

IUPAC Division VII - Chemistry and Human Health



The plan for the division for the next biennium (and beyond) remains :

- to develop new projects on the theme of Chemistry and Human Health
- to further strengthen our links with other Divisions to ensure broader collaboration (interdivisional projects)
- to support further collaborations with other scientific organizations (e.g. SAICM, IFCC, WHO, WADA, LOINC, SNOMED)

Division VII has interests ranging from research and training in medicinal chemistry and drug discovery, engineered nanomaterials, emerging problems with the use of 'designer drugs', explanatory dictionaries, terminology and nomenclature of properties in clinical laboratory science, advances in immunochemistry and applications to human health, among others.

The Division activities are presently carried out by 4 Subcommittees:

- Drug Discovery and Development (DDD), Chair Gerd Schnorrenberg
- Toxicology and Risk Assessment (TRA), Chair Vincenzo Abbate
- Nomenclature for Properties and Units in Clinical Chemistry (NPU), Chair Ulla Magdal Petersen ٠
- Public Relations and Election, Chair Tom Perun

The SubCommittee on Drug Discovery and Development.

Recent and ongoing projects:

- Revision of Glossary of terms related to Drug Metabolism (P. Erhardt), Computational Chemistry (Y.C. Martin), Medicinal Chemistry (D.R. Buckle) and Combinatorial Chemistry (A. Ganesan)
- Training Courses in the field: Medicinal Chemistry in Drug Discovery and Development. The project aims to build and optimize a basic medicinal chemistry course for industrial and academic scientists in India and other South Asian countries India 2019 and angina in 2024. (Balu Balasubramanian & William Greenlee)
- IUPAC book series: Successful Drug Discovery (Wiley Editor Prof. J. Fischer), last published: Volume 5



The Subcommittee on Toxicology and Risk Assessment.

The SC works to further strengthen links with other Divisions and International bodies (e.g. European Commission and World-Antidoping Agency) in new and ongoing projects.

Ongoing projects:

- The emerging problem of Novel Psychoactive Substances.
 - The objective of this project is to critically review the present status of "Novel Psychoactive Substances" (NPS) and how they are evaluated, with special regards to structure-activity relationships, synthetic and analytical aspects, and their potential biological effects. This will aid in increasing the awareness of NPS across the wider scientific



Technical Reports on: Human Drug Metabolism database. A survey is ongoing (P. Erhardt)

New projects:

- Analysis of Ph III Failures. Drug discovery and development most frequently fail during clinical trials as in vitro and pre-clinical studies do not effectively translate into success in humans, and attaining regulatory approval, many fail their commercialization goals. Medicinal chemists and scientists in drug discovery can benefit from understanding the cause of these failures. This project will create a database of such failures in Multiple Sclerosis as initial target. (M. Liebman)
- *Evaluation of the recent dynamic of the medicinal chemistry projects funding in academia.* The project task group plans to investigate this trend on a global level. The plan is to create a survey and distribute it among scientists in academia and grant agencies around the world to get exact information and statistics regarding this issue. (A. Gruzman)

The SC is involved in selecting an IUPAC-Richter Prize Winner every two years for outstanding achievements in medicinal chemistry. The 2022 IUPAC Richter Prize was awarded to Michael **E. Jung (UCLA)** in recognition of his research, which has afforded new drugs for the treatment of advanced prostate cancer. (Selection Committee, chair Prof. J. Fischer)



The D3 SC Newsletter aims to summarize information on SC D3 activities, inform on IUPAC news related to SC D3 and upcoming congresses in the field and attract new members for our subcommittee. The newsletter will facilitate D3's commitment to the challenges and opportunities in this area, both scientifically and in

the pharma industry. This electronic newsletter is complimentary to IUPAC's Chemistry International Journal. 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 much the broader pharma industry and academic communities to enhance the visibility of the D3 subcommittee, and facilitate recruitment of new subcommittee members.

c) The schedule for publication would initially be 2 times a year.



A database of chemical structures and identifiers used in the control of WADA Prohibited Substances. The aim of this project is to provide the anti-doping community with a database of relevant substances with the corresponding chemical structures and identifiers (InChI, InChIKey), guided by

IUPAC experts, for the identification and reporting of doping substances across and beyond World Antidoping Agency (WADA)-accredited laboratories.

A technical report will be published with these outcomes.



The Subcommittee on Toxicology and Risk Assessment in Interdivisional projects

Analytical chemistry of nanomaterials - critical evaluation (2017-005-3-500) Analytical chemistry of nanomaterials is an emerging issue. In addition to physicochemical characterization of shape, size, and structure of nanoparticles, analytical chemistry research considers isolation/purification and detectionidentification/ quantification/ spatial composition of pristine nanomaterials, nano-enabled products, and complex matrices of environmental, biological and food samples.



- Human Health Risk Consideration of Nano-enabled Pesticides for Industry and Regulators (2017-035-2-600)
 - The objective is to assist industry, contract research organizations and regulators to determine an acceptable and practical approach for generating the data relevant to human health risk assessment required for the registration of nano-enabled pesticide formulations.



Per and polyfluroalkyl substances (PFASs) in the environment: Information for emerging economies on PFASs analyses in environmental media and their impacts on human health (2019-029-1-600)

The objective of this project is to write a synthesis, based on critical evaluation of the current state of knowledge on per and polyfluroalkyl substances (PFASs), and to distill learnings that can be beneficial to



The SubCommittee on Nomenclature for Properties and Units (NPU).

Is a *joint committee* between IUPAC and the International Federation for Clinical Chemistry (IFCC) with membership from both organizations. Both parties have been – and still are – very active in providing *Terminology for Properties and Units in the Clinical Laboratory Sciences* – the **NPU Terminology.**

The NPU Terminology is a coding system and terminology for unique identification of examination results from clinical laboratories. It is extensively used in Denmark, Norway and Sweden - and in local use in other European countries.

This is expressed in a prescribed syntax and identified with a code: *NPUxxxxx* System— Component; kind-of-property = measurement unit NPU24866 Urine—Morphine; mass concentration = ? microgram per litre NPU02187 Blood—Glucose; substance concentration = ? millimole per litre

The basic principles and structure of the NPU Terminology are described in the 'Properties and Units' series of IFCC-IUPAC Scientific Publications and in international Standards on Metrology and Terminology.

Ongoing (and future) projects aim to support the further development of the NPU Terminology.

NPU codes for characterizing subpopulations of the hematopoietic lineage, described from their Clusters of Differentiation (CD) markers. (2021-022-1-700)

NPU03568 B-

 $? \times 10^{9}/L$

Thrombocytes; num.c. =

One of the significant trends in the Laboratory Scientific field is the use of immunotherapy treatment and the effect on cells. The project aims to establish an internationally accepted nomenclature for defining CD-markers for use in the NPU definitions.

Establishing definitions for nonreferenced terms in the NPU terminology. (2010-035-2-700) The objective is to establish a model for standardized definitions for non-referenced terms in the NPU Terminology. The project will be finalized during this year.

emerging economies.



Enhancing capabilities for the mitigation of chemical risk: the dissemination of the Emergency Response Guidebook (ERG) in Russian-speaking countries (2020-020-2-600)

A systematic dissemination of the ERG manual, previously translated into Russian, and a parallel awareness-raising campaign, with workshops and tutorials about its correct use in first responders' and chemical industrial workers' professional activities will allow Central Asian and Eastern European countries, where Russian is the common working language, to strengthen the preparedness of emergency operators and enhance their capability to cope with risks related to an unintentional or deliberate release of hazardous and/or toxic chemical substances.



- LC-MS Quantitative Method Validation and Performance: An Exemplified Guide (2021-036-1-500) The project aims to review the present status of validation methods critically and provide a broader and easy to follow guide for the validation steps in various application areas, with cross-references to definitions and further details.
- Personal Protective Equipment Disposal for the Future (2021-012-2-400)

Most personal protective equipment (PPE), such as disposable face masks, aprons and gloves, are made of synthetic or semi-synthetic organic polymers (i.e. plastics). During the pandemic use of PPE has increased significantly, as it is not only worn professionally but has become a permanent fixture in

society. The specific aim of this project is to critically evaluate existing data on the components used in PPE. Based on these data, possible ways of disposing of the waste related to PPE can be proposed. In order to raise awareness of the problems related to the use of PPE, educational material (a series of videos) and a technical note were produced; the first focus was on the general public, while recommendations to inform scientists, policy makers and industry will also be written.





IUPAC Co-owner of the

NPU Terminology

Representatives from the National Release

Centers on NPU (Repr. the users)

Committee on NPU

Danish Health Data Authority

IFCC Co-owner of the

NPU Terminology

The joint Committe-

SubCommittee on NPU (C-SC-NPU)

Completed project

An Online Dynamic NPU Manual

The NPU terminology is an evolving international medical laboratory terminology which is used in health care systems. However, the basic principle and structure of the terminology is described many publications, which are not updated. The objective is to establish an updated online manual of the NPU terminology, comprising the principles and special rules of the terminology. The manual is intended to provide easily searchable and updated information, and are freely accessible on the https://labterminology.com website.

The NPU terminology is overseen by *a Steering Committee* with members from the parties: IUPAC, IFCC, Danish Health Data Authority, joint SC-NPU and user representatives.

Terminological projects:

A collaboration on mapping the NPU and SNOMED terminologies

The SNOMED terminology is a worldwide clinical terminology limited for member countries. WHO-NPU cooperation

The Steering Committee on NPU has been invited to establish a terminological cooperation which has to do with enriching the WHO Family of International Classifications (WHO-FIC) with 'laboratory data specifications' from the NPU Terminology.

Representatives from DIV. VII have joined the major interdivisional project on Updating the Gold Book.

The task group, chaired by Doug Templeton, consists of members of each subcommittee: Gerd Schnorrenberg of DDD, Douglas Templeton of TRA and Helle Møller Johannessen of NPU. The work is ongoing according to advice from the JSIGB.

More information on the NPU Terminology:

- Website: www.npu-terminology.org
- Wikipedia entry: en.wikipedia.org/wiki/NPU terminology
- The NPU database for download of the Terminology:

www.npu-terminology.org/npu-database/

• Or the Danish NPU Terminology site: www.labterm.dk (download-eng.) For more information please contact; labterm@sundhedsdata.dk

