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.

For more information and comments, contact Task Group Chair Irina V. Perminova <iperm@med.chem.msu.ru>
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