



Minutes of

The 14th **MIRAGE** **Meeting**
WIBACE

June 19, 2023
9:00 – 17:30 CEST
Dom Hotel Limburg
Germany

January, 2024
Dr. Carsten Kettner

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List of Participants



Yuki Akune, Imperial College London

Kiyoko Aoki-Kinoshita (online), Soka University,
Tokyo

Catherine Costello, Boston University

Ten Feizi (online), Imperial College London

Niclas Karlsson, Oslo Metropolitan University

Carsten Kettner, Beilstein-Institut, Frankfurt

Frédérique Lisacek, SIB, Geneva

Yan Liu, Imperial College London

René Ranzinger, University of Georgia, Athens

Weston Struwe, Oxford University

Hiroaki Tateno, AIST, Ibaraki

Joe Zaia, Boston University

Excused: Jim Paulson, Guinevere Lageveen-Kammeijer, Maria Angeles Canales, Nicki Packer, Daniel Kolarich, Anne Dell, Kay-Hooi Khoo, Pauline Rudd, Erdmann Rapp, Stuart Haslam

Agenda and results

News and activities

- CE Guidelines published:
MIRAGE website:
https://www.beilstein-institut.de/en/projects/mirage/guidelines/#ce_analysis
Glycobiology, DOI:10.1093/glycob/cwac021
- Lectin array guidelines finalized, manuscript is in preparation
- all Guidelines are registered with FAIRSharing.org
- image flyer updated

ACTION POINTS

- Update of the MIRAGE landscape diagram (CK will make a proposal)
 - image flyer:
 - add group picture or institute logos
 - add In collaboration section and add logos (e.g. PSI)
 - graphical abstract instead of text?
 - add journals that adopted the guidelines
- CK will send out a draft for review

Update/revision of the MS Guidelines

Background: the description in the MIRAGE guidelines leaves a lot of space for interpretation which may lead to different sets of “MIRAGE compliant” datasets in different databases and software tools. Especially, if that interpretation is done by software developers that are not experts in the corresponding fields. Developer guidelines or let’s call them developer recommendations can give software developers information/blueprint in hand that they can easily implement without the need for interpretation. In addition, the aim of the revision is to start with a core document that is applicable to any MS experiment which

links to additional variants that describe additional MS experiments including on intact glycoproteins, glycoproteomics, N- and O-glycans and glycoconjugates.

NK proposed a modification of the MS guidelines after he and his team tried to apply them in the lab. They realized that the guidelines are now getting old, and that there are issues that needed to be updated/removed, because the field have moved on. He presented some of these issues at the MIRAGE meeting and received the suggestion to share his thoughts with the group. By widening the target group it is hoped to receive more input from the people on the benches on to to improve the guidelines towards an increase of practicality. It should be avoided to both request information that is not required, and information that we ourselves actually really don't understand what it is.

ACTION POINTS

- NK will circulate his proposal with a deadline for feedback by end of August.
- The group will give feedback.
- Another (updated) version will then circulate after August.

The latest versions are available on Google Drive at: <http://tinyurl.com/5wpycaaj>.

Glycan Microarray Guidelines

The MIRAGE array guideline template is a Word file that is flexible and allows a lot of free text but the content is not ready to transfer into software tools and databases.

An amended version of the Glycan array MIRAGE document planned which is suitable for ready download by bioinformaticians, also a smooth linkup with the Glycan Array Repository in which we are including metadata entries that are mandatory for the MIRAGE document.

RR and YL presented the latest status on the array data, the MIRAGE metadata file format and the result of their review of the MIRAGE guidelines.

The array repository provides metadata information on the assay, the print slide and print run (both are using the CFG metadata). The data upload front end provides the user with various templates that allows to enter data on the sample, the spots, the slide, the printer etc. In order to allow machine-readability, there are individual form fields rather than full text fields and some of them are mandatory reflecting the MIRAGE Array Guidelines.

The usability is increased by prepared metadata sets that describe standardized items such as the printer, the print run procedure and the slide. All metadata can be exported and read out in e.g. Excel.

However, Excel spreadsheets also could be used to collect data and to upload these into the repository. In contrast to the currently ,static‘ PDF or Word file, the Excel file would allow for more flexibility and user-friendliness. The proposal is to also allow Excel files to collect glycan microarray data although it does not 100% match the MIRAGE guidelines (section 8 is missing: „Interpretation and Conclusion from Microarray Data“). The list of glycans is not included as this data is part of additional files in the repository.

The review of the current version of the microarray guidelines as well as the implementation of the repository showed that some data and metadata in the guidelines are missing and thus are proposed to be added. This includes the glycan sequence in digital form, information on the nature and composition of the slide as well as the description and data from the image analysis. These tasks will be addressed starting in October by an extension of the working group by additional scientists. There are some open positions with regards to the extension of the MIRAGE Microarray Guidelines by additional array types such as bead arrays, liquid glycan arrays etc. But no decision has been made yet.

Template for the LC Guidelines in GlycoPOST

The creation of a template for the LC Guidelines has been delayed due to some reasons.

It has been concluded that a working group should be formed and CK and KAK become in charge to contact a number of suggested persons and to create first this working group.

ACTION POINTS

- CK and KAK contact suggested researchers and ask for their help,
- a spreadsheet (template) is proposed
- the spreadsheet will be used to create a data acquisition web form
- the working group performs a beta test and gives feedback
- Deadline set to end of August.

Lectin Microarray Guidelines

These guidelines were formerly called „Glycan Binding Protein Specificity Guidelines“ but later renamed to gain more flexibility.

The final and revised version of the guidelines is published on the MIRAGE website at https://www.beilstein-institut.de/en/projects/mirage/guidelines/#lectin_microarrays.

HT presented this version of the guidelines and noticed the need of some minor corrections in the published document. However, even after the corrections have been performed, the version will still stay 1.0.

ACTION POINTS

- CK will correct the document.
- HT will provide an example document for the webpage.
- HT will collect some papers that report lectin microarray data in compliance with the MIRAGE guidelines.
- The group (HT, JP, LM) will publish a paper on the guidelines.

Glycoproteomics Guidelines

The Glycoproteomic Guidelines were carefully evaluated by members of HGI (Human Glycoproteomics Initiative, part of HUPO, Human Proteome Organisation). Further changes were suggested as a testing ground for the practicability of the guidelines. The latest version (v06.4) is available on Google Drive at <http://tinyurl.com/2sxu7hd7>.

FL (ii) discussed comments and instructions with some of the reviewers to preserve the consistency of the guidelines, and (ii) added bioinformatics resources relevant to glycoproteomics in order to optimize standardization. New aspects have been introduced to refine the description of output, interpretation and validation as well as quantification.

Furthermore, with the aim of increasing the visibility of MIRAGE, cooperation with PSI (Proteomics Standardization Initiative) is envisaged. FL contacted PSI representatives and received the answer that a charter for adding glycans to PSI needs to be created (see also here: <https://www.psdev.info/proteomics-informatics-standards-working-group-charter>):

“3.3 Charter A charter is an agreement between a WG and the PSI-SG to work on the designated topics. Charters should be revised and resubmitted yearly, due before the annual Spring Workshop to reflect changes to the current status, organization, or goals

of the group. The formation of a WG requires a charter that is initially negotiated between the prospective WG Chair(s) and the PSI Chair in cooperation with the PSI-SG. When the prospective WG Chair(s) and the PSI Chair are satisfied with the charter form and content, and is approved by the PSI-SG, it becomes the basis for forming a WG. A PSI WG charter consists of two components: a. Administrative: Working group name, names, and contact information for the group Chair / coChair(s), name and contact information for the WG's Secretary, Editor, MIAPE Coordinator, Ontology Coordinator, Website Maintainer, and mailing list address. b. Description and Objectives: Description of group, goals for the group, and schedule of milestones (particularly important for working groups)." -PSI management doc

ACTION POINTS

- creation of the PSI charter (FL, CK)
- combine the glycoproteomics guidelines with the revised MS guidelines and merge whenever possible so that the MS guidelines for glycans, glycopeptides and glycoproteins will be described in the same document.
- circulation of this newly compiled document within the MIRAGE Commission.

It is very likely that there will be future discussions from the bioinformatics standards viewpoint from the upcoming Dagstuhl seminar

(<https://www.dagstuhl.de/en/seminars/seminar-calendar/seminar-details/23301>)

General Topics

MIRAGE Project Webpage

ACTION POINTS

- CK: Review member list on the webpage which also may include a redesign of the organizational structure of the initiative.
- People that help with the guidelines will become "guest" members
- CK, RR: Redesign of the repository and databases page on Beilstein webpage
- CK, RR: Emphasizing the use of both the SNFG Nomenclature and GlyTouCan IDs, add a clear statement on the recommendation of both services to the community.

Guidelines

- NMR guideline papers are still in the pipeline.
- Outreach to journals to promote guidelines is still an open task

Next meeting 2024

In connection with the next Warren workshop?