics 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 latest results on their work on these guidelines. After the NMR guidelines have been split into two separate ones (Guidelines for Reporting Nuclear Magnetic Resonance Data on Binding of Glycans to Receptors, and Guidelines for Reporting Nuclear Magnetic Resonance Data on Glycan Structures) with meaningful titles and individual introductory paragraphs for each and after they have been published on the MIRAGE website and registered with FAIRSharing.org, they are going to be published in a journal's publication. MDLA and colleagues are working on this.

Glycan Binding Protein Array Guidelines

The draft presented by JP, LM and HT was accepted by the Commission. For the further tasks, the working group has met over the past year several times. They concluded that they need to contact experts to review the guidelines in addition. In particular, they are also seeking for feedback from array developers and will then provide the revised version of the guidelines the MIRAGE Commission for approval.

With regards to repositories for microarray data, RR mentioned that data deposition of micro array data is part of the GlyGen project which has made good progress of the past year. In a short overview he presented some details on how the samples are described in metadata. He raised the question how the data from other array platforms such as shotgun arrays, beam search arrays etc. could be integrated be it either in the microarray guidelines or in separate guidelines. He defined the following tasks:

- Review of the array guidelines and template based on metadata collection from repository,
- Update of the guidelines as need to match array repository metadata but also keep them short,
- Evaluation of the integration of other array platforms.

These tasks are going to be worked on until the next meeting.

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 and the place of deposition of the raw dataset.

INTACT Glycoproteins Guidelines

WS presented the review of these guidelines and raised a number of questions deriving from the review's results. He presented some information on native MS which was intensively discussed by the group. There seem to be connections with top-down guidelines but WS recommends not to include top-down in the native MS guidelines. Thus, he suggested to introduce only minor changes to the sample preparation guidelines to include data on native MS. On the other hand, however, he asked for more input on the INTACT guidelines whether to make the top-down or native. CEC mentioned that one cannot really leave out top-down when determining complex stoichiometries but WS believes that the distinction is not to include top-down dissociation.

Glycopeptide Analysis Guidelines – nearly final

FL presented the close-to-final version (90% done, the remaining 10% are laborious) of the glycopeptide analysis guidelines.

NP points to the human glycoproteomics initiative because the same data are used around the world and that's why not only cooperation with other groups for the guidelines is recommended but they also should be published in larger journals such as Nature Methods. During the discussion, it could not be reached a clear consensus regarding the proper reporting of software conditions. There was a general agreement that further work on the guidelines will be done in a smaller group in order to finalize them soon. In addition, input is sought from a broader userbase.

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. Wuhler, 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.

Glycan binding protein specificity Guidelines

These guidelines may also include antibodies. JP has identified a number of scientists interested in this topic including Lara Mahal and is refocusing.

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.

KAK presented a list of metadata used in GlycoPOST. However, regarding the ontologies there is a long list (e.g. to be found on the Ontologies Lookup Server, OLS) of ontologies that are hard to interpret in terms of usability for the own purposes.

Data exchange format mzIdentML

JZ reported on the progress of the modification of mzIdentML, i.e. PSI data exchange format for protein MS data. For this purpose, mzIdentML will be extended by large glycoconjugate-metadata as PTM. Currently, HUPO-PSI is reviewing this proposal.

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		
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	

Task	Responsibility (lead)	Status
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	
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	

Task	Responsibility (lead)	Status
LC Guidelines Provide template and completed example	M. Campbell	
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 Update PPTX slide Update poster Update MIRAGE Wikipedia page	C. Kettner	
Promotion with journals JPR to adopt Guidelines Nature Letter template to Commission (requires modifications for the corresponding needs) PLOS (One and other) Mol. Omics (in particular special issue) JACS (L. Kiessling) via Jesús Jiménez-Barbero JBC (via Gerry Hart) ACS Chemistry Central Science via C. Bertozzi	J. Paulson J. Paulson, T. Feizi J. Paulson, T. Feizi F. Lisacek N. Packer A. Canales C. Kettner J. Paulson	In progress In progress In progress
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