

Report to Council 2021
Division VII Chemistry and Human Health
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I. Highlights and/or Executive Summary:

Due to the turmoil created by the Covid pandemic, members of Division VII had to adapt their lifestyle. They expressed limitations to the time that they could devote to IUPAC. I hope that in 2022 prospects will be better and face-to-face meetings restored. These are quintessential for stimulation and efficiency of the work within the subcommittees by scientists residing all over the globe. Teleconferences are not able to sustain cohesion between members to the same extent.

The three subcommittees (SC) of Division VII are structured as follows:

- Drug Discovery and Development (DDD), Chair Gerd Schnorrenberg
- Toxicology and Risk Assessment (TRA) Chair Vincenzo Abbate, succeeding John Duffus
- Nomenclature for Properties and Units in Clinical Chemistry (NPU) Chair Ulla Magdal Petersen, succeeding Helle Johannessen

The membership of the 3 subcommittees has been updated and new members joined. They are listed on the iupac.org site, Division VII.

The subcommittees will continue their actions as usual. The SC DDD has Teleconferences every trimester.. The subcommittees TRA and NPU continue to work on their projects.

The status of the ongoing projects (total 10 + 4 interdivisional projects) are given below. Seven projects were completed. The publications include 3 books. They all contribute to IUPAC's goal to provide an indispensable worldwide resource for chemistry related to human health.

The royalties of all books, past and new publications, contribute to the revenue of IUPAC, be it in a modest way. The quality of these books is outstanding and the amount of work the authors have put into these volumes is impressive.

Another gem of Division VII and more particularly of the DDD subcommittee is the attribution of the 2020 IUPAC-Richter Prize in Medicinal Chemistry to John Macor, PhD, Global Head Integrated Drug Discovery, Sanofi, for the development of drugs for the treatment of migraine

In 2020 Mike Schwenk was awarded the Emeritus Fellowship. He was Titular Member and Secretary of Division VII (2020 – 2016) and currently corresponding member with the Interdivisional Standing Committee on Green Chemistry for Sustainable Development.

A major priority of Division VII is the revision of the Goldbook. Doug Templeton has already initiated this. The project (#2021-004-2-700), entitled

Gold Book update of terms for chemistry and human health,

was approved March 2021. The task group consists of members of each subcommittee: Gerd Schnorrenberg of DDD, Brandon Presley and John Duffus of TRA and Helle Møller Johannessen of NPU.

II. Plans and priorities for this biennium, and beyond:

Goals for IUPAC Division VII Subcommittee Drug Discovery and Development (DDD)

_Generate new projects in line with IUPAC's strategic goals and the changing landscape in Drug Discovery and Development

-Progress and finalize ongoing projects successfully

_Implement new working modes in SC D3 to increase interactivity between SC members and external experts in the area D3

_ Utilize SC D3 NEWSLETTER as a vehicle to increase the IUPAC exposure and to explore potential funding mechanism for D3 specific projects that may fall within the broader scope of D3, for ex: other factors that influence the chemistry of D3 such as Chemistry–Biology feedback loop

_Increase visibility of SC D3 in the Drug Discovery and Development community

_Attract new members for SC D3

Goals for IUPAC Division VII Subcommittee on Toxicology and Risk Assessment (TRA)

_Coordinate projects relating to toxicology and risk assessment and to provide a forum for discussing their progress

_Provide a forum for initiating new project submissions in toxicology and risk assessment appropriate to Division VII

_Report to the Division VII President and the Division Committee on the progress of current projects and to initiate new projects

_Provide connections to other organizations concerned with toxicology, between others with OPCW

_Interact with chemists in the Chemical Industry worldwide in the field of toxicology and risk assessment

_Offer advice to the Division President and Committee on matters concerning toxicology and risk assessment, in all their aspects from the purely chemical to the protection of human health and the natural environment

_The SC's strategy for next biennium (and beyond) will be to strengthen links with other Divisions (e.g. new interdivisional project "A database of chemical structures and identifiers used in the control of WADA Prohibited Substances") between Divisions VII-VIII as well as create new links with appropriate International bodies (e.g. EC and WADA) to primarily harmonise and create a unique chemistry language with respect to drugs of abuse and misused drugs

Goals for Division VII Subcommittee on Nomenclature for Properties and Units (NPU)

The NPU coding system provides a terminology for Properties and Units in the Clinical Laboratory Sciences. The availability of electronic patient records would greatly increase the quality of health care, reduce health care cost and facilitate epidemiological surveys to the benefit of patients worldwide. In developing a generalized architectural build up and adherent structures, there is a need for systems and schemes in each of the medical domains to support and populate the electronic patient record. In the domain of clinical laboratory medicine the guidelines from IFCC-IUPAC on the structuring of properties, on kind-of-properties and on units are needed if a coherent system with global acceptance is to be worked out. The SC-NPU maintains its website www.npu-terminology.org. to make available the complete contents of the generic NPU database for electronic downloading of the NPU Terminology.

The goals are: _Make recommendations on NPU for reporting clinical laboratory data that conform to or adapt current standards of authoritative organizations, that will improve their utilization for health care

_Provide a connection with other organizations concerned with NPU, such as BIPM, CEN and ISO, and, by extension, clinical laboratory science societies, and the in vitro diagnostics industry, to ensure that problems encountered by health care professionals in the area of NPU are considered by those organizations

_Act as a consultant group on NPU in clinical chemistry and, by extension, in the rest of clinical laboratory sciences to international scientific panels, regional and national clinical laboratory sciences organizations, editors of scientific journals, manufacturers of clinical laboratory instrumentation and products, and to individual clinical laboratory professionals and other health care professional

_Develop activities with other Organizations: an upcoming collaboration between WHO, LOINC and NPU aims at coordinating the use of terminology and classifications in individual clinical laboratory professionals and other health care professionals.

III. Overall report of Division/Committee activities and achievements during the later part of the 2018-2019 biennium and through 2020 organized by the Goals and Objectives laid out in the current IUPAC Strategic Plan

Ongoing Projects

Project 2003-044-1-700, Ganesan

The manuscript was submitted to ICTNS for publication in PAC. It appears to be still under review.

Project 2010-035-3-700, Johannessen

Final Drafts have been circulated, and should be ready for publication very soon. Should not be difficult to finalize, but it is very important to do it right as it will be an increasingly important part of the NPU terminology work.

Project 2011-018-700, Erhardt

The project it is still scheduled for June 2021 but if COVID continues to slow things down Prof Erhardt may have to extend that. He will know better about such a forecast in the near future

Project 2014-017-1-700, Karlsson

The manuscript was approved by Division VII and submitted as a technical report for publication in PAC.

Project 2014-019-1-700, Abbate

The project on psychoactive drugs was extended until Dec 2020. However, the combination of the pandemic and paternity leave has meant there has not been much progress this year, except for two Skype meetings to discuss a potential way forward and make soon a decision whether to complete part 2 and publish a second paper or to close the project.

Project 2016-044-2-700, Hansen

The project is not finished yet, but about 80% of the main content of concepts (kind-of-properties) are listed. Links to the general NPU concept model is not completed. A review group consisting of members of the three release centers is considered.

Project 2017-040-1-700, Gubala

Four animations were created under this project and they were *Carbon cycle*, *2 x Plastics in the ocean*, *Cell cycle and medicine*.

In February 2020, the videos were embedded in a lesson plan, created by Claire Saunders (one of the task members) and supplied to chemistry teachers in three secondary schools: one in London, one in Broadstairs (county Kent) and one in Medway (county Kent). The aim was to collect feedback from teachers to improve the lesson plan and roll it out to multiple schools, firstly in the UK.

Unfortunately, the progress of this project was significantly slowed down due to Covid.

Project 2019-018-2-700, Liebman

The project has been somewhat delayed because of the involvement of the Chair in Covid modelling which had to be prioritized but progress has been made.

Project 2019-019-2-700 Liebman

The subject is: Impact of Objective Analysis of Clinical Trial Failures on Drug Discovery and Development Processes.

The members have formalized the relationship with Accelerated Cures, the patient advocacy group who has extensive data and is extending our interaction to the network of institutions and foundations. In addition, they are in discussion with the DOD and separately with the Veterans Health Administration, which is not in DOD but in HHS. Additionally they have connected with a group that is developing therapeutics and access comprehensive patient. Data have been brought in a senior data analyst.

To frame all of this the members have extended the data model and the approach for knowledge graph development. They are working with a biomarker database

Project 2021-004-2-700, Templeton

Gold Book update of terms for chemistry and human health,

The task group consists of members of each subcommittee: Gerd Schnorrenberg of DDD, Brandon Presley and John Duffus of TRA and Helle Møller Johannessen of NPU.

Interdivisional projects

Project 2020-016-3-020, Chiu and Cesa

IUPAC's role in extending the global gender project: A global approach to the gender gap in mathematical and natural sciences: how to measure it, how to reduce it. This project is a cooperation of 8 Divisions.

Project 2020-019-4-050, Apotheke and Saha

Examples of the introduction of sustainable development as well as green industrial processes for secondary school chemistry and introductory chemistry, a cooperation of CCE, COCI, Chemrawn, Divisions VI & VII.

Project 2020-017-2-700, Abbate

A database of chemical structures and identifiers used in control of WADA prohibited substances, a cooperation of Divisions VII & VIII

Enhancing capabilities for the mitigation of chemical risk. The dissemination of the emergency response guidebook (ERG) in Russian-speaking countries, a cooperation of the IUPAC Chemistry and the Environment Division (VI), the Chemistry and Human Health Division (VII) and the Committee on Chemistry Education (CCE).

Project 2020-020-2-600, Guidotti

In progress

COMPLETED PROJECTS

Project 2016-045-2-700, Johnston

Project is complete. A first paper has been published in NanoImpact: <https://doi.org/10.1016/j.impact.2020.100219> and a second one:

Linda J. Johnston, Norma Gonzalez-Rojano, Kevin J. Wilkinson, and Baoshan Xing, Challenges for evaluation of the safety of nanomaterials, Chemistry International, January – March 2021, pages 4 – 7

Project 2019-009-1-700, Johannessen

The project is finished, and we are working on a notice for CI. The resulting video was accepted for the Jubilee IUPAC conference in Paris. It can be viewed here: <https://www.youtube.com/watch?v=7Qw4d0uhxqQ>. It is suggested that the video technique may be useful for explanations and demonstrations of the more difficult NPU concepts.

Project 2017-012-1-700, Templeton

The project is completed. The book entitled 'Glossary of Terms Used in Molecular Toxicology' has been published by the RSC in May 2020.

Project 2018-006-1-700, Balasubramanian

Completed in 2019

Project 2018-001-3-700, Fischer

The project was completed according to schedule.

Vol-4 of Successful Drug Discovery, János Fischer (Editor), Christian Klein (Editor), Wayne E. Childers (Editor), has been published in 2019. It received a very positive review.

This book was also published in Chinese in 2021. The Chinese Publisher has purchased the license from Wiley

Project 2019-021-1-700, Fischer

The project was completed according to schedule

Vol 5 of Successful Drug Discovery, Janos Fischer, Christian Klein, Wayne E. Childers was published in February 2021

Project 2000-009-1-700, Erhardt

Glossary and tutorial of xenobiotic metabolism terms used during small molecule drug discovery and development (IUPAC technical report), Pure and Applied Chemistry 2021. Paul Erhardt*, Kenneth Bachmann, Donald Birkett, Michael Boberg, Nicholas Bodor, Gordon Gibson, David Hawkins, Gabrielle Hawksworth, Jack Hinson, Daniel Koehler, Brian Kress, Amarjit Luniwal, Hiroshi Masumoto, Raymond Novak, Phillip Portoghese, Jeffrey Sarver, M. Teresa Serafini, Christopher Trabbic, Nico Vermeulen and Steven Wrighton

This project originated more than 15 years ago with the intent to produce a glossary of drug metabolism terms having definitions especially applicable for use by practicing medicinal chemists. A first-draft version underwent extensive beta-testing that, fortuitously, engaged international audiences in a wide range of disciplines involved in drug discovery and development. It became clear that the inclusion of information to enhance discussions among this mix of participants would be even more valuable. The present version retains a chemical structure theme while expanding tutorial comments that aim to bridge the various perspectives that may arise during interdisciplinary communications about a given term. This glossary is intended to be educational for early stage researchers, as well as useful for investigators at various levels who participate on today's highly multidisciplinary, collaborative small molecule drug discovery teams.

IV Publications

Book Vol-4 of 'Successful Drug Discovery, J. Fischer, Christian Klein, Wayne E. Childers, Wiley, 2019
This book was also published in Chinese in 2021. The Chinese Publisher has purchased the license from Wiley

Linda J. Johnston, Norma Gonzalez-Rojano, Kevin J. Wilkinson, and Baoshan Xing, Challenges for evaluation of the safety of nanomaterials, NanoImpact, 18, 100219, 2020

Book entitled 'Glossary of Terms Used in Molecular Toxicology', authors: D. Templeton, J. Duffus and M. Schwenk, published by the RSC in May 2020

Linda J. Johnston, Norma Gonzalez-Rojano, Kevin J. Wilkinson, and Baoshan Xing, Challenges for evaluation of the safety of nanomaterials, Chemistry International, January – March 2021, pages 4 – 7

Glossary of terms used in molecular toxicology, D.M. Templeton. M. Schweik, J. Duffus, Commentary by Douglas Templeton, Chemistry International, January March 2021, page 40 – 41

Book, Vol 5 of Successful Drug Discovery, Janos Fischer, Christian Klein, Wayne E Childers, 2021

Paul Erhardt*, Kenneth Bachmann, Donald Birkett, Michael Boberg, Nicholas Bodor, Gordon Gibson, David Hawkins, Gabrielle Hawksworth, Jack Hinson, Daniel Koehler, Brian Kress, Amarjit Luniwal, Hiroshi Masumoto, Raymond Novak, Phillip Portoghese, Jeffrey Sarver, M. Teresa Serafini, Christopher Trabbic, Nico Vermeulen and Steven Wrighton,
Glossary and tutorial of xenobiotic metabolism terms used during small molecule drug discovery and development (IUPAC technical report), Pure and Applied Chemistry 2021.