

Annual report 2024

Division III Organic and Biomolecular Chemistry

Summary

Division III Organic and Biomolecular Chemistry covers a substantial part of chemistry. This is reflected by the wide range of topics in our project portfolio and the fact that a large fraction of our activities is facilitated through our 5 sub-committees. In addition, we are involved in interdivisional projects and activities. For the next biennium we will concentrate our efforts on three specific topics in addition to our traditional core activities.

Part 1. Highlights and/or Executive Summary

Division III (Organic and Biomolecular Chemistry) covers a vast part of chemistry, bordering with pharmacy/biology/medicine on one end and physics/physical chemistry on another. This is reflected by the wide range of topics in our project portfolio (see Part 4) and the fact that a large fraction of our activities is facilitated through our 5 sub-committees:

- (a) Biotechnology,
- (b) Photochemistry,
- (c) Organic Synthesis,
- (d) Structural and Mechanistic Organic Chemistry, and
- (e) Biomolecular Chemistry.

Our portfolio also includes a good number of long running IUPAC endorsed conferences (see Part 4). In addition, we are involved in several interdivisional projects and activities. We have also been reasonably successful in publishing one Scientific Recommendation and three conference proceedings in Pure and Applied Chemistry since 2023 (see Part 4). In all these activities, the Division fulfills IUPAC's strategic goal of providing added value to the international chemistry community, distinguishing it from any other body. We continue to do our best to maintain high scientific quality, uphold high ethical standards, and ensure to the best of our ability to include scientists worldwide, irrespective of political, ethnical, religious and gender borders.

The Division committee was assembled in den Haag during the IUPAC General Assembly in August 2023 and online in September 2024. The leadership has regular online meetings to discuss upcoming activities and tasks. The Division president receives information from the Secretariat, typically on a biweekly basis, and meets occasionally online with elected IUPAC officers for specific discussions. In general, we find communication to be good, but miss the opportunity for directly influencing decisions, since the Division President is no longer an ex-officio member of the Bureau (now Executive Board and Science Board).

The sub-committees are generally active and communicate efficiently to scientists in their respective subfields. The role of the Division is therefore to a large degree to coordinate, oversee and support the work of the subcommittees. In this sense, the subcommittees are essential to the operation of Division III, and should continue to exist as such. Critical voices could say that this way of organizing the work is conservative, at odds with the need for picking up new ideas and identifying emerging fields within Organic and Biomolecular Chemistry or Chemistry at large. There may be some truth in this, but we will remind the reader that the Division identified the coming of Green chemistry at a very early stage, organized the enthusiasts in a

sub-committee that later developed into an Interdivisional Committee. One important role of the Division is therefore to be on the alert for upcoming topics and take necessary measures to include new subfields into our organization, when relevant. For topics that are interdivisional by their nature, we will help to identify such, and communicate with the Science Board.

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

For the rest of this biennium and onwards we will continue to curate and support our ongoing projects and conferences. Traditional IUPAC activities (nomenclature, terminology and symbols) will remain at the core. At the same time, we realize the need for renewal. We identify three areas that will be important for the development of the Division and for IUPAC at large, see below for details: (i) Recruitment of officers to IUPAC, (ii) Dissemination to young chemists, (iii) Digitalization of chemistry. None of these topics is unique to Organic and Biomolecular Chemistry, so we will seek interdivisional cooperation to address these challenges when relevant.

The limited finances available for the rest of the current biennium, unfortunately hinders us in supporting new initiatives from our own funds, at best one. If we identify new projects and initiatives that will need additional economical support in order to be realized, we will support application to the Project Committee or externally—to the extent that funds are available.

(i) Recruitment of officers to IUPAC. IUPAC officers tend to be chemists in the late stage of their careers and many continue to work for IUPAC many years after retirement. This is quite natural, since the older generation has more time available for volunteer work, have valuable professional experience, and do not have to worry so much about spending time doing work not directly relevant to their CV as younger scientists have to these days. In fact, IUPAC depends strongly on this grey-haired work force, and should realize this and be grateful. Despite this, we need to work continuously to recruit new officers for renewal. It is more realistic to aim at well-established middle-aged people for this specific task, rather than the very young, and we need a strategy for attracting the best people in this category to work with us. This does not mean that we will ignore the young generation. On the contrary, we think that the arrangement with inviting Young observers is excellent, for a number of good reasons. First, it provides valuable insights and ideas. Second, it makes IUPAC visible to the younger generation. Third, in the long run, when the observers are no longer young, they have established a good relationship with IUPAC that will be valuable for recruitment.

(ii) Dissemination to young chemists. There are two target groups for dissemination, (a) the general public and (b) young chemists including chemistry students. For the first group, IUPAC should play a minor role, since our national organizations are responsible for informing the general public in their country about the benefits of chemistry and the pros and cons of chemicals. Instead, IUPAC should take a major role for setting standards for excellence in chemistry and help cultivating talents in chemistry, focusing on the younger generation. To this end, our division's humble contribution is to oversee the biannual awarding of the Thieme-IUPAC Prize for Organic Synthesis for scientists under the age of 40 years in the field of synthetic organic chemistry. But, we need to be more ambitious than that. We need to involve young chemists in making IUPAC visible to the worldwide chemistry community. It turns out that many chemists only have vague ideas about what IUPAC does. In particular, we need to conquer places where young professional chemists from universities and industry meet, which means social media, social media influencers and discussion fora. In order to achieve this goal, we need to involve young chemists to work with us to better understand this landscape and

define a work plan. On our own side, we have recently supported and now host project 2024-007-4-300 "Human Wellness and Environmental Sustainability: How Chemistry can make the difference", which we think is an important first step in this direction.

(iii) *Digitalization of chemistry.* Electronic computers were introduced in chemistry already in the 1950s. Even before that, mechanical computers were used to solve specific numerical tasks in physical and theoretical chemistry. From 1970 and onwards methods for representing molecular structures by graph theory helped introducing computer tools for planning syntheses, nowadays assisted by direct access to large data bases of reaction data and literature. Although not being perfect, these tools have become more and more powerful and are now quite useful to the the organic chemist. A parallel path of development has been seen for the application of multivariate analysis methods for process optimization and analysis of spectral data. The practising organic chemist employs a wide range of physical methods for measurement and characterization in the daily work, of which NMR spectroscopy, mass spectrometry, X-ray crystallography and optical spectroscopy are most important. All these methods generate vast amounts of data that often remain in printed version in the lab for a period of time after publication. There is a need to change this situation, and push towards general open source publication of raw data in suitable formats in repositories generally available to the community. Although such data formats and repositories exists, it is still fragmented and very often of limited value, if not correctly/comprehensively taken. IUPAC should 1) provide guidelines to satisfactorily reach a good standard of data and 2) facilitate the transfer to an open access integrated information system. More and more powerful artificial intelligence algorithms that will allow more efficient analyses of data are emerging, whether the data are on chemical reactions, spectroscopic data or results from environmental field missions. The democratic question is to which degree these data will be privately controlled and owned or to be in the public domain. The latter would require substantial public funding.

We are aware of the valuable and important work of the IUPAC Interdivisional Subcommittee on Critical Evaluation of Data* in this field, but suggest a broader discussion on how to deal with the questions rised here.

*) See the Technical Report in *Pure and Applied Chemistry* in Issue 10 (2023)

Part 3. Overall report of activities and achievements of Division/Committee since the last report to Council and organized according to the priorities listed below:

We have decided to include this information in the section below (Part 4), and use the letters (a)-(d) to identify the four categories for IUPAC priorities set by the Scientific board:

- (a) *Global scientific cooperation and collaboration that creates a common language of chemistry, including data or technical standards, nomenclature, terminology, and symbols;*
- (b) *Interaction with chemistry organisations, professional societies, industry and other relevant bodies to facilitate best practice in chemistry and chemistry education, or which support educational initiatives in data standards and management;*
- (c) *Connections with cognate disciplines and educational communities, including outreach or engagement initiatives and those that contribute to sustainable development;*
- (d) *Promotion of diversity and inclusiveness in the profession of chemistry, or of values and ethics in science through responsible practice.*

Part 4. Tabular material

Publications

IUPAC recommendation "Definition of the pnictogen bond" by Giuseppe Resnati et al, Pure and Applied Chemistry 96(1) 135-145 (2023).

(From project: 2016-001-2-300)

Special issue of the 25th International Conference on Physical Organic Chemistry, edited by Manabu Abe, Pure and Applied Chemistry 96(4), (2023).

Special Issue of the 28th IUPAC Symposium on Photochemistry, edited by Fred Bouwer, Pure and Applied Chemistry 96(8), (2023).

Special issue for the 30th International Carbohydrate Symposium edited by Ivone Carvalho, Amélia P. Rauter and Nikolay E. Nifantiev, Pure and Applied Chemistry 96(9), (2023).

Conferences

International Conference on Organic Synthesis (ICOS)

ICOS23, Shanghai, October 15-20, 2023. ICOS24, Łódź, Poland from in 2026.

Int. Conf. on Biodiversity and Natural Products (ICOB and ISCNP)

ISCNP31/ICOB11, Naples, October 15– 19, 2023. ISBOC-13, December 18-20, 2023, Singapore.

ISCNP32/ICOB12, 2025, August 24-28, Sydney, Australia ISBOC14, 2026, 21-24 June, Milano, Italy, ISCNP33 & ICOB13, 2027, Japan, ISBOC15, 2028, Paris, France

International Biotechnology Symposium (IBS)

IBS2024 Rotterdam, June 30 – July 3, 2024 .

IUPAC Conference on Physical Organic Chemistry (ICPOC)

26th ICPOC, Beijing, China, 18-23 August 2024. 27th ICPOC, München, Germany, First week of September, 2026.

IUPAC Symposium on Photochemistry

29th, Valencia, Spain, 14–19 July, 2024. 2026 in Zagreb (Croatia) and 2028 in Hiroshima and probably 2030 (somewhere) in Canada.

International Carbohydrate Symposium (ICS)

XXXI ICS Shanghai, July 14- 19, 2024. Slovakia, 2026; Canada, 2028; Italy, 2030; Thailand, 2032; Ireland, 2034; Australia, 2036; Japan, 2038, USA, 2040.

Int. Symp. on Organometallic Chem. Towards Organic Synthesis (OMCOS)

21st OMCOS, Vancouver, Canada, July 24-28, 2023.

Division projects

2024-007-4-300 - Human Wellness and Environmental Sustainability: How Chemistry can make the difference (Nativi).

Status: Recently started up

Category: c – Dissemination

2021-020-1-300 - Gold Book Update of Terms for Organic and Biomolecular Chemistry (Rauter)

Status: The task chair continues not to respond. From another member we hear there is some activity by individual members but there appears to be little general direction given by the chair. The Division will now consider whether it is necessary to re-organize the task group of this important project.

Category: a

2019-046-3-300 - Guidelines on developing robust biocatalysts for biorefinery (Bai).

Status: Progress of this project will be reported in 2025 during the division meeting in Kuala Lumpur.

Category: a

2017-037-2-300 - Bridging Ethnic Food Cultures through Chemistry (Rauter)

Status: The task chair continues not to respond.

Category: c

2016-023-2-300 - A critical review of reporting and storage of NMR data for spin-half nuclei in small molecules (Harper)

Status: To be terminated and merged with project 2019-031-1-024 - "Development of a Standard for FAIR Data Management of Spectroscopic Data".

Category: a

2016-001-2-300 - Categorizing Chalcogen, Pnictogen, and Tetrel Bonds, and Other Interactions Involving Groups 14-16 Elements (Resnati).

Status: A Scientific recommendation has been published in PAC and a meeting was held in 2024.

Category: a

2015-027-1-300 - Strategic Planning for a Network for Heterocyclic Chemistry among Countries of the Mediterranean Sea Area, including Europe and North Africa (Florio).

Status: Likely to be terminated in the near future if it still is impossible to come in contact with project chair.

Category: c

2013-054-2-300 - Healthy life and active ageing - the contribution of functional food ingredients (Rauter)

Status: The task chair continues not to respond.

Category: c

2013-040-1-300 - Measurement of Photoluminescence Quantum Yields (Brouwer)

Status: Plans to finish draft for Technical note by the end of 2024.

Category: a

2011-044-1-300 - Rules for Abbreviation of Protecting Groups (Brimble)

Status: The task chair did not respond in August 2024. A reminder will be sent.
Category: a

2008-037-2-300 - Standard Photochemical Processes (Griesbeck).

Status: It was reported by e-mail in September 2024 that the project is still running but was slowed down by Covid.

Category: a

Other projects

2021-005-1-041 Green Chemistry in Sub-Saharan Africa (partner,
Interdivisional Committee on Green Chemistry for Sustainable Development -ICGCSD)

2020-016-3-020 The Gender Gap in Chemistry – Building on the ISC Gender Gap Project
(partner)

2019-041-3-400 Nomenclature of Sequence-Controlled Polymers (partner)

2019-032-1-024 Development of an IUPAC Recommended Term Management System for
expansion of the Coverage of the IUPAC Compendium on Chemical Terminology (partner,
Committee on Publications and Cheminformatics Data Standards)

2019-026-2-600 The Environment, Health and Food Safety Impact of Microplastics (partner,
Chemistry and the Environment Division)