

IUPAC Organic and Biomolecular Division III

Report to IUPAC Bureau Meeting
Montreal, Canada

Margaret Brimble

I. Executive Summary

The mission of the Division of Organic and Biomolecular Chemistry is to oversee activity in the field of organic and biomolecular chemistry in the broadest sense. Division III consists of a Division Committee (comprising 10 Titular members, 6 Associate Members and 10 National Representatives) and 6 Sub-committees.

Major activities comprise conference organization and projects (both evaluation and involvement); a Divisional newsletter is produced at intervals. The Division oversees the awarding of two IUPAC prizes, the guidelines for one of which (the CHEMRAWN prize for Green and/or Atmospheric Chemistry) was reviewed during 2015.

Highlights of the 2014-2015 biennium include the hosting of nine international conferences and the funding of four new projects, as detailed below.

II. Division Activities against IUPAC Strategic Goals and Objectives

1. IUPAC will improve the vitality, effectiveness and efficiency of our Union.

IUPAC will enhance interdivisional interaction and collaboration.

IUPAC will emphasize multidisciplinary projects addressing critical global issues.

The scientific interests of Division III cover the fundamental and applied aspects of organic chemistry. Central to the Division is the topic of organic synthesis, an enabling science, covering topics as diverse as new reactions and reagents, the asymmetric synthesis of natural products, transition metal catalysts, organocatalysis, organometallic chemistry, enzyme aided synthesis and methods for green synthesis. In the biomolecular area, key topics include chemical biology, notably glycomics, linking across to the more applied topic of biotechnology. The Division has always had strong links into physical chemistry through spectroscopy and/or organic analysis. The Division also has close association with inorganic chemistry especially in the area of catalysis. The discipline of green chemistry first emerged within Division III, and continues to connect the Division to other Divisions of IUPAC.

The main program of activities is conducted in two forms: firstly via a series of well-established international conferences, and secondly through the IUPAC project system. This Division coordinates these scientific topics through six sub committees as well as by involvement in interdivisional activities. Rotation of leadership and succession planning within the six sub committees is actively encouraged. The six sub committees and their elected Chairs are:

Sub-Committee on Organic Synthesis (2016-2017 Chair: Nikolay Nifantiev, Russia)

Sub-Committee on Biomolecular Chemistry (2016-2017 Chair: Zhen Xi, China)

Sub-Committee on Biotechnology (2016-2017 Chair: Fengwu Bai, China)

Sub-Committee on Green Chemistry (2016-2017 Chair: Pietro Tundo, Italy)

Sub-Committee on Photochemistry (2016-2017 Chair: Silvia Braslavsky, Germany, retiring)

Sub-Committee on Structural and Mechanistic Chemistry (2016-2017 Chair: Einar Uggerud, Norway)

Four of these sub-committees meet annually, either at the most relevant scientific conference or at the biannual General Assembly. The photochemistry sub-committee also meets annually at one of their specialist conferences. The sub-committee on structural and mechanistic chemistry has been inactive in recent years, but maintains carriage of the ICPOC series of conferences (see below). The sub-committee on green chemistry will meet in Venice in September 2016.

To date, the Division has approved six project proposals during the 2014-2015 biennium:

Strategic Planning for a Network for Heterocyclic Chemistry among Countries of the Mediterranean, including Europe and North America (2015-027-1-300) - continuation of project (2011-006-2-300 see below);

Continuation of the Revision of IUPAC Recommendations on Carbohydrate Nomenclature (2015-035-2-800) – continuation of project (2012-039-2-800 see below);

An introduction to Computational Chemistry and in-silico visualization; a Workshop for sub-Saharan Africa scientists (2015-016-2-300);

Nomenclature of Homodectic Cyclic Peptides Produced from Ribosomal Precursors (2015-003-2-300);

Healthy Life and Active Ageing: the Contributions of Functional Food Ingredients (2013-054-2-300);

Chemistry beyond Chlorine (2013-057-3-300).

The following five projects approved during the 2012-2013 biennium remain current:

Glossary of renewable chemistry (2013-036-2-300);

Green chemistry curricula in Latin America/Africa (2013-041-3-300);

Photoluminescence quantum yields (2013-040-1-300) – joint with Division I; this project was chaired by Enrique San Roman and Fred Brouwer and resulted in the publication of several very valuable documents on fluorescence standards and related matters.

Nomenclature of phosphoryl transition states (2013-039-2-300) - A manuscript titled 'How to Name Atoms in Phosphates, Polyphosphates, their Analogues, and Transition State Analogues for Enzyme-catalysed Phosphoryl Transfer Reactions' is available as provisional recommendations and for public review until 30 June 2016.

Carbohydrate nomenclature (2012-039-2-800) – joint with Division VIII and continued as project 2015-035-2-800.

The following three projects are close to conclusion or have concluded:

Abbreviations for protecting groups (2011-044-1-300);

SE Asian network for organic chemistry (2011-041-1-300);

Mediterranean heterocyclic chemistry network (2011-006-2-300) - TRAMECH VIII, Antalya, Turkey 11-15 November 2015 (www.tramech8.org) was very successful. TRAMECH IX will be organized at Fes (Morocco) in November 2017 continued as project 2015-027-1-300.

A list of Division projects (2012-2016) is provided at the end of this report.

Focusing on communication: The new initiative of the Istanbul General Assembly was the holding of inter-Divisional meetings. Division III participated in meetings with Division VI, in which joint interests in green chemistry were explored, as well as with Division VIII given the joint interests in various aspects of organic nomenclature. These meetings continued at the

General Assembly in Busan (2015) with an additional meeting with Division I to discuss the concept of a standardization of NMR data project. An abbreviated version of the Division newsletter was published in *Chemistry International* (2013, Sept./Oct., pp29-32). In this way, national representatives have been kept informed of Divisional activities.

2. IUPAC will brand IUPAC in the minds of stakeholders.

IUPAC will improve quality and frequency of communication with stakeholders.

Through the work of the Sub-Committee on Photochemistry, Division III provides tools for international standardization thus branding IUPAC as the leading authority in this area. Examples of projects coordinated by members of the group include: *Measurement of Photoluminescence Quantum Yields* (2013-040-1-300; Brouwer); *Standard Photochemical Processes* (2008-037-2-300; Griesbeck). Nomenclature projects are also important: recent examples include *Nomenclature of Homodectic Cyclic Peptides Produced from Ribosomal Precursors* (2015-003-2-300); *Nomenclature of Transition State Structures and their Analogs for Phosphoryl Transfer Reactions* (2013-039-2-300); *Rules for abbreviation of protecting groups* (2011-044-1-300). In general, the documents produced over the years, first by the Committee on Photochemistry and afterwards by the Division III Sub-Committee on Photochemistry are very well referred to in the scientific literature and have been very well received by the photochemical community (a well-organized community with three major Photochemical Associations, one in the Americas: I-APS, one in Europe: ESP, and one in Asia and Oceania: APA) who have always been integrated in the work of the Sub-Committee. The very active participation of many photochemists in the activities related to the Year of Light all over the world has also been well supported and often triggered by several members of the Sub-Committee on Photochemistry.

Scientific discussion: During the 2014-2015 biennium, the Division oversaw arrangements for nine international conference series, many of which are meetings of long-standing within the IUPAC conference calendar. These meetings were:

- 5th International Conference on Green Chemistry (ICGC, August 2014, South Africa);
- 8th International Conference on Biodiversity and 28th International Symposium on the Chemistry of Natural Products/ (ICOB/ISCNP October 2014, China);
- 20th International Conference on Organic Synthesis (ICOS, June 2014, Hungary);
- 10th International Conference on Biomolecular Chemistry (January 2015, India);
- 16th International Symposium on Biotechnology (IBS, September 2014, Brazil);
- 11th International Conference on Heteroatom Chemistry (ICHAC, June 2015, France);
- 18th International Symposium on Organometallic Chemistry directed towards Organic Synthesis (OMCOS, June 2015, Spain);
- XXVth IUPAC Symposium on Photochemistry (July 2014, France);
- 22nd International Conference on Physical Organic Chemistry (ICPOC, August 2014, Canada).

Division conferences are traditionally well supported by younger chemists, and several activities within these meetings target this age group. The majority of these meetings provide poster prizes to student delegates, and some host workshops designed for young researchers to meet with plenary speakers. Details of Division conferences are provided elsewhere in this report.

The Division oversees the awarding of two prizes to outstanding young chemists. The Thieme-IUPAC prize in Synthetic Organic Chemistry, which is generously supported by the scientific publisher Thieme, is awarded to a chemist under the age of 40 whose research has had a major impact on the field of synthetic organic chemistry. The 2014 prize was presented at ICOS20 (Hungary) to Professor Martin Burke (USA) for the synthesis and study of small molecules with

protein-like functions. The CHEMRAWN VII Prize for Atmospheric and Green Chemistry is presented biannually to a chemist under the age of 40 and from a developing country for research in green and/or atmospheric chemistry. The 2014 prize was awarded at SICGC (South Africa) to Dr Vania Zuin (Brazil) in recognition of her significant contributions in developing green analytical methodologies used to analyze bioactive high-value organic substances extracted from agro-industrial residues.

In relation to the public appreciation of science, the year 2015 was chosen by UNESCO as the Year of Light (including light technological applications). The photochemical community, and members of the Sub-Committee on Photochemistry, have contributed to this UNESCO-sponsored celebration.

Other projects, notably those coordinated through the Sub-Committee on Green Chemistry, seek to engage young people; for example, project 2013-036-2-300 *Glossary on Renewable Chemistry* (led by Silvio Vaz) is developing content related to biomass chemistry and green chemistry, and is aimed at students as well as at researchers. An earlier project, 2013-041-3-300 *Green Chemistry in Higher Education: towards a Green Chemistry Curriculum for Latin American and African Universities* (led by Vania Zuin) has considered the development of general modules for up-to-date university Green curricula within Chemistry courses (Bachelor and Teacher Training), and also has an emphasis on public awareness of green chemistry principles. Finally project 2013-057-3-300 *Chemistry beyond Chlorine* led by Pietro Tundo seeks to improve the perception of chemistry.

3. IUPAC will provide scientific expertise to address critical world needs.

The Sub-Committee on Green Chemistry has provided project activity connecting to the economical growth and activity of the chemical industry, particularly in developing countries. In other activities, Division III conferences, particularly the International Biotechnology symposia and the various Green Chemistry meetings, provide an opportunity to link industry-based chemists with those from universities and the government sector. A project funded in 2015 (*Healthy Life and Active Ageing: the Contributions of Functional Food Ingredients*, 2013-054-2-300, Rauter) seeks to bring chemistry to the general public, demonstrating through the implementation of an interactive website, how chemistry offers unique solutions for society needs in terms of a healthy living and a better ageing.

4. IUPAC will support chemistry education, particularly in developing countries

The 5th International IUPAC Conference on Green Chemistry (5th ICGC) was held in Durban (South Africa), 17-21 August 2014. It was co-hosted by the South African Chemical Institute (SACI), the University of Kwazulu-Natal (located in Durban) and the University of Venda (located in Thohoyandou). This was the first time that the ICGC came to the African continent, and so offered a great opportunity to facilitate interactions of African scientists with colleagues from all over the world and to promote green chemistry in Africa. The main objective of the conference was that of emphasizing the importance of green chemistry for sustainable development; it was a multidisciplinary event considering all the major areas of green chemistry. There were joint sessions with other IUPAC divisions or committees for selected themes (environmental chemistry, green chemistry education, and polymers). A session on sustainability and security, conducted by the Organisation for the Prohibition of Chemical Weapons (OPCW) emphasized the links between scientific knowledge, education and policies with regard to the production and use of chemicals.

A number of Division III projects are strongly linked to chemistry in developing countries. Recent examples include the following geographic areas:

Africa - a workshop in computational chemistry for sub-Saharan chemists (2015-016-2-300, Whitehead); biomass burning in sub-Saharan Africa (2007-025-1-300, Mammino); network for heterocyclic chemistry in North Africa (2011-006-2-300, Florio); green chemistry in higher education (2013-041-3-300, Zuin);

Central/South America - green chemistry in higher education (2013-041-3-300, Zuin); glossary on renewable chemistry (2013-036-2-300, Vaz);

East and South East Asia - network for organic chemistry (2011-041-1-300, Isobe).

5. IUPAC will expand and retain member and volunteer base with an emphasis on diversity and inclusion.

In terms of geographical representation in the 2014-2015 biennium, the Division III committees for 2014-2015 comprised representatives from Asia (1 x TM, 2 x AM, 4 x NR), Africa (1 x NR), the Middle East (1 x AM) in addition to the traditional bases of Europe and North America. The Division has lacked representation from Latin or South America, other than a Provisional Member from Mexico, and various members of project task groups.

In diversity matters, the Division has excellent representation with two female Titular Members serving as Division President and Division Vice President, respectively, two female Associate Members and two female National Representatives. Indeed women comprise 23% of the 2014-2015 Divisional committee. The age profile within the Division still requires attention, although it should be noted that National Representative Dr Oleg Demchuk (Poland) has previously been a Young Observer at Division III meetings. Dr Demchuk has been retained on the Division committee as an Associate Member for the 2016-2017 biennium.

The recent Division ballot for the 2016-17 biennium has resulted in election of Prof Amelia Rauter (Portugal) as Division Secretary, and Dr Janet Scott (UK) as a Titular Member, thereby increasing the number of women Titular Members to 4 out of the 10. Membership from the Latin and South American region is considered high priority ahead of the IUPAC meetings in Brazil in 2017, therefore Associate Members have been selected from Brazil and from Puerto Rico for the next biennium. In the 2016-2017 biennium, women will represent 27% of the Division committee.

III. Plans and Priorities for the 2016-17 Biennium and Beyond

During 2015, the Division reviewed past projects within the field of NMR spectroscopy, and convened email discussions with members of the NMR community and with representatives from Division I about the standardization of NMR data in scientific manuscripts, and the level of accuracy associated with the reporting of NMR data. Members of the NMR community belonging to Division III have diverse technical interests ranging from metabolomics, natural products and synthetic structure elucidation, through to NMR methods development, and consequently express a wide range of views on these issues. During the latter part of 2016, a project submission is envisaged, ideally in concert with interested members of Division I.

Future meetings in the Division III conference series are envisaged as follows: 21th International Conference on Organic Synthesis (ICOS21, 11-16 December 2016, Mumbai, India); XXVth IUPAC Symposium on Photochemistry (3-8 April 2016, Osaka, Japan); 23rd International Conference on Physical Organic Chemistry (ICPOC23, 1-8 July 2016, Sydney, Australia.); 6th

International Conference on Green Chemistry (6ICGC, 4-9 September 2016, Venice, Italy); 17th International Symposium on Biotechnology (IBS17, 25-28 October 2016, Melbourne, Australia); 29th International Symposium on the Chemistry of Natural Products/9th International Conference on Biodiversity (ISCNP29/ICOB9, Turkey, September 2016); 11th International Conference on Biomolecular Chemistry (October 2017, Konstanz, Germany).
Dates and venues for the 12th International Conference on Heteroatom Chemistry and the 19th International Symposium on Organometallic Chemistry are under discussion.

III. Additional Information:

Finance: Historically, Division III has had considerable difficulty creating worthwhile projects, or allocating its entire project budget; in contrast, the Divisional operating funds that support attendance at subcommittee meetings are under pressure every biennium. One view that is worthwhile considering is that Division III Sub-Committees effectively represent broader scale “project taskforces”, and as such merit a portion of the funds that might otherwise be earmarked solely for Division III project activity. The majority of Division business is put forward to the main Divisional meeting from individual Sub-Committee meetings; it is therefore essential that Sub-committee meetings are well attended.

Structure and governance: The Division has an Executive Committee comprising the current President (Prof Margaret Brimble), the Past-President (Prof Mary Garson), the President-elect (Prof Francesco Nicotra) and the Secretary (Prof Amelia Rauter). The current Executive has sought to ensure that Division practices and decisions are clear to all members, and that all Division members are informed as well as active and involved in Division business. In particular, Division members seeking officer and/or Titular member status are reminded of the need to be involved in Divisional business, for example by suggesting new project initiatives or in project evaluation, or by acting as Chairs of Divisional Sub-Committees.

Division minutes and reports are now archived on the Division website, and the process associated with the biannual Division election for President and new Titular members has been provided to the current Division membership.

IUPAC prizes: At its 2014 meeting, the Green Chemistry Sub-Committee expressed some concerns about the small number of individuals applying for the CHEMRAWN prize for Green and/or Atmospheric Chemistry. The group reviewed the guidelines that govern the award of the prize, and made some recommendations to the Division and to the CHEMRAWN. The IUPAC secretariat was informed; the new guidelines will be adopted when awarding the next CHEMRAWN Prize.

IV. Tabular Material:

The following pages provide additional details of projects and conferences as well as the membership of Division III for the 2016-2017 biennium.

Margaret Brimble

President of Division III (Organic and Biomolecular)

Auckland, report 19 February 2016

**Summary of Division III (Organic and Biomolecular) Projects (most recent first)
(February 2016)**

BIENNIUM 2016-2017

Project No: 2016-xxx-x-xxx

Title: *Categorizing Chalcogen, Pnictogen, and Tetrel Bonds, and Other Interactions Involving Groups XIV-XVI Elements*

Objective: This Project extends the inspiring IUPAC Recommendations on halogen and hydrogen bonds (Project No. 2009-032-1-100 and 2004-026-2-2 100) to the categorizing of interactions involving Groups XIV-XVI elements. Definition(s) will be proposed:

- enabling a consistent and unambiguous terminology for most interactions given by Groups XIV-XVI elements;
- registering the emerging consensus on proposals suggesting to use terms chalcogen bond, pnictogen bond, and tetrel bond exclusively for interactions wherein Groups XIV-XVI elements are the electrophile. Proposed definition(s) will balance wide applicability (i.e., generality) and robust descriptive power (i.e., specificity), and convey specific information on the interactions, e.g., polar characters, geometries.

Chairs: Giuseppe Resnati, Pierangelo Metrangolo, Anthony Legon, Jane Murray, Francesco Nicotra, Steve Scheiner

Members: David Bryce, Antonio Frontera,

Webpage: objectives are related to those of a successfully concluded IUPAC project (2009-032-1-100; <http://www.iupac.org/project/2009-032-1-100>).

Start Date: June 1st 2016

End Date: April 31st 2018

Budget in USD: 15k

Progress: under review

BIENNIUM 2014-2015

Project No: 2015-027-1-300

Title: *Strategic Planning for a Network for Heterocyclic Chemistry among Countries of the Mediterranean, including Europe and North America*

Objective: The principal objective of this project is to continue and exploit the excellent results of the previous project which achieved resounding success in establishing a strong collaborative network involving countries, especially less developed countries of North Africa, in terms of collaborative stages for PhD work in research laboratories of more developed nations and participation to international meetings (Tramech VII at Rabat, Morocco, 27-30 November 2013, fifteen grants for young people and Tramech VIII, Antalya, Turkey, 12-15 November 2015, ten grants for young people). This will help to build and foster a sustainable program of high-quality heterocyclic chemistry research, education and chemistry-based applications in all the Network countries.

Chair: Saverio Florio

Members: Brancko Stanovik, Jose Elguero, Jean Louise Gras, Essassi El Mokhtar, Metin Balci, Hussein El-Kashef, Maamar Hamdi, Hassen Amri, George Varvounsis

Webpage: [http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1\[project_nr\]=2015-027-1-300](http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1[project_nr]=2015-027-1-300)

Start Date: January 2016

End Date: 31 December 2018

Budget in USD: 13k

Progress update: not yet available

Project No: 2015-035-2-800**Title:** *Continuation of the Revision of IUPAC Recommendations on Carbohydrate Nomenclature***Objective:** IUPAC/IUBMB document of 1996 has served as an immense help for authors and editors to name the compounds unambiguously. Since 1996, the number of compounds that have been discovered and/or synthesized has grown enormously. The number of constituting monomers and substituents has increased, i.e. due to study of carbohydrates and glycoconjugates in a larger range of organisms in the animal and plant kingdoms, and to the progress in analytical and synthetic methods. The revision of the 1996 document by the IUPAC Task group was started in January 2013 and has led to a partial revision of the 2-Carb document. The current project is focused on completion of the revision and extension of the existing 2-Carb document in order to bring it up-to-date in the light of the enormous progress made in the areas of glycoscience, biotechnology and bio-informatics in the past 20 years.**Chair:** Hans Vliegthart**Members:** Amelia Rauter, Gerald Moss, David Baker, Sandro Sonnino, Nuno Xavier, Martin Frank, Thomas Lutteke**Webpage:** [http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1\[project_nr\]=2015-035-2-800](http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1[project_nr]=2015-035-2-800)**Start Date:** tba**End Date:** tba**Budget in USD: proposed 10k (Div III 2.5k, Div VIII 7.5k)****Progress update:** not yet available**Project No: 2015-016-2-300****Title:** *An introduction to Computational Chemistry and in-silico visualization; a Workshop for sub-Saharan Africa scientists***Objective:** The objective of the proposed Introduction to Computational Chemistry & In-silico Visualization Workshop for Sub-Saharan Africa scientists is to provide an introduction to computational chemistry, similar to the set of workshops that have already been delivered at the University of Kinshasa but which would now be provided with a larger regional remit. The Sub-Saharan Africa workshop would provide an introduction to molecular modeling in structural chemistry, medicinal chemistry and drug discovery. Application examples would be given, showing the value of these methods for research purposes but also for teaching purposes, as the visual illustration of chemical concepts has been shown to enhance their understanding by students. Existing local chemoinformatics resources such as the Kenyan Mitishamba database of about 2000 compounds would be used to demonstrate the value of such databases and how software can be used to extract valuable information from such sources. The overall aim is to help develop the ability to use software suites to build structural chemistry knowledge among the teachers who can then themselves train others, such that the knowledge transfer process can become self-perpetuating.**Chair:** Lewis Whitehead**Members:** Evans Changamu, Solomon Derese, Colin Groom, Juliette Pradon**Webpage:** [http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1\[project_nr\]=2015-016-2-300](http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1[project_nr]=2015-016-2-300)**Start Date:** 01-06-2015**End Date:** 01-06-2016**Budget in USD: 4k (2 k from Div III with 2k from COCI)****Progress update:** The Cambridge Crystallographic Data Centre will be performing computational chemistry workshops in Kenya for scientists from the sub-Saharan region during the week of 7th September 2015 at Kenyatta University & the University of Nairobi. For more information & the application process, e-mail kongamano@ccdc.cam.ac.uk

Project No: 2015-003-2-300

Title: *Nomenclature of Homodetic Cyclic Peptides Produced from Ribosomal Precursors*

Objective: to disseminate through the scientific community guidelines for nomenclature of homodetic cyclic peptides produced from ribosomal synthesis. Specifically this includes N-to-Clinked peptides belonging to the groups cyanobactins, cyclotides, orbitides, amatoxins, phallotoxins and circular bacteriocins. By selection of a narrow focus we are hoping to develop a template that can be applied to develop nomenclature systems for other groups of peptides. Although peer-reviewed journals have published nomenclature recommendations the objective is also to consolidate literature and provide a IUPAC supported nomenclature recommendation. The project will expand and elaborate on the prior "Nomenclature of Cyclic Peptides" (<http://www.iupac.org/project/2004-024-1-800>) in the naming of the homodetic peptides.

Chair: Martin Reaney

Members: David Craik, Ulf Göransson, Gerard Moss, Ninghua Tan

Webpage: [http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1\[project_nr\]=2015-003-2-300](http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1[project_nr]=2015-003-2-300)

Start Date: 01-06-2015

End Date: 01-06-2017

Budget in USD: 10K (7.5 k from Div III and 2.5k from Div VIII)

Progress update: first meeting scheduled October 2015

Project No: 2013-054-2-300

Title: *Healthy Life and Active Ageing: the Contributions of Functional Food Ingredients*

Objective: to bring Chemistry to the general public demonstrating, through the implementation of an interactive website, how chemistry offers unique solutions for society needs in terms of a healthy living and a better ageing.

Chair: Amelia Rauter

Members: Amal-al-Aboudi, Mary Garson, Melissa Fitzgerald, Francesco Nicotra, Livia Sardaki

Webpage: not yet accessible

Start Date: 21-11-2014

End Date: 21-11-2017

Budget in USD: 7.5 k from Div III

Progress update: filming of video clips undertaken in March 2015 (Rauter, Garson, Sardaki, Nicotra) and website clips/recipes in preparation (June 2015).

Project No: 2013-057-3-300

Title: *Chemistry beyond Chlorine*

Objective: Publication of a book to improve the perception of the role of chemistry in issues of general interest. The book (comprising 23 chapters) will be published by Springer as a research publication (ISBN: 978-3-319-30071-9). This project will return a profit to IUPAC as the royalties from publication of the book will go to IUPAC instead of the Editors. A signed contract confirms this agreement.

Chair: Pietro Tundo

Members: Lian-nian He, Ekaterina Lokteva, Murray McLaughlin, Claudio Jose de Araujo Mota, Bo Olssen, Qianghao Qu, Yehudah Shevah.

Webpage: [http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1\[project_nr\]=2013-057-3-300](http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1[project_nr]=2013-057-3-300)

Start Date: 1-5-2014

End Date: 01-05-2016

Budget in USD: 5.6 k (\$4.8k Div III, \$0.8k COCI)

Progress update: *June 2014.* Website advises planning group will meet 22 July 2014. No updates available as of February 2016

BIENNIUM 2012-213

Project No: 2013-036-2-300

Title: *Glossary on Renewable Chemistry*

Objective: Construction and publication of a nomenclature guide – an IUPAC Glossary – related to biomass chemistry and green chemistry. Aimed at students (under graduation and graduation), professionals, and researchers from all countries.

Chair: Silvio Vaz Jr.

Members: Monica Damaso, Birgit Kamm, James Clark, Vincenza Faraco, Vitor Ferreira, Claudio Mota, Vania Zuin, Pietro Tundo.

Webpage: [http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1\[project_nr\]=2013-036-2-300](http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1[project_nr]=2013-036-2-300)

Start Date: 30-12-2013

End Date: 30-12-2015

Budget in USD: 5k

Progress: website updated (Jan 2014) with additional details of methodology and timelines. A draft glossary was circulated to TCG members and to Division members (May 2015). A range of comments were received, and the draft glossary is currently under revision.

Project No: 2013-041-3-300

Title: *Green Chemistry in Higher Education: towards a Green Chemistry Curriculum for Latin American and African Universities*

Objective: 1) Proposing general modules for up-to-date university Green curricula in general and subareas of chemistry of Chemistry courses (Bachelor and Teacher Training), together with their responsible lecturers;

2) Development (generation and/or adaptation) of Green Chemistry contents in theoretical and experimental disciplines of the involved universities in Latin America and Africa, considering the specific context of each region;

3) Contributing to establish permanently Green Chemistry in the education of Chemistry professionals in their initial courses and facilitating the public understanding of Green Chemistry principles showing its involvement in most aspects of common life and current demands nowadays;

4) Putting together universities, industries and governmental/non-governmental sectors in order to approach relevant themes and contents in the Green Chemistry modules

Chair: Vania Gomez Zuin, Lilliana Mammino

Members: Moacir Rossi Forim, Peter Seidl, Claudia Moraes de Rezende, Claudio Jose de Arajo Mota, Fernando de Carvalho da Silva, Carlos Alberto Marques, Patrocoa Vasquez, Gustavo Romaneli, David Gonzalez, Patricia Morales Bueno, Andoni Garritz Ruiz, Neil Coville, Temechegn Engida, Geoffrey Kamau, Egid Mobofu, Pietro Tundo, James Clark

Webpage: See

Start Date: 26-09-13

End Date: 26-09-17

Budget in USD (Expenditure to July 2013): 5k

Progress update: website not up-to-date last update Dec 2013

Project No: 2013-040-1-300

Title: *Measurement of Photoluminescence Quantum Yields*

Objective: The quantum yield (QY) is one of the most important quantitative properties of a luminescent sample, and robust ways to measure it are essential in the application of luminescence techniques. In the project we will perform an inter-laboratory comparison of the two main methods for QY measurements, the classical relative method based on standards, and the absolute method using integrating spheres which recently gained popularity.

The outcomes will be: (i) insight into the reproducibility and inter-laboratory variability of QY measurements using the two methods; (ii) an extended set of standards and protocols for QY measurement.

Chair: Fred Brouwer

Members: Suzanne Fery-Fourges, Stephan Landgraf

Webpage: See [http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1\[project_nr\]=2013-040-1-300](http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1[project_nr]=2013-040-1-300)

Start Date: 26-09-13

End Date: 26-09-16

Budget in USD (Expenditure to July 2013): 4.5k

Progress update: *In October 2014, a decision has been made which samples to measure, and samples have been shared among the labs during November 2014. An announcement of this project was published in the Sep 2015 issue of Chemistry International, p. 31, <http://dx.doi.org/10.1515/ci-2015-0521>. By September 2015, most of the teams have delivered their results, and the task group expected to be able to start the analysis of the data. Website updated 19 Oct 2015.*

Project No: 2013-039-2-300

Title: *Nomenclature of Transition State Structures and their Analogs for Phosphoryl Transfer Reactions*

Objective: This Project seeks to establish a rational, logical, and practical system of nomenclature to identify discrete axial and equatorial ligands in both t_{bp} and octahedral transition states and their analogues for phosphoryl transfer reactions. In many cases, these will be chirally defined only as a result of coordination to components of the enzyme active site where they are located. It will apply to TSs for “in-line” and/or for (theoretical) “adjacent” attack systems and be independent of considerations about “associative” and “dissociative” TSs. It will link to established IUPAC nomenclature systems and usage, in particular to IUPAC Red Book (2005). It will aim to be directly comprehensible to and useable by stakeholders who may not be specialized inorganic chemists

Chair: Michael Blackburn

Members: Jacqueline Cherfils, Gerry Moss, Nigel Richards, Jon Waltho, Nick Williams, Alfred Wittinghoffer

Webpage: See [http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1\[project_nr\]=2011-044-1-300](http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1[project_nr]=2011-044-1-300)

Start Date: 26-09-13

End Date: 26-09-15

Budget in USD (Expenditure to July 2013): 10k

Progress: *A manuscript titled 'How to Name Atoms in Phosphates, Polyphosphates, their Analogues, and Transition State Analogues for Enzyme-catalysed Phosphoryl Transfer Reactions' is available as provisional recommendations and for public review until 30 June 2016.*

Project No: 2012-039-2-800

Title: *Carbohydrate Nomenclature – revision and extension of IUPAC recommendations*

Objective: The aim of this revision and extension is to bring up-to-date the existing Carbohydrate document in the light of the enormous progress made in the areas of glycoscience, biotechnology and

bio-informatics in the past 20 years. Furthermore, the explosion of data stemming from glycomics and glycoproteomics, necessitates the connection with databases for presenting adequately carbohydrate structure and sequence information. There exist a number of databases, each covering different collections of data. Developing guidelines for harmonizing these data are within the goals to be achieved. Another aspect deals with the correction of some names.

Chair: J. Vliegenthart

Members: Jonathen Brecher, Frank Martin, Karl-Heinz Hellwich, Derek Horton, Thomas Lutteke, Gerard Moss, Stefan Oscarson, Amelia Rauter, Sandro Sonnino, Xavier Nuno

Webpage: See [http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1\[project_nr\]=2012-039-2-800](http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1[project_nr]=2012-039-2-800)

Start Date: 01-01-2013

End Date: not listed

Budget in USD (Expenditure to July 2013): \$5.5k from Division III

Progress: *December 2013* –website updated.

Details of projects initiated during 2008-2009 and 2010-2011 have been provided in previous Divisional reports, for example the Division III report to the 95th Bureau meeting held in Coimbra (12-13 April 2014). A Special Issue of Pure and Applied Chemistry dedicated to “Chlorine-free Synthesis for Green Chemistry” (*Pure Appl. Chem.* **2012**, Vol. 84, Issue 3) has been edited as part of Project No: 2008-016-1-300.

IUPAC Conferences Organized under the Auspices of Division III

International Conference on Green Chemistry (ICGC) series

ICGC4 (Foz do Iguazu, Brazil; co-chairs Arlene Gomea and Vania Gomez Zuin, August 2012; IUPAC representative: Pietro Tundo

ICGC5 (Durban, South Africa) chair Lilliana Mammino (sasdestria@yahoo.com;), 17-21 August 2014; <http://www.saci.co.za/greenchem2014/>; IUPAC representative Pietro Tundo.

ICGC6 will be held in Venice, Italy 4-9 September 2016 (chair Pietro Tundo).

2014 meeting: The main objective of the conference was to emphasize the importance of green chemistry for sustainable development, and to promote novel research and collaborations, by bringing together experts and interested parties from all over the world – from academia, industry and government. The conference considered all the major areas of green chemistry, including green synthesis processes, catalysis, environmentally benign solvents, energy storage, biofuels, green chemistry education, policies, and many other interesting topics. Interfaces with other sciences and other research areas were actively encouraged. Special attention was given to the roles of green chemistry in fast-growing economies and to the promotion of green chemistry in the African continent. A session on sustainability and security, conducted by the Organisation for the Prohibition of Chemical Weapons (OPCW) emphasized the links between scientific knowledge, education and policies with regard to the production and use of chemicals.

International Conference on Biodiversity and Natural Products (ICOB and ISCNP) series

ISCNP27/ICOB7 (Brisbane 2011); IUPAC representative David Black

ISCNP28/ICOB8 (Shanghai); Yang Ye (yye@mail.shcnc.ac.cn; yeyang@live.cn), October 20-25 2014; website address-<http://iupac.simm.ac.cn>; IUPAC representative Mary Garson.

ISCNP29/ICOB9 (Izmir, Turkey) chair Bilge Sener, September 24-27, 2016; IUPAC representative Mary Garson.

Greece has expressed an interest to host ISCNP30/ICOB30.

International Conference on Organic Synthesis (ICOS) series

ICOS19 (Melbourne, 2012); IUPAC representative Krishna Ganesh

ICOS20 (Budapest, Hungary); chair Péter Mátyus (matyus.peter@pharma.semmelweis-univ.hu); Janos Wolfling; June 29-July 4 2014; <http://www.icos20.hu/>; IUPAC representative Mary Garson

ICOS21 (Mumbai, India) chair Krishna Kaliappan, December 2016. Florence, Italy will host ICOS22 16-21 September 2018, Florence, Italy (chair: Alberto Brandi).

Update on ICOS20: ICOS-20 was held in ELTE Convention Centre at 29 June - 4 July 2014.

Topics included new reactions and new reagents, applications and new trends in bioorganic chemistry, natural product synthesis, organic synthesis in materials research, organic synthesis in drug discovery and process development, and catalysis in organic synthesis. Plenary lecturers were: Prof. Margaret Brimble (New Zealand) Prof. Marco Ciufolini (Canada) Prof. Minoru Isobe (Taiwan) Prof. Eusebio Juaristi (Mexico) Prof. Max Malacria (France) Prof. Johann Mulzer (Austria) Prof. Jay Siegel (China) Prof. Lutz Tietze (Germany) Prof. Mark A. Rizzacasa (Australia). Professor Martin Burke (USA) was awarded the Thieme-IUPAC Prize for Organic Synthesis, and gave the award lecture.

International Conference on Biomolecular Chemistry (ISBOC) series

ISBOC9 (Beijing, 2012); IUPAC representative Krishna Ganesh

ISBOC10 (Pune, India, January 2015; Co-chairs Ganesh (ganesh1953@gmail.com) and Yamuna Krishnan (yamuna@ncbs.res.in). IUPAC representative: Mary Garson.

ISBOC11: September 27-29, 2017, Konstanz, Germany; Chair Andreas Marx (andreas.marx@uni-konstanz.de)

12th ISBOC – suggestion of Ireland (Marie Migaud) presented to Biomolecular S/C.

International Biotechnology Symposium (IBS) series

IBS 14 (Rimini, Italy) September 2010

IBS15 (Daegu, Korea) 2012; IUPAC representative Francesco Nicotra

IBS16 (Fortaleza, Brazil) chair Osvaldo Carrioca (jkriok@gmail.com), September 14-19; website <http://ibs2014.org/>; IUPAC representative Francesco Nicotra

IBS17 (Melbourne) contact: Glenn Cross, Ausbiotech (gcross@ausbiotech.org), 24-27 October 2016; <http://www.ibs2016.org/>

IBS18 Montreal has made a preliminary bid; Dr Robert Hart NRC Canada and others)

Update on IBS16: The meeting was well supported by R&D Brazilian Scientific Agencies and Brazilian Federation of Industry-CNI, as well as by the Brazilian Association of Chemical and Pharmaceutical Industries. For the first time the IBS-Symposium held a Biobusiness Forum to promote innovation in the country, as well as, the construction of an International Research Platform to promote and engage young students, doctors and researchers into an international biotechnology network leading to collaboration with members of the European Federation of Biotechnology. For that initiative, CAPES- Brazilian Agency for Advanced Post-graduation Studies provided financial support. The participation is confirmed of a Nobel Prize in Chemistry (2004) plus four distinguished scientists as Plenary Lecturers; six experts on Bioeconomy and thirteen outstanding invited speakers for the six parallel scientific sessions.. Elsevier Publishers (Journal on Biotechnologies Advances) offered an Special Issue on Bioeconomy and Biotechnology containing selected works by indicated guest editors.

International Conference on Heteroatom Chemistry (ICHAC) series

ICHAC10 May 2012 (Kyoto, Japan); chair Norohiro Tokitoh (tokitoh@boc.kuicr.kyoto-u.ac.jp) <http://oec.kuicr.kyoto-u.ac.jp/~ichac10/>; Name of IUPAC representative – unknown.

ICHAC11 June 2015 (Caen, France); chair Annie-Claude Gaumont; website http://www.lcmt.ensicaen.fr/96621202/0/fiche_article/&RH=LCMT_FR.

ICHAC 12: no advice provided (July 2015)

International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis (OMCOS) series

OMCOS16 (Shanghai, 2011)

OMCOS17 (Fort Collins, July 28-August 1 2013); chair Peter Kundig (peter.kundig@unige.ch);

OMCOS18 (Barcelona, Spain) 28 June - 2 July 2015; chair: Antonio M. Echavarren, Rubén Martín, Kilian Muñoz; website <http://www.omcos2015.com/>

OMCOS19 is suggested to be held in South Korea

IUPAC Symposium on Photochemistry series

XXIV Symposium on Photochemistry, Coimbra, Portugal (15-20 July 2012); contact Hugh Burrows

XXV Symposium on Photochemistry, Bordeaux, July 13-18, 2014; chair: Dario Bassani (d.bassani@ism.u-bordeaux1.fr); website <http://www.photoiupac2014.fr/>. Contact: photoiupac2014@ism.u-bordeaux1.fr.

IUPAC representative Silvia Braslavsky

XXVI Symposium on Photochemistry, Osaka, Japan. April 3-18, 2016. Conference chair: Tetsuro Majima. Preliminary website: <http://web.apollon.nta.co.jp/iupac2016/invitation.html>

Update on XXV Symposium on Photochemistry: The organization of the XXVth IUPAC Symposium on Photochemistry (Bordeaux, France from July 13 to 18, 2014) proceeded smoothly. The financial operations were the responsibility of the CNRS through their conference organization office of the local delegation, and the number of sponsors obtained was very satisfactory: 10 industrial exhibitors (2 more in negotiations) and 3 publishers. The local government provided substantial financial aid, which has been used to offset the relatively high organizational costs in France in order to maintain low inscription fees and lunches. Additionally, a dozen PhD grants (free inscription) were distributed. The city of Bordeaux agreed to provide free bus and tram tickets to all participants for the duration of the meeting. The IUPAC representative, Prof.

Sylvia Bravlaskey, provided a brief historical perspective of the meeting in commemoration of its 50th anniversary.

IUPAC Conference on Physical Organic Chemistry (ICPOC) series

ICPOC21 (Durham, UK) September 2012; RSC; IUPAC representative Krishna Ganesh

ICPOC22 (Ottawa, Canada) 10-15 August 2014; chair: Paul Meyer (pmmayer@uOttawa.ca);

<http://events.science.uottawa.ca/icpoc22/committee.html>; IUPAC representative Heidi Muchall (Concordia)

ICPOC23 (Sydney, Australia) July 3-8 2016; contact: Jason Harper. Website: <http://www.icpoc23.unsw.edu.au/>

ICPOC24 (Faro, Portugal) Chair: Maria de Lurdes Christiano – U. Algarve

ICPOC25 preference for South America or Asia declared

Other IUPAC Conferences supported by members of Division III

80th Prague Macromolecular Meeting Self-assembly in the World of Polymers

PMM80 (Prague, Czech Republic) 10-14 July 2016;

contact: Dr. Petr Štěpánek, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic Heyrovsky Sq. 2, 162 06 Prague 6, Czech Republic, E-mail: stepanek@imc.cas.cz

Website: www.imc.cas.cz

<http://www.imc.cas.cz/sympo/80pmm/>

The 21st International Conference on Phosphorus Chemistry

ICPC21 (Kazan, Russia) 5-10 June 2016;

contact: Prof. Andrey Karasik, A.E. Arbuzov Institute of Organic and Physical Chemistry, Arbuzov str. 8, Kazan, 420088 Russian Federation, Email: karasik@iopc.ru

Website: <http://icpc2016.ru>

3rd International Conference on Bioinspired and Biobased Chemistry & Materials

NICE2016 (Nice, France) 16-19 October, 2016

contact: Prof. Elena Celia, Université de Nice Sophia Antipolis, IMREDD – MQM, 1-3 bd Maurice Slama, 06200 Nice, France, Email: elena.celia@unice.fr

Website: www.nice2016-conference.com

MEMBERSHIP OF DIVISION III (2016-2017)

Name	Status	Proposed Term	NAO
Prof. Margaret A. Brimble	TM – President	2016-2017	New Zealand
Prof. Francesco Nicotra	TM – Vice-President	2016-2017	Italy
Prof. Amelia Rauter	TM – Secretary	2016-2017	Portugal
Prof. Mary J. Garson	TM – Past President	2016-2017	Australia
Prof. Pher Anderson	TM	2016-2017	Sweden
Prof. Jon Clardy	TM	2016-2017	USA
Prof. Nikolay E. Nifantiev	TM	2016-2017	Russia
Prof. Ganesh Pandey	TM	2016-2017	India
Prof. Janet Scott	TM	2016-2017	UK
Prof. Zhen Xi	TM	2016-2017	China
Prof. Vanderlan Bolzani	AM	2016-2017	Brazil
Prof. Nestor Carballeira	AM	2016-2017	Puerto Rico
Prof. Thomas Carell	AM	2016-2017	Germany
Prof. Oleg Demchuk	AM	2016-2017	Poland
Prof. Bilge Sener	AM	2016-2017	Turkey
Prof. Einar Uggeraud	AM	2016-2017	Norway
Prof. Amal Al-Aboudi	NR	2016-2017	Jordan
Prof. Munawar Ali	NR	2016-2017	Pakistan
Prof. Lilliana Mammino	NR	2016-2017	South Africa
Prof. Emilia Naydenova	NR	2016-2017	Bulgaria
Prof. Koop Lammerstsma	NR	2016-2017	Netherlands
Prof. Miroslav Ludwig	NR	2016-2017	Czech Republic
Prof. Sylvain Marque	NR	2016-2017	France
Prof. Viktor Milata	NR	2016-2017	Slovakia
Prof. Injae Shin	NR	2016-2017	Korea
Prof. Ken-Tsung Wong	NR	2016-2017	China-Taipei
	10 TMs, 6 AMs, 10 NRs		

AM = Associate Member

NR = National Representative

TM = Titular Member