

## Database on Molecular Compositions of Natural Organic Matter and Humic Substances as Measured by High Resolution Mass Spectrometry

The investigation of non-living organic matter at the molecular level is a chief focus of modern environmental chemistry. Fourier transform ion cyclotron resonance mass spectrometry (FTICR MS) is a method of choice due to its unprecedented resolution capacity (Hertkorn *et al.* 2007; <https://dx.doi.org/10.1007/s00216-007-1589-0>). It resolves millions of carbon atoms with distinct chemical environments, both in terrestrial and extraterrestrial organic matter. The data on the molecular diversity of non-living organic matter, coupled to numerous data on biomarkers, can be used to draw conclusions on various biogeochemical processes, past and present. Further progress in this field is conditional on the development of a publicly accessible electronic database containing information about detected compounds and their concentration in non-living organic matter, defined as natural organic matter (NOM) in waters and humic substances (HS) in solid systems (e.g. soils, coals, peats, or bottom sediments).

A recently approved project supported by the Chemistry and the Environment Division (Division VI), the Organic and Biomolecular Chemistry Division (III), and the Analytical Chemistry Division (V), have the following specific objectives:

- develop a database architecture for storage, visualization, and classification of large datasets of molecular constituents of non-living organic matter
- compile initial data on molecular compositions of HS and NOM from different environments, with fully annotated protocols of their isolation, FTICR MS data acquisition, and data treatment and upload them into the developed database.

This will enable the elaboration of criteria for further evaluation of data on the molecular composition of NOM and HS. To achieve the formulated tasks, the project brings together researchers with long-term experience in FTICR MS data acquisition and treatment who work with HS and NOM of various origin (water, soil, coal, peat, and bottom sediments) in different geographic regions, using different isolation techniques and data treatment approaches. In addition, the task



group includes professionals in the fields of geostatistics, information technologies, and big data treatment.

The combination of diverse expertise and rich FTICR MS data pools available to task group members is a key prerequisite for the compilation of initial data on molecular constituents of NOM/HS into a user-friendly database. The task group will use the existing Biogeochemistry Database architecture developed by the task group members of the Lomonosov MSU, adapt it to the project needs, and distribute upload tasks among other TG members in accordance with their specific expertise (freshwater NOM, marine DOM, terrestrial HS from different sources) to come up with the demonstration database at the end of the project.

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[www.iupac.org/project/2016-015-2-600](http://www.iupac.org/project/2016-015-2-600)

## Integrating Green Chemistry and Socio-Sustainability in Higher Education: Successful Experiences Contributing to Transform Our World

More than ever, Green Chemistry can be considered a powerful tool to modify unsustainable practices in chemistry, engineering, and correlated areas all over the world. It is well known that the contextualized insertion of Green Chemistry principles into the curricula of higher education institutions (HEI) can contribute to a better professional education, engaging students to learn conceptual content associated with procedural and attitudinal subjects.

In order to promote Chemistry Education and Education for Socio-sustainable Development in Latin America and Africa, the project 2013-041-3-300 has

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*From left to right Prof. Liliana Mammino, Prof. Paul Anastas and Prof. Vânia Zuin*

been developed to study, adapt, and create new contents for HEI. Coordinated by Prof. Zuin (Brazil) and Prof. Mammino (South Africa), the project involves researchers, lecturers, professors, students, and related HEI representatives from 14 different countries. The resulting webpage, available in Portuguese, Spanish, and English, can be seen at <http://greenchemed.iupac.ufscar.br/>

At the Federal University of São Carlos (UFSCar), São Paulo, Brazil, for instance, a number of teaching experiments and related didactic initiatives have been conducted at the undergraduate and post-graduate levels since 2013, considering locally important topics, mostly associated with sustainable agriculture, agro-resilience, green chemistry, and socio-environmental technologies, especially for the bio-rational control of plagues. As an example, multifactorial mechanisms to repel, control, or eliminate *Aedes aegypti* have been studied, since they are the main type of mosquito that

spreads Zika, dengue, chikungunya, and other viruses. Such scientific approaches have been transformed and adapted to make them suitable to be used as learning objects at UFSCar [1-3].

As a consequence of multiple actions in the Chemistry Department, another collective initiative was the elaboration and implementation of a new curriculum for teaching education at UFSCar at the beginning of 2017, emphasising Green Chemistry principles in several theoretical and practical subjects, including one dedicated exclusively to green chemistry and sustainability projects.

At the University of Venda, South Africa, the Chemical/science education at the tertiary level is a type of educational research fully integrated within tertiary-level science teaching. Its aims are the continuous enhancement of the quality of teaching through the investigation of students' difficulties, through general-character reflections on contents and approaches, and through active participation in international meetings and debates. Particular attention is given to crucial issues, like the language-related difficulties encountered by science students studying in a second language, or the exploration of approaches to suitably and effectively incorporate education for sustainable development into course activities, and to the educational aspects of advanced chemistry courses.

The courses provide a firm foundation in chemical ideas, processes, applications, and the context of chemistry in society. The full picture, from raw materials

## Participation by Member Organizations Worldwide

### **The Pontificia Universidad Católica del Perú**

Currently, in Peru, the state is implementing a policy to support the development of science and technology. Among other strategies, it is providing financial support to graduate schools, specifically to the master's programs showing the best conditions for the formation of new researchers. Our master's program is one of the winners of this subsidy program, so the conditions to promote research in Green Chemistry are favorable. We focus particularly on the following objectives of the project:

- Proposing general modules for up-to-date university Green Chemistry curricula for chemistry courses, and developing of Green Chemistry contents for the theoretical and experimental components of such courses.
- Contributing to the establishment of Green Chemistry as a component in the training of professionals

and promoting the public understanding of Green Chemistry principles.

In 2013, a new curriculum for the Master's program in Chemistry was implemented, including a Green Chemistry course as one of the elective courses. In this course, the fundamental concepts of green chemistry are presented and the application of its principles is discussed by means of a review and critical analysis of the research reported in the relevant scientific literature.

### **The Universidad Nacional de La Plata, Argentina; Universidad Pedagógica y Tecnológica de Colombia, Universidad del Cauca, Colombia;**

A number of short courses on green chemistry for the undergraduate level, as well as outreach activities (school, communities), are being developed.

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through beneficiation to research, including management aspects, is presented. Experimental and field work form an integral part of all courses and self-initiated research is encouraged at the postgraduate level.

Apart from the current courses, several main meetings and workshops have been organised by the coordinators, as is the case for:

- *Green Chemistry Education session on the 4th, 5th, and 6th International IUPAC Conference on Green Chemistry (2012-2016)* [4-5]: [www.ufscar.br/icgc4](http://www.ufscar.br/icgc4), [www.saci.co.za/greenchem2014](http://www.saci.co.za/greenchem2014) and [www.greeniupac2016.eu](http://www.greeniupac2016.eu)
- *Green Chemistry session in the Brazilian Chemical Society Annual meeting, Brazil (2013-2016)*: [www.s bq.org.br/36ra/workshops.php#hiddenDiv6](http://www.s bq.org.br/36ra/workshops.php#hiddenDiv6), [www.s bq.org.br/37ra/coordenadas-qve.php](http://www.s bq.org.br/37ra/coordenadas-qve.php), [www.s bq.org.br/37ra/workshops.php](http://www.s bq.org.br/37ra/workshops.php), [www.s bq.org.br/38ra/programacao-completa/conferencias-convidadas](http://www.s bq.org.br/38ra/programacao-completa/conferencias-convidadas), [www.s bq.org.br/38ra/programacao-completa/sesoes-coordenadas](http://www.s bq.org.br/38ra/programacao-completa/sesoes-coordenadas)
- 2nd African Conference on Research in Chemical Education: <https://sites.google.com/site/acrice2015/>

Material about the project has been prepared and disseminated by magazine articles, web pages, scientific papers, and a didactic book published by the Royal Society of Chemistry in 2015 (*Worldwide Trends in Green Chemistry Education*, <http://pubs.rsc.org/en/content/ebook/978-1-84973-949-8>)

Another book focusing on the topic will be published by UFSCar, involving many members of the project. It is important to emphasise that we aim to mobilise efforts to achieve the United Nations 2030 Agenda for Sustainable Development and its 17 Sustainable Development Goals. These objectives are discussed together with industries and governmental/non-governmental organisations, as well as with schools.

Some members are actively participating: see box included below and continued on the following page.

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### The Brazilian Green Chemistry School, Brazil

The Brazilian Green Chemistry School is based at the School of Chemistry of the Federal University of Rio de Janeiro (UFRJ), which offers undergraduate courses in chemical engineering, industrial chemistry, food engineering, and bioprocess engineering, as well as a graduate program in Technology of Chemical and Biochemical Processes. The Green Chemistry School has access to a staff made up of professors from UFRJ and other universities, as well as researchers from technology centers and companies. It conducts surveys on the state of the art in bio-based chemicals from raw materials abundant in Brazil; organises courses, workshops and meetings on green chemistry and related topics; and develops materials, experiments, and demonstrations for students at a high school level that can also be used for outreach activities.

### The Faculty of Sciences and Technology, Portugal

A four-year doctoral programme was established in the

largest Centre of Excellence / Laboratório Associado para a Química Verde (LAQV) at REQUIMTE and has been hosted by three Portuguese Universities (NOVA Lisbon, Porto, and Aveiro) since 2014. During the first year of the course, the students attend mandatory and optional courses offered by the three Universities. During the 2nd, 3rd, and 4th years, the students develop projects covering different fields of Sustainable Chemistry, taken from a very wide view of the research agenda of the SusChem platform (the European Technology Platform for Sustainable Chemistry).

FCT-NOVA is highly committed to the dissemination of Green Chemistry to the general public, hosting different activities for high school students. The students have the opportunity to do research together with Master and PhD students in projects focused on the development of sustainable processes for the production of novel products for different applications. The training period starts with a lecture introducing the Principles of Green Chemistry and Sustainable

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Engineering. Special effort is made to give practical examples of the applicability of concepts to the real world. On-going research activities foster a new philosophy in the industry, instilled alongside chemical reactions and processes. The methodology includes the co-supervision of Masters and PhD students developing collaborative projects with national companies.

### The Green Chemistry Centre of Excellence, University of York, UK

In addition to the successful Masters course in Green Chemistry & Sustainable Industrial Technology that has been running at the University of York for the past 15+ years, green chemistry will now be incorporated in the undergraduate chemistry curriculum at York, in both taught and practical material.

The Greener Reagents and Sustainable Processes (GRASP) project has been running for the past 2 years with the aim of addressing the use of hazardous/un-sustainable chemicals in teaching labs and providing chemistry undergraduates with the requisite skills and knowledge to prepare them for future careers in the chemical industry.

The The Green Chemistry Centre of Excellence (GCCE) recently launched the RenewChem initiative, which incorporates graduate training as one of its core activities. The training will be specifically aimed at equipping future employees of the chemical industry with the requisite skills and knowledge to make an

immediate impact on the transition to green manufacturing and circular economy within the chemical industries.

A bespoke e-learning platform has been developed with the aim of promoting the uptake of green and sustainable methodologies, with a particular focus on the synthesis of pharmaceuticals. The CHEM21\* online learning platform comprises a range of free, shareable, and interactive educational and training materials that have been created in collaboration with industry.

Also via the CHEM21\* project, the GCCE, in collaboration with other CHEM21\* academic and industry partners, have organised a series of face-to-face training workshops aimed at graduates, PhDs, and post-docs covering topics such as metrics, route selection, safety, and biocatalysis, to name but a few.

We continue to engage Masters-level students and provide them with hands-on experience organising and delivering public engagement activities to a wide range of audiences, from primary school children to members of the general public. Many of the experiments and exhibitions have focused on obtaining chemicals from food waste in order to introduce green chemistry principles in a way that is directly relevant to a non-technical audience. The GCCE also continues to engage with our international partners to share knowledge and examples of best practice, in particular through the Global Green Chemistry Centres or G2C2 network (<http://g2c2.greenchemistrynetwork.org>).

## NUTRIAGEING: Combining Chemistry, Cooking, and Agriculture

The website NUTRIAGEING was created to bring chemistry to the general public by demonstrating how chemistry offers unique solutions for society's needs in terms of healthy living and better ageing. It is now open to academic partners and the general public at <http://nutriageing.fc.ul.pt>. Offering modules to promote healthier nutrition, and showing the contribution of food chemistry to health, the website educates, not only on how to improve eating habits, but also on how to grow vegetables and condiments, demonstrating the added value of their chemical activity. In addition, games on the site offer entertainment and allow the user to confirm the knowledge acquired.

Developed within the scope of the IUPAC project "Healthy life and active ageing-the contribution of functional food ingredients" (2013-054-2-300) and the EU Project "Personalized ICT Supported Service for Independent Living and Active Ageing" (GA 610359),

this new platform was built for the transfer of scientific knowledge into usable personal advice, with a clean, easy-to-use, "app-like" interface with minimal menus. The responsive layout ensures device-independent accessibility and a good viewing experience for the user.

The website is structured around three major themes: (1) Healthy eating, (2) Recipes and videos, and (3) Vegetable gardens.

