

## Part 1. Highlights and/or Executive Summary

For Division VII, the biennium 2024/2025 was an active period, with several notable achievements. As a division, we were able to manage our budget very well, endorse two new projects in 2024, hold and organize two meetings: one formal meeting held in Cambridge, UK, on May 18-19, 2024, one virtual in September 2024 (DP, VP, Secretary) and one all-members virtual meeting on February 5<sup>th</sup> 2025.

2024/2025 Division/Committee achievements:

### 1. Projects

- a. Completed - 2 projects were completed in 2024. As an example, project 021-022-1-700 was completed with the announcement published in *Chem. Int.* A technical report was published in PAC. (<https://doi.org/10.1515/pac-2023-0806>).
- b. Ongoing project highlights – several Division VII projects had a considerable progress in 2024. Of all active projects, led by or supported by Division VII, 65% were interdivisional projects, many of which also forge strong global cooperation with organizations such as WADA, WHO, UNDRR, ACS and several industrial partners, for example in medicinal chemistry. A more detailed report on the activities and achievements is presented in Part 3.
- c. New projects highlights – 2 new projects were funded in 2024, and both have started and are already ongoing. Another interdivisional project (2023-020-2-600) was approved in late 2023 and started in 2024. All new projects (i.e. 100%) are interdivisional collaborations. Project 2024-008-2-700 was funded as an interdivisional project between Div VII and Div I. This project aims to create comprehensive and standardized vocabulary for the field of photodynamic medicine. Project 2024-007-4-300 is also an interdivisional project, funded by Div VII, Div II and CCE. The main focus of this project is to explore and highlight the role of chemistry in addressing challenges related to human wellness and environmental sustainability. Project 2023-020-2-600 aims to develop a global Weigh of Evidence framework, which may be used by the crop protection registrants and regulators to inform hazard and risk assessment decisions.

### 2. Publications and conferences/symposia/workshops

Overall, 6 publications were published under the umbrella of Division VII. Four of them were published in Pure and Applied Chemistry, one was published in J. Med. Chem. and one online (<https://labterminology.com> website). IUPAC sponsored (organized under the Division VII umbrella) a drug discovery & development course for industrial and academic scientists (MCADDI 2024), held from September 22-27 in Bangalore. This course brought together leading scientists, industry professionals, and academics for an intensive five-day program. The event was co-sponsored by the American Chemical Society (ACS) Division of Medicinal Chemistry (MEDI), ACS Publications, and the Human Health Division of the International Union of Pure and Applied Chemistry (IUPAC). With close to 100 participants from the pharmaceutical and biotechnology sectors, the course provided in-depth training on the principles of medicinal chemistry and drug discovery.

Relevance to the IUPAC Strategic Plan: All Division VII outputs are strongly aligned with IUPAC Science board priorities and IUPAC Core Values, particularly in creating a standard language for the academic and industrial community, fostering outreach and engagement activities relevant to the role of chemistry, establishing new and strengthening existing cooperation with other global organizations.

## Part 2. Plans and priorities for the remainder of 2024-2025 biennium, and beyond

Division VII priority plan for 2025 – the overall priorities cover the following 5 points:

1. Project completion – specific focus will be on projects that started before 2020 and are either dormant or require specific input to restart the intended activities to drive completion.

There are currently 5 projects that started before 2020. The combined unspent budget across these projects is \$15,689.51. One of the Division VII priorities will be to drive the completion of the projects through frequent interactions with the task chairs and setting up realistic deadlines for both project completion and effective use of the remaining budget. Projects that are more than 5 years old and have no updates in 2025, despite increased divisional efforts to re-activate the project, will be terminated.

2. Highlight/Showcase/Support successful projects – successful projects will be highlighted for the division members in Div VII memos and showcased during the GA in Kuala Lumpur in July 2025.

Projects such as 2022-023-2-700, 2017-035-2-600 and 2023-036-1-700 are great examples of successful projects that are being/were carefully managed and completed in a timely manner. They are also excellent examples of projects that were disseminated in PAC and other high-impact scientific journals (e.g. Nature Nanotechnology) and these projects involved multidisciplinary task group and have links to international organizations such as WHO, OPCW and UNDRR. We aim to showcase these projects as examples and set them up as standards any other projects should aspire to as a goal in the 2024/2025 biennium and beyond.

We also aim to continue with the strong recognition and support of Division VII IUPAC Richter Prize in 2025 and beyond the 2024/2025 biennium.

3. Support of new (interdivisional) projects – specific emphasis will be placed on the support of the new interdivisional projects with task groups built across multiple chemistry sub-disciplines. This can encourage diversity, increase global scientific cooperation and interactions with other chemistry organizations and industry.

Several new projects are/were being presented for consideration. One specific example is a new opportunity for IUPAC to organize a multidisciplinary workshop as part of a potential EU project (Exploration of Plastic particles Origin, Solutions and Effects on Human Health). This would provide a new type of opportunity to have an IUPAC-organized workshop that would be funded by an external partner.

4. Integrate/recruit new members – in addition to integrating new members, we aim to keep frequent communication and engagement with existing members to keep their activity for IUPAC at a high standard.

Division VII will continue with integrating new members/observers to our divisional meetings and engaging with project task members. Good examples are two young and very efficient / active scientists currently involved in project 2023-036-1-700 (Dr Sully and Dr Pinero).

5. Increase impact from projects – reach a wider audience to increase impact from existing and successful divisional projects.

We will encourage task chairs/members to go beyond the traditional PAC dissemination and for every project, each task group chair will be asked to summarize it in a form of a 'highlight' in Chem. Int. or in a form of a short video clip that will be shared through IUPAC YouTube channel and other social media channels (Instagram, Facebook, X and TikTok etc.)

### **Part 3. Overall report of activities and achievements**

#### **A) Global cooperation that creates a common language for chemistry**

A new Division project in 2024 focuses on development of terminology relevant to biomedical and environmental effects of the photodynamic effect. The project team led by Francesca Giutini has members from 13 countries and has drafted a list of ~100 terms for inclusion which are now allocated to sub-groups for drafting definitions. The creation of a coherent glossary will reduce confusion and enhance acceptance of the approach within the scientific community.

The development of a database of chemical structures and identifiers used in control of World Antidoping Agency (WADA) Prohibited Substances aims to provide a common language to identify and report doping

substances which will include chemical structures with WADA names, their InChI and InChI Keys and other relevant identifiers. The first draft of terms has been compiled and the task group, led by Vincenzo Abbate, is engaging experts for input on the database format and debating the inclusion of additional terms. An IUPAC technical report is planned.

An inactive project led by Helle Johanessen on establishing definitions for non-referenced in the Nomenclature for Properties and Units (NPU) terminology database has been restarted and will be completed in this biennium. This project supports correct and standardized exchange of data across clinical laboratories and e-health systems, ensuring similar interpretation of results between laboratories and across countries.

The update of Division VII terms for inclusion in the Gold Book led by Doug Templeton completed the initial compilation of terms in late 2023, providing information on minor changes and changes that would require review. The joint Interdivisional Committee for this project has resumed regular meetings and the Division will review modified terms and work with other Divisions to reconcile terms that are duplicated between Divisions in the next year.

A project on development of a human health metabolism database led by Paul Erhardt has distributed a survey to gather input on the topics. The results are being summarized for publication in either PAC or Chemistry International. There have significant shifts in philosophy towards improved preclinical in vitro methods that impact how drug metabolism research is approached, and an extension of the project scope is being considered.

A partner project started in 2024 and led by Division VI aims to develop a global Weight of Evidence framework that can be used by crop protection registrants and regulators to inform hazard and risk assessment decisions. This will help to accelerate a greater adoption of novel approach methods to reduce the use of animal testing for crop protection chemicals.

## **B) Interactions that facilitate best practices in chemistry and chemical education**

Chemical hazard information profiles (HIPs) for United Nations Disaster Risk Reduction are being reviewed and updated by a team led by Richard Hartshorn. This high-profile project for the UN aims to reduce disaster risk and the IUPAC review is designed to account of the evolving nature of disaster risk. The project recognizes IUPAC's role as an authoritative organization for chemical nomenclature and standards. The HIPs are currently in the final review stage by UNDRR and WHO.

A week-long workshop was held in Bangalore, India in September 2024, co-sponsored by the IUPAC Medicinal Chemistry in Drug Discovery project, led by Balu Balasubramanian, and the American Chemical Society Medicinal Chemistry Division and ACS Publications. This workshop brought together 100 people including leading scientists, industry professionals, and academics and provided in-depth training on the principles of medicinal chemistry and drug discovery.

Michael Liebman leads a project on Analysis of Clinical Trial Failures and their impact on Drug Discovery and Development that aims to identify gaps in treatment options that impact drug discovery. Initial work focusing on multiple sclerosis was published in Journal of Translational Research in 2023 and an extension to infant/maternal mortality during pregnancy and hypertension will be completed in 2025.

The Drug Discovery and Development Sub-Committee will publish the next issue of its Newsletter in spring 2025 and will feature a summary of the project on recent trends in funding for medicinal chemistry research. A poster highlighting sub-committee activities is planned.

A project led by Arie Gruzman that aims to evaluate recent trends towards decreased funding for academic medicinal chemistry programs has published a summary of a global survey in *Journal of Medicinal Chemistry*. The data is now being used to develop recommendations for governments and funding agencies for continued investment in medicinal chemistry, particularly in emerging fields.

A partner project with Division III aims to highlight how chemistry can influence human wellness and environmental sustainability by running a video competition for young scientists that will involve young scientists in IPUAC and highlight IUPAC's mission and activities. Jaana Rysä will be one of the judges for the competition and winning videos will be widely disseminated.

Two other partner projects with Division V focus on (a) assessment of the present state of electroanalytical flow methods and devices for effective monitoring of selected chemical species and (b) development of guidelines for validation of LC-MS studies. A draft technical report is in preparation for the first project and the second project has completed a survey and is currently writing a technical report.

### **C) Connections with cognate disciplines and educational communities that contribute to sustainable development**

The most relevant project that contributes to sustainable development is project 2023-020-2-600. It will convene an international group of experts from academia, industry, government, and other institutions through a series of international workshops to review, evaluate, and disseminate the principles of WoE (Weight of Evidence) that integrates New Approach Methods (NAMs). The primary goal will be the development of a global WoE framework, which may be used by the crop protection (CP) registrants and regulators to inform hazard and risk assessment decisions. Such a framework will help accelerate and transition to a greater adoption of NAMs to reduce the use of vertebrates in human health and ecological assessments for CP.

### **D) Promotion of Diversity and Inclusiveness or values and ethics in science through responsible practice**

## **Part 4. Tabular Material**

### **a) Publications (2023-Feb 2025)**

J. Labuda, L. J. Johnston, Z. Mester, Z. Gajdosechova, H. Goenaga-Infante, J. Barek, S. Shtykov, Analytical chemistry of engineered nanomaterials: Part 1. Scope, regulation, legislation, and metrology (IUPAC Technical Report), *Pure Appl. Chem.*, 95, 133-163 (2023). <https://doi.org/10.1515/pac-2021-1001>

*Online Dynamic NPU Manual*, Young Bae Hansen (Chair of Task Group), <https://labterminology.com> website.

J. Labuda, J. Barek, Z. Gajdosechova, S. do Couto Jacob, L. J. Johnston, P. Krystek, Z. Mester, J. Costa Moriera, V. Svitkova, K. J. Wilkinson, Analytical chemistry of engineered nanomaterials: Part 2. Analysis in complex samples, *Pure Appl. Chem.* 95, 1159–1196, (2023). <https://doi.org/10.1515/pac-2022-0401>

M. Liebman, *Journal of Translational Medicine* 2023

E. M. Lindholm, E. Taraldsrud, J. T. Bay, M. Bemark, J. M. B. Jensen, R. Ceder, E. Abrahamsen, F. M. Yilmaz, S. Devaraj, E. van der Hagen and H. M. Johannessen,\* Properties and units in the clinical laboratory sciences. Part XXVIII. NPU codes for characterizing subpopulations of the hematopoietic lineage, described from their clusters of differentiation molecules (IUPAC Technical Report), *Pure Appl.*

*Chem.* 96, 1573-1582 (2024).

<https://doi.org/10.1515/pac-2023-0806>

A. Rothstein, M. Chorghade, H. Ibrahim, A. Ganesan, P. W. Erhardt, G. Schnorrenberg, A. Gruzman, Evaluation of the Recent Dynamics for Funding Medicinal Chemistry Projects in Academia. Results of a Survey Conducted by IUPAC Division VII (Chemistry and Human Health), *J. Med. Chem.* 68, 2095–2104 (2025). <https://doi.org/10.1021/acs.jmedchem.4c01466>

## b) Conferences, symposia and workshops

*Medicinal Chemistry and Drug Discovery & Development India 2024 (MCADDI 2024)*, held from September 22-27 in Bangalore, brought together leading scientists, industry professionals, and academics for an intensive five-day program. The event was co-sponsored by the American Chemical Society (ACS) Division of Medicinal Chemistry (MEDI), ACS Publications, and the Human Health Division of the International Union of Pure and Applied Chemistry (IUPAC). With close to 100 participants from the pharmaceutical and biotechnology sectors, the course provided in-depth training on the principles of medicinal chemistry and drug discovery.

## (c) Division-led projects (Task group leader)

2024-008-2-700 - [Glossary of terms, quantities and units used in photodynamic medicine and related fields](#) (Francesca Giutini)

2023-036-1-700 - [Updating Chemical Hazard Information Profiles for United Nations Office of Disaster Risk Reduction](#) (Richard Hartshorn)

2023-033-2-700 - [Medicinal Chemistry in Drug Discovery & Development, India](#) (Balu Balasubramanian)

2022-023-2-700 - [Evaluation of the recent dynamic of the medicinal chemistry projects funding in academy](#) (Arie Gruzman)

2021-004-2-700 - [Gold Book Update of Terms for Chemistry and Human Health](#) (Doug Templeton)

2020-017-2-700 - [A database of chemical structures and identifiers used in the control of WADA Prohibited Substances](#) (Vincenzo Abbate)

2019-018-2-700 - [D3 Subcommittee Newsletter](#) (Michael Liebman, Gerd Schnorrenberg, Balu Balasubramanian)

2019-019-2-700 - [Impact of Objective Analysis of Clinical Trial Failures on Drug Discovery and Development Processes](#) (Michael Liebman)

2014-017-1-700 - [Piloting NPU-SNOMED CT mapping](#) to be terminated

2011-018-1-700 - [Human Drug Metabolism Database \(hDMdb\)](#) (Paul Erhardt)

2010-035-3-700 - [Establishing definitions for non-referenced terms in the NPU terminology](#) (Helle Johanessen)

## Partner projects (Lead Division)

2024-007-4-300 - [Human Wellness and Environmental Sustainability: How Chemistry can make the difference](#) (Division III)

2023-020-2-600 - [A Global Framework Using Weight-of-Evidence incorporating New Approach Methods for Risk assessment of crop protection chemicals](#) (Division VI)

2023-010-2-500 - [Electroanalytical flow through systems for monitoring of biologically active species](#) (Division V)

2021-027-2-600 - [The global scenario and challenges of radioactive waste in the marine environment](#) (Division VI)

2021-036-1-500 - [LC-MS quantitative method validation and performance: an exemplified guide](#) (Division V)

2019-026-2-600 - [The Environment, Health and Food Safety Impact of Microplastics](#) (Division VI)

2019-029-1-600 - [Per and polyfluoroalkyl substances \(PFAS\) in the environment: Information for emerging economies on PFAS analyses in environmental media and their impacts on human health](#) (Division VI)