Nomenclature Committee of IUBMB (NC-IUBMB) and IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN)

Minutes for the Annual NC-IUBMB and JCBN Nomenclature Meeting

Killarney, Ireland, May 11th 2017, 9:00

Present Members: Gerard Moss (GPM, Chairman); Ron Caspi (RC, Secretary); Kristian Axelsen (KA); Ture Damhus (TD); Karl-Heinz Hellwich (KHH); Andrew McDonald (AGM); Amélia Rauter (AR); Ida Schomburg (IS); Keith Tipton (KT); Hans Vliegenthart (JFGV).

Observers: David C. Baker (DB); Gareth Owen (GO); Avadhesha Surolia (AS).

Apologies: Dietmar Schomburg (DS).

1) Welcome to the participants and apologies

The chairman welcomed the participants. He introduced GO, who is a curator at the ChEBI database, and AS, who is the IUBMB Member for Publications. The participants introduced themselves briefly. GPM gave a short review of the two websites that are operated by AGM and GPM, respectively. GPM announced that Marcus Ennis, who was a member of the commission in previous years, has resigned.

2) Approval of the agenda.

KHH asked to add a new topic to the agenda: IUPAC believes that its rules limiting the duration of service should apply to membership in JCBN. If that is to be the case, KHH, AR and TD may not be able to serve much longer. This topic was discussed again at the end of the meeting (see section 17, Changes in Membership), and is covered there.

3) Approval of the minutes of the Copenhagen meeting, May 2016

The minutes from the 2016 meeting in Copenhagen were accepted following two minor changes. RC will incorporate the requested changes and transfer the document to TD, who would transfer it to the IUPAC Secretariat on behalf of the Secretary of IUPAC Division VIII, to be published on the IUPAC website.

4) Matters arising

There were no further matters arising.

5) Reports

a) Chairman's Report

KFT suggested that since this report overlaps with the more specific presentations to be given during the meeting, it should be skipped.

b) Treasurer's Report

RC reported that 2017 was the third year of the current triennium, which is funded by IUBMB at $6000/year.

RC will prepare a short annual report following the meeting and submit it to the IUBMB General Secretary, Michael Walsh. In addition to summarizing the achievements of the commission over the past year, the report will include a request to renew the budget for the next triennium. These reports are presented to the IUBMB executive committee in their annual meetings during the International Conference of Biochemistry and Molecular Biology.

KHH reminded the members about the reimbursement policies of IUPAC.

c) IUBMB Report

AS reported that IUBMB is very pleased with the performance of JCBN, that he is personally overwhelmed by the commitment and performance of the committee members, and that he will make this opinion known to other members of the IUBMB executive committee when he meets them.

d) IUPAC Division VIII Report

KHH gave a review of some of the current projects at Division VIII.

i) The project "Recommendations on nomenclature of flavonoids" has been delayed because KHH has found some significant inconsistencies in the document. A solution to the problems has been found, but at that time KHH did not have the time to continue the review of the document. A 5th of July 2017 deadline for resubmission has been decided upon, before which time KHH will provide his final comments to AR (see also section 9 below).

ii) Another project, "Preferred names of constitutional units for use in structure-based names of polymers", is in its final stages. Following a final revision, the document was resubmitted and sent again to review by ICTNS, resulting in no further comments. On May 9th the document was finally accepted for publication.

iii) A recent publication, Source-based nomenclature for single-strand homopolymers and copolymers [Pure Appl. Chem. (2016) 88(10-11): 1073-1100], is the product of long-lasting discussions between members of the Subcommittee on Polymer Terminology (SPT) and Division VIII on the basic approach to the naming of polymers. It is the first polymer naming document that is fully consistent with nomenclature of organic chemistry. This goal was achieved by the introduction of a limited number of frequently encountered polymer names as "retained polymer names".

iv) The project Nomenclature and terminology for dendrimers with regular dendrons and for hyperbranched polymers has now produced a document that is available for public review until the end of May 2017.

v) KHH pointed out some technical problems with the Manuscript Central-managed review system used by IUPAC. For example, repeatedly resubmission reminders were issued while the public review process was still ongoing. In another case, a review could not be uploaded during the review period with the explanation that the document was already in the process of publishing. KFT suggested using a different provider (ScholarOne). However, these are, in fact, two names for the same system.

vi) KHH brought to the attention of the group that Division VIII has funds for up to 5 new projects within this biennium.

vii) KHH reminded that the origin of Division VIII stems from the ever-increasing interdisciplinary work, and as a consequence, the aim to concentrate the nomenclature activities and to unify the recommendations. He stated that in the remaining time of his Presidency he will try to intensify the Division activities towards this goal. Since the current Secretary General has served as a president of Division VIII in the past, he may be receptive to projects aimed at implementing a uniform nomenclature approach among all fields.

viii) TD described his involvement in two projects; the first project, "Preferred IUPAC Names (PINs) for inorganic compounds", is delayed by new difficulties that keep arising. The project "Nomenclature for polyhedral boranes and related compounds" is also delayed due to inconsistencies between it and other projects.

6) Report from the Carbohydrate Nomenclature Group (JFGV)

JFGV described the progress made by members of the carbohydrate group regarding the project "Carbohydrate nomenclature - revision and extension of IUPAC recommendations".

a) The discussion on the revision of the 2-Carb document was concluded. Important decisions were taken on cyclocarbohydrates in terms of numbering the rings and positions in the rings where one or more substituents exist. The possibility of hetero-oligomers was also considered.
b) In view of recent developments, one of the entries of 2-Carb, viz. glycoconjugates, was singled out and treated separately.
c) Glycoconjugates were defined as compounds consisting of one or more carbohydrate moieties covalently attached to a non-carbohydrate constituent. This class comprises both natural and synthetic compounds.
d) The compounds described in the "Glycoprotein" document and in the "Glycolipid" document are now included in the carbohydrate document under the item Glycoconjugates.
e) The glycoprotein/glycopeptide recommendations were revised and extended. A systematic classification, based on the type of linkage to the protein or peptide, was introduced. Linkages via C or S are now discussed.

f) Since glycosaminoglycans are now considered as consisting of only carbohydrate, they are covered in the carbohydrate document.
g) Further definitions of Proteoglycans, Peptidoglycans and of the products arising from glycation were given. Glycation is conceived as a non-enzymatic reaction between carbohydrate and protein, starting with a Maillard-type reaction and followed by an Amadori rearrangement. Further conversions may ultimately take place.
h) The glycolipid document was reconsidered. Although a large part of it can be kept as is, many items need a careful update due to new developments and the need for a uniform type of presentation in the whole carbohydrate document.
i) Lipopolysaccharides are still in need for details to be described properly.
j) For the nomenclature of Glycodendrimers, the dendrimer document is leading (see section 5d, iv above).
k) Glyconanoparticles still need further definition.
l) As to the graphical representation of carbohydrate structures, the group adheres to the recommendations in SNFG (Symbol Nomenclature for Glycans). The group members Martin Frank and Thomas Lütteke have contributed significantly to arrive at well-defined symbols for the common monosaccharides.
m) A second draft of the glycoinformatics document was discussed. Changes and additions are necessary to bring carbohydrate chemistry and informatics further in a consistent manner.
n) In summary: a draft 3-Carb document containing all items can be prepared. Many of the corrections and suggestions that remain can be handled by e-mail correspondence. However, a meeting in person will be essential for finalizing the document. At the moment there are no funds available for such a meeting.

7) Enzyme Nomenclature and Classification

a) Report on enzymes classified (AGM)

AGM presented some statistics about the activity of the Enzyme Taskforce in 2016. 230 new enzyme entries were created, 68 existing entries were modified, 35 were transferred, and 7 were deleted, for a total of 340 new and modified entries. In addition, during the first 4 months of 2017 67 new entries were created, 19 modified, and 6 transferred. GPM mentioned that two new subclasses were created. KFT pointed out one reason for the need to reclassify existing entries – some enzymes were originally characterized with artificial electron acceptors since their native electron acceptors were not known at the time. Such enzymes are classified under the corresponding 1.99 subclasses. As more information becomes available and the native electron acceptors are identified, these entries are moved into their proper place.

b) Report from the enzyme taskforce meeting (KFT)
   i) KFT listed the members of the enzyme task force.
   ii) A new subclass is introduced for conformational isomerases (subclass 5.6). This class will be used to classify enzymes that act on proteins (5.6.1) or nucleotides

(5.6.2) and hydrolyse nucleoside phosphates to drive changes in the conformation of those substrates.

iii) A new upper class (class 7) is introduced for ATP-hydrolysing transporters ("translocases"). This is a significant change, as it is the first upper class to be added to the enzyme list since its inception.

iv) A decision has been made to acknowledge the contributions of the people who submit requests for new enzymes or error reports. A list of these people will be posted on ExplorEnz.

v) Another addition to ExplorEnz will be a (partial) list of databases that use (or have used) the EC system.

vi) The ExplorEnz website has a section for Newsletters. A few of those have been published in 2016, and a few more are expected soon. The Enzyme Taskforce would like to have these news items also included in the IUBMB newsletter, which is published on the IUBMB website. RC will ask for this when he submits his annual report to the IUBMB chair.

vii) AGM and KFT have previously written a manuscript named a 'brief guide' to enzyme nomenclature (as described in last year's minutes). KFT expressed concerns that IUPAC will not accept the manuscript without a formal project, which involves applying for a project and requesting unnecessary funds. KHH pointed out that IUPAC can approve projects that do not involve a budget. He also mentioned that IUPAC documents are now published under the Creative Commons license, which could simplify the issue of copyrights. GPM questioned whether the issue of copyright is indeed resolved, based on his recent experience. TD suggested that the brief guide could be published on ExplorEnz. KFT stated that he would like to ensure that doing so would not prohibit future publication in IUPAC.

8) Progress on the Small Molecule Glossary Project

GPM introduced the project "Glossary of small molecules of biological interest", which was started under Richard Cammack and later transferred to Marcus Ennis, who has recently resigned. As a result, there has been no progress in this project during 2016. The remaining budget of the project is $1845. The team needs to decide how to continue, and specifically which molecules to include, what exactly should be published, and most importantly, who should lead the project. A survey is in progress to establish which of the entries currently present in the project's database should be included in a printed document.

9) Progress on the Flavonoid Project (AR)

AR reported on the progress of the project "Recommendations on nomenclature of flavonoids". The project was completed in 2013, and has been reviewed by ICTNS and ca. 25 reviewers. A second version that incorporated the comments made by the reviewers was prepared and sent back to the taskforce members the following year. During 2015 all members have sent their revisions to AR, with the exception of KHH, who committed to do so by the end of June 2016. As already mentioned above (section 5d, i), KHH discovered

some inconsistencies that resulted in further delay. A new deadline of July 5th 2017 has been agreed upon.

10) Progress on the Phosphoryl Transferases Project (GPM)

GPM reported on progress in the project "How to name atoms in phosphates, polyphosphates, their analogues, and transition state analogues for enzyme-catalysed phosphoryl transfer reactions". The project has been finalized, and the document was published in Pure and Applied Chemistry (2017) 89: 653-675. GPM will prepare a short news item for ExplorEnz about this publication.

11) An extended appendix to the tetrapyrrole document (Moss)

There has been no progress regarding this tentative project.

12) Progress on the Conjugates Project (GPM)

GPM has described the progress on another project he participates in, "Nomenclature for polymeric carriers bearing chemical entities with specific activities and names". The name of the project has been changed to "Nomenclature and Terminology of Conjugates". The project was announced in Sep 2015, and the last draft was submitted in January 2017.

13) Progress on any other projects

GPM mentioned a non-IUPAC project called "HELM RNA polymer nomenclature recommendations". The project aims to develop nomenclature that clearly indicates what the modifications are in modified RNA polymers, and uses the Hierarchical Editing Language for Macromolecules (HELM), a machine readable notation system developed by a consortium of pharmaceutical companies known as the Pistoia Alliance to render the composition and structure of peptides, proteins, oligonucleotides, and related small molecule linkers. GPM raised the question whether IUPAC should endorse this document in some sort of official manner.

14) Reports from Databases

IS gave a short presentation about BRENDA. The team has moved to a new building. IS provided some statistics about data growth, which has slowed recently due to a smaller staff. New features include word maps (calculated by literature mining, providing quick linking to related terms in the database), metabolic pathways, and overview maps for pathways.

15) Recent Biochemical Nomenclature Publications of Interest

A relevant paper about phosphoryl transferases has already been mentioned by GPM (section 10 above). KHH mentioned the paper "The use of IUPAC names in glossaries", published in Chemistry International in May 2016.

16) Future projects

a) **Nomenclature of phosphorus-containing compounds of biochemical importance**. The proper terminology of phosphorus compounds is an issue that often surfaces during enzyme classification. Existing recommendations for the nomenclature of phosphorus-containing compounds have not been revised since 1976. A newer document, created in 2006 by Hal Dixon, has not been published, and has been present since its creation in multiple parts in different formats, hindering efforts to finalize and publish it. GPM has just transferred the different parts to KA, who formatted them into a single Microsoft Word document. A discussion was held about the need to update the phosphorus document. AR has accepted upon herself to submit a proposal for a new IUPAC project for this purpose. The team will include GPM and KHH. GPM mentioned that he would like to include morpholine analogues of nucleotides in the updated document.

b) As the current carbohydrate nomenclature project is about to end, a potential new project for the nomenclature of glycoconjugates was discussed briefly.

17) Changes in Membership

a) IUPAC's policy on maximal tenure. As mentioned by KHH at the beginning of the meeting, IUPAC has indicated that it considers enforcing its policy on JCBN, which would limit the membership duration to 4 consecutive years for IUPAC Titular or Associate Members. As KHH, TD and AR have now served for 4 years or more, enforcing this policy will prevent their future participation as TMs or AMs. KFT suggested that the IUPAC rules should not apply to JCBN, as it is an independent commission sponsored equally by IUPAC and IUBMB. AS pointed out that unlike IUPAC, IUBMB appreciates the importance of continuity. GPM stressed that had JCBN followed these rules, there would be no enzyme list. KHH suggested that a meeting should be arranged soon between IUPAC, IUBMB and JCBN to resolve these issues, as well as clarify the financial commitments. A potential opportunity to do so may be the upcoming IUPAC congress.

b) Minoru Kanehisa, currently listed as an emeritus member of JCBN, has indicated his interest to attend the enzyme group/JCBN general meeting next year, and thus his status will be changed to a representative of the KEGG database.

c) Hellen Berman (HB), currently listed as the representative of the PDB database, has retired. GPM will contact Dr. Shuchismita Dutta, who has represented PDB in past meetings, to see if she is interested in replacing HB.

d) Richard Cammack is now listed as an emeritus member.

e) GO has been nominated as a Titular Member of JCBN (funding provided by IUPAC) instead of Marcus Ennis who resigned. RC reminded that since GO replaced Marcus Ennis, his participation in the 2017 meeting should be covered by IUPAC.

f) GPM mentioned that in accordance with the decision during last year's meeting he has tried to contact A. Cornish-Bowden, who is still listed as an associate member of the commission but has not participated in its activities for several years, to find out whether he is still interested in maintaining his membership. However, GPM's emails have not been answered. GPM will send a letter by regular mail.

g) GPM will approach two potential candidates that were recommended by Dr. Henrissat last year. KA will provide the contact details.

18) Any other business

a) During the discussion of the phosphorus document the issue was raised that many of the previous documents issued by JCBN are only available via the private website operated by GPM, and not posted on the websites of either IUPAC or IUBMB. It was proposed that IUBMB should host these documents. RC will bring up this possibility in the annual report that he will send Mike Walsh.

b) KHH has a new postal address which is:
Dr. Karl-Heinz Hellwich
Beilstein-Institut zur Förderung der Chemischen Wissenschaften
Trakehner Str. 7 - 9
60487 Frankfurt
Germany,
e-mail unchanged (hellwich.iupac@gmx.de).

c) KHH pointed out that the symbol of the new element tennessine, Ts, is identical to the two-letter abbreviation of the tosyl group, raising some opposition to the new symbol. It remains to be seen whether the new symbol will go through the IUPAC Council.

19) Date and Place of the 2018 Meeting

a) AR offered to host the 2018 meeting in Lisbon provided it could be scheduled in July instead of May. However several members will not be able to attend in July.

b) GPM suggested Cambridge as an alternative location. The meeting will tentatively be held during the 29-31 of May.

GPM thanked AGM on behalf of the commission for his great help in hosting and organizing this very pleasant meeting. The meeting was adjourned at 13:32.