IUPAC DIVISION VII Chemistry and Human Health

Division VII Meeting, Paris, July 6 & 7, 2019

Draft Meeting minutes

Dates

- Saturday July 6th 2019, 9-17 hours, Venue: Palais des Congrès de Paris. Room: 305
- Sunday July 7th 2019, 9-17 hours, Venue: Palais des Congrès de Paris. Room: 305

DAY 1 (Saturday):

1. Welcome and introductions (Rita Cornelis)

Rita Cornelis welcomed all members of Division VII, guests and Young Observers Each of the attendees introduced himself/herself.

In attendance: Rita Cornelis (President), Tom Perun (Past-President), Helle Møller-Johannessen (Vice-President), Vladimir Gubala (Secretary), Vincenzo Abbate, Gerd Schnorrenberg, A. Ganesan, Geok Bee Teh, Balu Balasubramanian, Brandon C. Presley, Janos Fischer, Linda Johnston, Hassan Ibrahim, Ling Peng, Doug Templeton (Past President), Lewis Whitehead (lewis.whitehead@me.com; guest), Claudia Contini (c.contini@imperial.ac.uk, Young Observer), Janos Fischer, Claude Guillou (claude.guillou@ec.europa.eu; guest), Lyoma Guillou (lyoma.guillou@me.com; guest), Natalie LaFranzo (Vice President - Market Development | Cofactor Genomics Councilor | St. Louis Section American Chemical Society (nlafranzo@gmail.com), guest)

Apologies: John Duffus, Mike Schwenk, Nestor Carballeira, Paula Gomes, Chulbom Lee

2. Approval of Agenda

The agenda, which was sent out by email, was approved.

3. Approval of Minutes of Previous Meeting (Boston)

The minutes of the Division VII meeting in Boston (August 2018) were approved.

4. **Report of the Division President**

Rita Cornelis gave a brief summary of her Report to Bureau 2019 (available on the Division VII IUPAC page: https://iupac.org/who-we-are/divisions/division-details/?body_code=700). She outlined a summary of the activities in Division VII and highlighted the role of the four Subcommittees (SC): Drug Discovery and Development (SC-D3) Chair G. Schnorrenberg,

Toxicology and Risk Assessment (SC-TRA) Chair J. Duffus, Nomenclature for Properties and Units in Clinical Chemistry (SC-NPU) Chair H.M. Johannessen and SC on Public Relations and Election, chair Tom Perun. The subcommittees reported the progress of their ongoing projects.

5. Achievements of Division VII in the frame of IUPAC 100

Rita Cornelis is a member of Project No 2016-024-2-020, Planning and coordination of global activities for the celebration of IUPAC 100 in 2019. She organized the event "Empowering Women in Chemistry' a Global Networking Event" in Brussels on February 12, 2019 attended by 150 participants.

Division VII congratulated Geok Be Teh with her recent appointment as President of the Varsity College, Kolej Universiti Selaton, Malaysia. She is the first woman ever to be appointed to that position since its foundation. An article about her success can be read on the site:

https://www.thestar.com.my/metro/metro-news/2019/02/26/varsity-college-welcomes-firstwoman-president/#3zA7vxI7Z6OeBKZL.99

At the meeting in Paris, Vladimir Gubala organized a game of post-it notes with the attendees. The purpose was to generate ideas not only about the state of the art of Division VII, but also about its future and that of IUPAC. Suggestions popped up, such as a switch from less standard-style dissemination to more modern ways using any available technology, more attractive to younger audiences

Janos Fischer gave a brief expose about his achievements. He presented the cover pages of all his books and he also discussed his next goals.

6. Update on Division membership (Tom Perun)

Tom Perun explained that only two members from the nominating committee can be from the Division. These were Tom Perun and Helle Møller-Johannessen. The third person was supposed to be John Duffus, but the Secretary General Richard Hartshorn objected because John was too closely associated with the Div VII. He was replaced by Birger Heinzow, who has been a member of the Commssion on Toxicology in the past.

The membership list of Division VII for the biennium 2020-2021 reads as follows:

The **Titular Members** are: Rita Cornelis, President Helle Møller Johannessen, Vice President Vladimir Gubala, Secretary Gerd Schnorrenberg Linda Johnston Tom Perun Geok Bee (Sharon) Teh Balu Balasubramanian Xiaohong Fang Brandon Presley

The Associate Members are:

Vincenzo Abbatte, UK Nestor Carballeira, Puerto Rico Paula Gomes, Portugal Chulborn Lee, Korea Ling Peng, France Milena Popova, Bulgaria

The National Representatives are:

Hassan Ibrahim, Egypt Janos Fischer, Hungary Henna Veijaleinan, Finland Michele Saviano, Italy Roland Pieters, The Netherlands Abdullah Nuhu, Nigeria Igor Opsenica, Serbia, Tun-Cheng Chien, Taiwan

7. Finances of the Division (Rita Cornelis)

The budget allocation of Division VII for the biennium 2018-2019 reads as follows: Total \$ 52 300 Projects 30%: \$ 36 610; actuals July 2019: \$ 14 500, positive balance \$ 22.110 Operation 70%: \$ 15 690; actuals July 2019: \$ 17 644, (negative balance \$1 954)

Due to financial restrictions, the budget for operations has been scrapped in the biennium 2020-2021. This implies that there is no money for a Division VII meeting in 2020. The expenses to attend the General Assembly in 2021 are not on the Division budget, but directly on that of the IUPAC treasury. The Division will be allocated in 2020 part of its budget for projects, and the remaining part in 2021.

The group explored the possibility to have a face-to-face division meeting in 2020. Those members, who find their own financial resources, may convene in a location where a free of charge meeting room is available. The Royal Academy in Brussels or the Danish Health Data Authority in Copenhagen are possible locations. Those who cannot attend in person may then join in a teleconference. It could also be that only a teleconference for all members can be envisaged.

Doug Templeton reminded the audience that there is an alternative source of funding, i.e. from the Project Committee. They fund interdivisional activities. In the current biennium, the Project Committee budget is still under spent.

8. Structure and competency of the subcommittees, its chair and membership Updates from Subcommittees

A. Drug Discovery and Development (SC-D3) (Gerd Schnorrenberg)

Gerd Schnorrenberg presented his update in three parts:

1. Ongoing projects

a. <u>Medicinal Chemistry in Drug Discovery and Development, India 2019</u>, Project <u>2018-006-1-700</u>

The project leader: Balu Balasubramanian, said this event was very successful, and counted 200 participants.

As this course has already been financially endorsed four times by our Division, Balu Balasubramanian said that he may now go ahead with mainly funding from the industry.

b. <u>The emerging problem of Novel Psychoactive Substances</u>, Project <u>2014-019-1-700</u>, The project leader Vincenzo Abbate explained it consists of 2 parts:

i) synthetic cannabinoids – A first technical report has been published: The ongoing challenge of novel psychoactive drugs of abuse. Part I. Synthetic cannabinoids (IUPAC Technical Report), *Pure and Applied Chemistry*, 90(8), pp. 1255-1282, 2018, <u>https://doi.org/10.1515/pac-2017-0605</u>.

ii) synthetic cathenones – in preparation. Vincenzo reported that the team has two new members: Claude Guillou and Azell Carter.

Vincenzo presented a talk at the 7th Seminar of European Customs Chemists in Budapest, titled: NEW PSYCHOACTIVE SUBSTANCES: WHY IUPAC STANDARDS MATTER TO CUSTOMS CHEMISTS? under the umbrella of IUPAC on the topic of harmonising the nomenclature and structural representation of drugs and chemicals.

This project lead by Vincenzo Abbate is a joined SC-D3 + SC-TRA activity.

The group discussed how best to engage with ACS (new compound class drugs) and with Committee of Chemical Education to disseminate the summary of this project to laymen, particularly to young audiences. The Young Observer (Claudia Contini) commented that at the Imperial College London, many other Schools and young learners are keen to engage with the scientific activities of IUPAC. Division VII welcomes its participation.

- c. Human Drug Metabolism Database (HDMDB) Project 2011-018-1-700, Chair Paul Erhardt. The issue is that some task group members do no longer respond to emails about their involvement in the project. However, the project has been finalized and papers have been / will be published to disseminate the results.
- d. Glossary of terms used in combinatorial chemistry, Project No.: 2003-044-1-700, Chair A. Ganesan
 Ganesan informed the group that a 20-page manuscript (with unknown number of definitions) has been prepared in 2018 and it would be submitted for publication to PAC.
 In the mean time a draft manuscript was received for review by Gerd Schnorrenberg. The manuscript was distributed to SC-D3 members, feedback was forwarded to A. Ganesan.

- d. Implementation of regular project updates, as requested by the IUPAC secretariat.
 The chair must update on the progress of each project, more particularly its milestones. These will then be reviewed during the subcommittee meetings.
 Project updates at every SC-D3 meeting/teleconference have been implemented.
- 2. New projects:
 - a. IUPAC proposal 2019-019-1 by Michael N. Liebman entitled "Impact of Objective Analysis of Clinical Trial Failures on Drug Discovery and Development Processes

The project leader solicits the co-operation of the SC-TRA and SC-NPU.

b. IUPAC proposal 2019-018-1 SC-D3 Newsletter by M. Liebman.

The aim of this project is to develop and support a newsletter to facilitate D3's commitment to the challenges and opportunities in this area, both in academia and in the pharma industry. This electronic newsletter is complimentary to IUPAC's Chemistry International journal and will be focused on "Drug Discovery and Development Chemistry". The objectives include: a) Highlighting contemporary scientific topics, pertinent to Drug Discovery and Development Chemistry

b) Circulation to all Division and subcommittee members as well as the much broader pharma industry and academic communities to enhance the visibility of the D3 subcommittee and facilitate recruitment of new subcommittee members.

c) The proposed schedule for publication would initially be 3 times a year.

Tom Perun suggested creating a link to the ACS Medicinal chemistry division, which currently has 7000 members.

c. Janos Fischer – Successful Drug Discovery – book series: volume 4 will be published in 2019. Volume 5 is in the pipeline. Some discussion was held around the need to include section editors, but Janos said it would complicate future books. He also said that today the new trend between readers consists in purchasing chapters on line instead of the hard copy book

3. The IUPAC-Richter Prize 2018 was awarded in Nashville to Peter D. J. Grootenhuis of Vertex Pharmaceuticals for the invention, discovery and development of the drug ivacaftor (Kalydeco) for the treatment of cystic fibrosis.

Next prize will be awarded in Basel in 2020. Nominations are open until December 2019.

So far only one or two women were nominated for this prize; hopefully this will change in the future.

In summary, Gerd presented some changes in how the SC operates. The traditional meetings will be replaced with 2 x teleconferences + 1 x face-to-face meeting, alternatively held in the US and EU. He will also update the membership list.

B. Nomenclature for Properties and Units (NPU) (Helle Møller Johannessen)

Report from the meetings in the Steering Committee on NPU

Helle gave two reports: a first one about the NPU subcommittee and a second one on NPU steering committee.

the

NPU SUBCOMMITTEE

- a) Joint IFCC-IUPAC committee Helle introduced the objectives of the SubCommittee on NPU (SC-NPU), and explained how the SC-NPU is organized. The IUPAC projects aims to improve the NPU coding system, as well its technicality as its terminology. The NPU terminology is a collection of more than 27 000 NPU IDs and their definitions of clinical laboratory result items. They are used to communicate patient examination results safely between laboratory information systems, hospital patient records, GPs and local and national data repositories.
- b) Since 2014, there has been an increased demand for new NPU definition
- c) and their codes, partly because of:
- d) several Scandinavian users of the NPU terminology
- e) development of new technologies in the laboratory area, especially in the genetic field
- f) increased demand in the area of substance abuse
- g) SC-NPU the members are getting used to Skype meetings, although information is more difficult to pass through than by face-to-face
- h)
- i) Project 2014-017-1-700 SNOMED CT very useful in the context of NPU definitions; The NPU codes cover 598 elements of which 376 (63 %) could be assigned a SNOMED CT code. A large groups of non-matching elements e.g. antibodies (n=99) and genes (n=20) are however represented slightly differently from those in SNOMED CT.
- a) **IUPAC Project 2016-044-2-700** *Online Dynamic NPU manual* The objective is to establish an updated manual of the NPU terminology, comprising the principles and special rules in the terminology. The Dynamic NPU manual will be a freely accessible online manual on the www.NPU-terminology.org website.
- b) Project 2019-009-1-700 What is the NPU Terminology and how is it used
- c) This project aims to increase the general knowledge of the NPU Terminology, create interest and demonstrate the use and the value of terminology. The outcome of the project is a Youtube video:

<u>https://www.youtube.com/watch?v=7Qw4d0uhxqQ&t=55s</u>. Div VII watched the Youtube video and it was very well received.

NPU STEERING COMMITTEE

In 2014 IUPAC, IFCC and the Danish Health Data Authority made an important agreement. One of the key points was to establish the Steering Committee on NPU Terminology.

They defined:

i) Roles of the steering committee:

- ii) Responsible for the Governance and Strategic planning
- iii) Work out rules and operation procedures
- iv) 'Licensing' of NRC' for translation and publication rights

v) Establishing high level of external links with other organizations, departments, companies etc.

For more information: http://www.npu-terminology.org

C. Subcommittee on Toxicology and Risk Assessment (TRA) (John Duffus)

Rita Cornelis presented the update on TRA instead of John Duffus.

Completed Projects:

Project 2009-034-2-700, Chair G. Nordberg, Risk assessment of effects of cadmium on human health, Published Online: 2018-01-10, DOI: <u>https://doi.org/10.1515/pac-2016-0910</u>, PAC 90(4) pp 755 – 808, 2018.

Project 2013-007-1-700, Chair V. Gubala, Nanomaterials.

Two separate technical reports have been submitted to PAC with the following title:

– Engineered Nanomaterials and Human Health: Preparation, Functionalization and Analytical characterization, PAC, 90(8), pp 1288 – 1324

Engineered Nanomaterials and Human Health: Applications and Nano toxicology, 90(8), pp 1325
 1356, 2018

Cover feature titled "Nanomaterials – On the brink of evolution? or the endless pursuit of something unattainable?", published in *Chem Int* April 2017, pp. 10-13.

Project 2016-045-2-700, Chair N.González Rojano and <u>L. Johnston</u>, Safety of engineered nanomaterials, The workshop was held in Quertaro, Mexico, Sept 28-29, 2017. Report published in CI, October 2018

Current Projects:

Project 2017-005-3-500, Chair V. Gubala, Analytical chemistry of nanomaterials - critical evaluation, In development. Last progress report 25 May 2017

Project **2017-012-1-700**, Chair D.M.Templeton (with J.H.Duffus and M.Schwenk), Glossary of Terms in Molecular Toxicology, Final draft has been submitted to the Division for approval. It will next be submitted to ICTNS and finally to RSC Publishers.

Project 2017-040-1-700, Chair V. Gubala, Chemistry in the classroom, In progress.

Project **2017-035-2-600**, Chair L. Johnston and Rai Kookana, Human health considerations of nanoenabled pesticides for industry and regulators, Recent ref of relevance: Melanie Kah, et al. 'A critical evaluation of nanopesticides and nanofertilizers against their conventional analogues', *Nature Nanotechnology*, 2018, published online 7 May 2018, https://doi.org/10.1038/s41565-018-0131-1

John Duffus is unfortunately unable to continue as Chair of the SC TRA. The Division welcomed Vincenzo Abbatte as the new chair of TRA.

D. Subcommittee on Public relations and Election (Tom Perun)

Tom Perun explained that Division VII has a set of representative slides and a poster to present at conferences and symposia. However, he needs input from the project chairs to update these slides and the poster. Tom pointed out that some projects should continue to be promoted because of their high value, despite the fact that some were completed some time ago.

9. New Projects

The group was urged to submit new projects a.s.a.p., because although there is still a remaining balance, new project proposals need to be reviewed and accepted before December 2019 to get funding in the current biennium. Till now there is no transfer of remaining project money to a next biennium.

Recent submissions are: two project proposals by M. Liebman, and one by J. Fischer, as outlined under SC DDD.

10. Social Media + IUPAC Division VII Website (Vladimir Gubala)

Updates on IUPAC webpage - information from members

The Division VII webpage on the IUPAC site has a new photo of the members attending the meeting in Paris. As a group, we do not have a separate Twitter, Instagram and Facebook accounts. Some other divisions have this but since IUPAC as an organization has become more active on social media, the group did not propose that we should have our own.

DAY 2 (Sunday):

11. Meetings attended by members

- Report on Bureau meeting 2019 (Rita Cornelis)
- IUPAC 100 (all members)
- IYPT (all members)

Rita Cornelis summarized the outcomes of the Bureau meeting in Bratislava and the festivities organized to celebrate IUPAC100 and IYPT. More details can be read on the IUPAC.org page.

• OPCW

Vladimir Gubala reported on a meeting he attended in November 2018 and the request from OPCW to collaborate on mapping of chemical substances that can be used as chemical weapons, as well as on creating educational material to educate young people about the danger of chemical weapons

12. Interdivisional Activities

CCE (Sharon Teh)

The ACCC7 invitation was made for all Division VII members. The fees are waived for this meeting. Sharon will need to be in contact with CCE.

The group was informed about signature conferences NICE, which are scheduled every two years. It has become compulsory that organizers involve teachers.

COCI (János Fischer)

The connections with COCI have faded away. This will be restored as Carolyn Ribes accepted to have Gerd Schnorrenberg and Balu Balasubramanian as representatives of Division VII within COCI. Whereas Gerd would be present at the COCI meetings in Europe, Balu would do so in USA and Asia.

•

ICTNS

Rita Cornelis was present at the ICTNS meeting.

The President of ICTNS Jürgen Stohner stated that all manuscripts, be it in PAC or as a book, needed approval of the Division prior to submission to ICTNS. This may in principle be extended to video films.

Draft manuscripts may also be available on the IUPAC.org site (world leaders) for public scrutiny.

ISMC

Vladimir Gubala reported on the activities of ISMC. He explained the concept of ISMC and invited members to attend a follow-up ISMC meeting on Monday July 8th.

13. Cooperation with Other Organizations

- ACS (American Chemical Society) (Tom Perun) Tom Perun reported that he was on the executive committee of Medicinal Chemistry. Tom participates regularly in these meetings, representing our Division.
- IFCC (International Federation of Clinical Chemistry) (Helle Møller-Johannessen) Helle reported on the analytical/clinical aspect of this committee (See Helle's report under 8. B). IFCC pays members for meetings. Michael Liebman should be informed about this project.
- RSC (*Royal Society of Chemistry*) (John Duffus –to be Vincenzo in the near future) John Dufus was unfortunately not present, Vincenzo Abbate has updated on the RSC-IUPAC committee, chaired by Colin Humphries, Vincenzo was invited to join the meeting a few months ago. He is willing to share the meeting minutes – some of them speak about the financial problems in both organizations. Brazil left IUPAC and China rejected the new algorithm to calculate the annual subscription to be paid by its National Adhering Organization.
- OPCW (Organization for the Prohibition of Chemical Weapons) (Mike Schwenk and Vladimir Gubala) Covered in point 11
- any other organization with whom members cooperated

Vincenzo Abbate commented on the new partnership with the European Commission. Div VII has hosted Claude Guillou member of EC (Senior Expert, Directorate General Joint Research Centre, Directorate F – Health, Consumers and Reference Materials) during the GA meeting. Claude said that many of the projects he has heard about while being a guest might be of great interest to the EC as well. So there scope for a close collaboration.

14. Conferences of Interest for IUPAC Sponsorship

Application for IUPAC Endorsement

The group was informed about this but nothing specific came up for further discussion

15. Any additional business

- Claudia Contini suggested that IUPAC should issue a newsletter that could be distributed to young people. IUPAC could then provide innovative tools for chemists to do their work more efficiently. Fabienne Meyers of the IUPAC secretariat would be the person to contact to achieve this.
- Claudia Contini also suggested creating a Division VII Twitter account (similar to Division IV) to communicate the achievements of Division VII.

16. Next Division meeting

- Possibility for face-to-face meeting only either in Europe (Brussels/Copenhagen) or having it in the US. Tom pointed out that we use the division meetings to elect future presidents.
- Any future teleconferences should be organized as 3 hours blocks, rather than the whole day. Perhaps in July 2020.
- Nominations for Emeritus member were discussed. Mike Schwenk will be nominated for an Emeritus Fellowship of Division VII during the next biennium.