

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

Cambridge, England, May 31st 2018, 9:00

Present Members: Gerard Moss (GPM, Chairman); Ron Caspi (RC, Secretary); Ture Damhus (TD); Karl-Heinz Hellwich (KHH); Minoru Kanehisa (MK); Andrew McDonald (AGM); Gareth Owen (GO); Amélia Rauter (AR); Ida Schomburg (IS); Keith Tipton (KFT); Hans Vliegthart (JFGV).

Observers: David C. Baker (DB).

Apologies: Kristian Axelsen (KA); Dietmar Schomburg (DS); Avadhesh Surolia (AV).

1) Welcome to the participants and apologies

The chairman welcomed the participants, who introduced themselves briefly.

2) Approval of the agenda.

The agenda was approved.

3) Approval of the minutes of the Killarney meeting, May 2017

KHH pointed out that in section 7b of the minutes KFT introduced the enzyme taskforce but did not list the names of its members. He also mentioned that he found a few small typographic issues. Since these were not significant, the minutes were approved, and it was agreed that KHH will contact RC by email, so that he could incorporate these small changes before transferring 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 arising matters.

5) Reports

a) Chairman's Report

The report was skipped because all relevant issues will be discussed in more detail during the meeting.

b) Treasurer's Report

RC reported that 2018 is the first year of a new triennium period for IUBMB funding. He has presented the IUBMB General Secretary, Michael Walsh, with a short annual report following the last meeting. In addition to summarizing the achievements of the

commission over the past year, the report included a request to renew the budget for the following triennium. The report was presented to the IUBMB executive committee during their annual meeting and the new budget was approved at a level of \$6000/year.

c) IUPAC Division VIII Report

KHH gave a review of developments in IUPAC and some of the current projects at Division VIII.

- i) The document "[Nomenclature of flavonoids](#)" has been finalized and sent for publishing, and is now waiting for the 3rd round of proofs.
- ii) The project "[Preferred names of constitutional units for use in structure-based names of polymers](#)" has been published.
- iii) The project "[Alignment of principles for specifying ligands and substituent groups across various areas of nomenclature](#)" intends to provide the basis for completion of several ongoing projects, including "Boron hydride nomenclature", "Metallacycles nomenclature", "Preferred names for inorganic compounds" (the kappa document), "Inorganic and coordination polymers", as well as the revision and extension of the Blue Book. So far there has only been an initial meeting during which the general principles were discussed and decided upon. Details remain to be clarified later.
- iv) The previous chair of the Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS), Ron D. Weir, has terminated that role and is now the President of Division I. The new ICTNS chair, Jürgen Stohner, has changed the review process by returning to past procedures. After addressing the issues raised during the ICTNS review, there will be a public review as a separate step prior to publication. GPM added that the review process will include 15 external reviewers.
- v) KHH described a project initiated by Michel Vert, "[Terminology relevant to lactic acid-based polymers: synthesis, structure, properties, applications and degradation](#)". The document, with the current title "Nomenclature and terminology for lactic acid-based polymers", passed a lengthy divisional review and has - after 10 revisions since the beginning of this year - now been submitted to ICTNS review.
- vi) A new book issued by Division VII, "Comprehensive Glossary of Terms Used in Toxicology" (RSC 2017), is a compilation of glossaries published previously. The appendix with 35 p. list of toxic substances with their corresponding IUPAC names was heavily revised by KHH, GPM and TD.
- vii) TD explained how several of the ongoing projects he is involved in, such as the "[Nomenclature for polyhedral boranes and related compounds](#)", which involve

both inorganic nomenclature and coordination nomenclature, have exposed the need for more accurate terminology of kappa substitutions, strengthening the need for the project described by KHH earlier (see 5/c/iii).

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 task group was established in 2015 and the project was expected to be completed by the end of 2017. However, the complexity of the carbohydrate structures made it impossible to finish the revision of the 2-Carb document within that time frame. An extension of the project for three more years was requested and granted by IUPAC in 2018.
- b) In the present meeting the revision of the 2-Carb document was nearly completed.
- c) The section on Glycoconjugates, planned to include glycoproteins and glycolipids, which were previously discussed in separate documents, still awaits further discussion.
- d) Regarding the section on glycoinformatics, it is clear that combining the two desired aspects of the document: serving the carbohydrate community while being useful for information specialists, is not easy. The task group feels that it has reached a stage wherein its members have provided their expertise. To bring this section further, other experts will have to be consulted. In particular, the group will seek experts from PDB, who are facing the problem of describing glycans attached to glycoproteins, and experts that have taken initiatives to develop their own glycoinformatics standards. Much exchange of opinion is now needed to harmonize the various ideas as far as possible.
- e) The symbolic representation of carbohydrates, as developed by the Society for Glycobiology, has been accepted by the task group. This representation has been published in Glycobiology.

7) Enzyme Nomenclature and Classification

- a) Report on enzymes classified (AGM)

AGM presented some statistics about the activity of the Enzyme Taskforce during 2017. 249 new enzyme entries were created, 48 existing entries were modified, 33 were transferred, and one entry was deleted, for a total of 331 new and modified entries. In addition, during the first 4 months of 2018 68 new entries were created, 22 modified, 9 were transferred, and 3 were deleted. GPM has mentioned the introduction of the new class 7 and the new subclass 5.6, which were mentioned last year. Much work has taken place transferring existing entries to the new classes, and the first examples of such entries will be introduced to the public soon.

- b) Report from the enzyme taskforce meeting (KFT)

- i) KFT pointed out the absence of Richard Cammack. After many years of outstanding service in the enzyme taskforce, as well as in JCBN, Richard has withdrawn owing to ill health. KFT mentioned Richard's significant contribution to the enzyme taskforce over the years and the commission's gratitude to him.
- ii) A key principle of the enzyme classification system is that enzymes are classified by the reactions they catalyze. In certain cases, this principle results in difficulties, as sometimes enzymes that are quite different from each other catalyze very similar reactions. The enzyme taskforce is still grappling with those cases.
- iii) To make the enzyme list more accessible to biologists, reaction equations are often written using compound names in common use, while the IUPAC official names are provided in a glossary entry. It has been pointed out by TD that some glossary entries are no longer correct. TD will work with the enzyme taskforce to correct these errors.
- iv) Several new newsletters will be published soon. One newsletter will discuss classification rules for cytochrome P-450 hydroxylases. Two other newsletters will introduce the new class EC 7 for translocases and subclass EC 5.6 for conformational isomerases.
- v) A communication from Rong Guan, a research investigator from DuPont – Industrial Biosciences, pointed out the need to classify two new glycosyltransferases: sucrose—1,6- α -glucan 3- α -glucosyltransferase and sucrose—1,6- α -glucan 2- α -glucosyltransferase.
- vi) A new Acknowledgements section in ExplorEnz lists the names of people who had contributed to the database by submitting requests for new enzymes or by pointing out errors in existing entries.
- vii) As discussed in the minutes of previous meetings, AGM and KFT have previously written a 'brief guide to enzyme nomenclature' with the intention of publishing it in a format that would help introducing the enzyme list to larger audiences. KFT asked KHH for guidance regarding its publication. KHH thought that it may be possible to publish the guide in Chemistry International without a new IUPAC project. GPM will consult with Dr. Fabienne Meyers, the standing secretary of the Project Committee in IUPAC, regarding the best path forward.
- viii) AGM described a problem he has recently experienced with the NIST database. The database contains thermodynamic data for many enzymes, and it used to be possible to link to that data from the ExplorEnz site using EC numbers. Following a recent change to the structure of the NIST website it is no longer possible to link to that data using EC numbers. When AGM contacted NIST he was informed that they do not plan to reinstate this ability. AGM will remove the non-functional links and may ask to download their data.

8) Progress on the Small Molecule Glossary Project

The project "[Glossary of small molecules of biological interest](#)" was started under Richard Cammack, transferred to Marcus Ennis (ME), who has recently resigned, and is now headed by GO, who is a ChEBI curator and project leader. Owing to significant cuts in ChEBI's workforce last year, GO had little time for the project. So far he had simply caught up with what was done before he joined the project. He has found that a survey has been conducted by ME regarding which structures should be included but did not find answers from the project's members. KHH pointed out that he did respond to the survey, and GPM thought that he has also done so. Both will resend their replies to GO.

9) Progress on the Flavonoid Project (AR)

AR reported on the completion of the project "[Recommendations on nomenclature of flavonoids](#)" (see item 5)c)i) above). The recommendation will be published this year. However, technical issues with the proofing process slow the publishing process. The team is currently waiting for the third round of proofs, which hopefully will be the last one.

10) Progress on the Phosphorus document (AR)

A project named "[Nomenclature of Phosphorus-containing Compounds of Biochemical Importance](#)" was started by the late Hal Dixon in 2006, and never finished. A preliminary document was created at the time but was never published. Last year the different parts of that document were formatted into a single Microsoft Word document by KA, and AR has accepted upon herself to submit a proposal for a new IUPAC project for renewing this project.

AR reported that she has gone over the material and concluded that much was missing, and that a new project should be started. AR has also pointed out that in addition to GPM and KHH, who have volunteered last year to participate in the project, she would like to include additional members specializing in fields such as inorganic chemistry, synthetic chemistry, and bioinformatics. TD has volunteered to participate as well.

GPM reiterated his statement from last year regarding the inclusion of morpholine analogues of nucleotides in the updated document.

KHH pointed out that since the original project was never terminated officially, it should be clarified whether this project should be processed as a new project or as a continuation of the old one, in particular since the original project had no budget. It was agreed that if possible it will be preferable to start a new project.

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

There has been no progress regarding this tentative project.

12) Progress on the Conjugates Project (GPM)

This project, headed by Michel Vert, appears on the IUPAC website as "[Nomenclature for polymeric carriers bearing chemical entities with specific activities and names](#)" even though it has been decided more than a year ago to change its name to "Nomenclature and Terminology of Conjugates". GPM thought that KHH would know more about the status of this project. KHH mentioned that the project team met in Sao Paulo but encountered some unexpected problems, in particular concerning the use of INNs. KHH has recently been invited to join the task group but hasn't decided yet.

13) Progress on any other projects

GPM described the project "[Chemical and Biochemical Thermodynamics Reunification](#)", which has been initiated by Division I. The project, initiated by Stefano Iotti, aims to unify chemical thermodynamics (that employs conventional thermodynamic potentials) and biochemical thermodynamics (that employs Legendre-transformed thermodynamic potentials).

14) Updates from the databases

MK provided a brief presentation discussing difficulties in the correlation between EC numbers and protein sequences. He showed an example of the three types of tryptophan halogenases (EC 1.14.19.58, tryptophan 5-halogenase; EC 1.14.19.9, tryptophan 7-halogenase; and EC 1.14.19.59, tryptophan 6-halogenase). Sequence analysis of these proteins does not always match the biochemical activity observed with the purified proteins.

15) Recent Biochemical Nomenclature Publications of Interest

KHH reminded of the document "[Preferred names of constitutional units for use in structure-based names of polymers](#)", which has been published in Pure Appl. Chem. 89(11), 1695–1736 (2017). This is not of general relevance to biochemistry but gives an outline of the principles, which might be helpful when encountering synthetic analogues of biopolymers.

16) Future projects

- a) The current carbohydrate nomenclature project has been extended for three years. In the coming years it will focus on the nomenclature of glycoconjugates.
- b) The phosphorus project has already been discussed (see section 10).

17) Changes in Membership

- a) These are the current members of NC-IUBMB and JCBN:

Full members:

NC-IUBMB: AGM, GPM (Chairman of both Committees), IS

JCBN: RC (Secretary of both Committees and Treasurer), GO

NC-IUBMB and JCBN: KA, KFT

Associate members:

NC-IUBMB: A. Cornish-Bowden, M. Kotera, JFGV

JCBN: TD, AR

Ex Officio:

KHH

Database Representatives:

DS, MK, H. Berman (USA), R. Apweiler (UK)

Emeritus Members:

R. Cammack

- b) GO's membership has been formally approved by IUPAC.
- c) According to the decision last year, Richard Cammack is now listed as an emeritus member.
- d) GPM has contacted Athel Cornish-Bowden, who is currently listed as an associate member but has not participated in JCBN activities for several years. Due to failing health he has decided to withdraw from the committee.
- e) GPM has also contacted Shuchismita Dutta from PDB to see if she would be interested in replacing Helen Berman, who has retired, as the PDB representative. He has not received an answer. He will try to contact her again.
- f) GPM has not approached two potential candidates that were recommended by Dr. Henrissat during the 2016 meeting (Professor Harry Gilbert of Newcastle Institute for Cell and Molecular Biosciences, University of Newcastle; and Professor Paul Walton, Department of Chemistry, University of York). He will follow up on this soon.
- g) IUPAC no longer objects to members serving on the committee for longer periods. Continuity in JCBN membership is essential for its functionality. TD will thus continue to serve on the committee.
- h) The JCBN recommends a meeting between IUBMB and IUPAC representatives to clarify their positions regarding the funding of JCBN and the terms and limits of participation. A potential opportunity is the upcoming meeting in Basel. KHH and GPM will follow up on this matter.

18) Any other business

- a) Many of the documents issued by JCBN are only available in digital format via the private website operated by GPM and are not posted on the websites of either IUPAC or IUBMB. During the 2017 meeting it was proposed that IUBMB should host these

documents. RC has inquired with Mike Walsh (president of IUBMB) about this option, but it turned out that doing so would be too costly. AGM has pointed out that he keeps backup copies of these documents.

19) Date and Place of the 2019 Meeting

The next meeting will take place in Braunschweig, Germany on 12-14 of June 2019.

JCBN thanks GPM and Stuart Govan from the Royal Society of Chemistry for their help in organizing the meeting.