



ECETOX NEWSLET

RECETOX NEWSLETTER is a quarterly newsletter by the Research Centre for Toxic Compounds in the Environment (RECETOX), Brno, Czech Republic



RECETOX is an independent REsearch CEntre for TOXic Compounds in the Environment operating within the Faculty of Science, Masaryk University, Brno, Czech Republic. The Centre fulfils three roles: an academic institution providing university education, a research institution working on transformation of research into practical applications and a body supporting implementation of the Stockholm Convention on Persistent Organic Pollutants (POPs) and of sound chemicals management in general, nationally and internationally.

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- ▶ RECETOX works with the next generation



Editorial

Dear readers,

This issue is full of good news. The year 2014 means the beginning of the five-year period of sustainability for the RECETOX Centre and we have high expectations for this time. It is the period in which we will capitalize on all previous investments. We have a new facility, modern instrumentation, an international team, and a large and broad cooperation network.

We have just received a certificate of accreditation for the Trace Analytical Laboratories for analyses of food, feeds, biological and environmental samples until April 2017. In addition, we are happy to announce that new version of the environmental information system GENASIS was just launched (www.genasis.cz) and that our researchers succeed in publishing their work in top international journals.

This newsletter also describes several new research projects that we were recently granted, shows examples of our capacity building activities abroad and provides more information on our work with talented youngsters.

Enjoy reading! Katka Šebková, on behalf of the editors

P.S. — The RECETOX newsletter is also available automatically if registered through www.recetox.muni.cz or newsletter@recetox. muni.cz and exists in English, Czech and Russian. The next issue will be out in late June 2014.



Calendar of Events

- March 29, 2014, Young Scientist Event, RECETOX, Brno
- April 11, 2014, Students from Slezské gymnázium, Opava in RECETOX
- May 11-15, 2014, SETAC Europe, Basel, Switzerland
- May 17, 2014, 10th Anniversary of Entry into Force, Stockholm Convention on POPs
- May 24, 2014, Day of Science Event, RECETOX, Brno
- June 4, 2014, 17th meeting of the Council of National Centre for Toxic Compounds, Brno
- June 22–26, 2014, Summer School on Protein Engineering, Loschmidt Laboratories, Brno
- June 23–28, 2014, 10th International Summer School on Toxic Compounds, RECETOX, Brno
- June 27–30, 2014, CSI Marie Curie project meeting, RECETOX, Brno
- July 8–9, 2014, EDCs Experts Meeting, WHO ECEH, Bonn, Germany
- September 2014, DENAMIC project partners meeting, RECETOX, Brno





Spring 2014 in RECETOX

RECETOX laboratories Accredited

We are very happy to announce that our Trace Analytical Laboratories began new stage of life on April 2, 2014. That day, the Czech Institute for Accreditation issued an accreditation certificate for our laboratories to perform chemical analyses of food, feeds, biological material (cellular tissues, secretions and excretions) and environmental samples (ambient and indoor air, surface waters, sediments and soils) and to analyze the following persistent organic pollutants: dibenzodioxins and furans, dioxin-like and indicator polychlorinated biphenyls and polybrominated diphenyl ethers. The Certificate is valid for three years, however we intend to further broaden its scope in 2015.

Congratulations to the whole team – Petra Přibylová, Anton Kočan, Rostislav Červenka who worked extensively on the documentation – and Lenka Vaňková, Petr Kukučka, Šimon Vojta, Iva Poláková and Ondřej Audy – who will pass the proficiency exam each year and are also instrumental to the whole process.



What are ANDROMEDE, BioGate and WaterChem?

All three titles are abbreviated titles of new research grants for distinguished incoming or resident researchers at the RECETOX Centre. In this issue, we describe the objectives of the projects, and the next newsletter will include interviews with the researchers, as two of the projects have already started, and the third one will begin in November 2014.

ANDROMEDE

The ANDROMEDE (Anthropogenic and Natural Drivers of Releases and Occurrence of Mixtures of Endocrine Disruptors in the Environment) project was granted to Dr. Luca Nizzetto for July 2013-June 2015. The overall goal is to develop a tool to assess the influence of natural factors (e.g., hydrology, climate, biogeochemistry) and anthropogenic factors (e.g., land use and socio-economic indicators) on ecosystem exposure to waterborne chemical pollutants. The reason for this tool is a clash between the protection of the environment and human health from chemical pollution and socio-economic development, demand for new products, sophisticated life styles and contemporary consumption habits. A particular focus will be paid to endocrine disrupters. In addition, consumer behaviour is a very important factor in the release of anthropogenic chemicals into the environment, but this also complicates prediction of exposure. A mathematical model will be compiled detailing the relationship between these elements in a holistic and quantitative way. The project will also collect data detailing the kinetic and mechanisms of reactions of chemicals in the environment for model calibration and validation. The output will be a quantitative tool for assessment of environmental exposure to chemicals from wastewaters.

BioGate

Dr. Sérgio Manuel Marques has recently started work on a BioGate project (March 2014–December 2016). Gates are structural features that control key functions in various biological systems and molecular machines. In spite of their importance, the knowledge about their structure and function is still limited, and to date there have been no attempts to rationally construct them. The project, therefore aims at developing novel concepts and methods for engineering enzyme properties by de novo design of gates.

Haloalkane dehalogenases will be used as model enzymes, representing a wide class of enzymes characterized by a buried active site connected to the surface by tunnels. The redesign of dehalogenase tunnels has been accomplished in previous work and has proven successful in increasing enzyme activity, enantioselectivity and stability. Herein the dynamics of the tunnels and their gates will be investigated in a systematic study. Then, the researchers will rationally design new gates and optimize their function in order to maximize the reaction rate. This procedure will allow design and experimental productions of mutant enzymes with improved catalytic properties. We expect to deliver new concepts and methods of protein engineering, which will be applicable to a wide range of technologically important enzymes to be used in practice.

WaterChem

The project "Effects of organic lining materials of water pipes to the chemical burden of water", WaterChem, was granted to Dr. Johanna Rajasärkkä for November 2014 to December 2016. She will look at the releases of chemicals from



renovation of aged water pipes (sewage pipes and household pipes) into water and their impact on the chemical burden of water and subsequently on water quality.

Different lining materials and chemicals (i.e., bisphenol A and F and their derivatives, volatile organic compounds, amines, amides, isocyanates, and organotins) as well as fac-

tors influencing the leaching pattern (physico-chemical properties of water, flow-rate, temperature) and time scale will be studied. The possible risk of chemicals in different lining materials to humans and the environment will be assessed. The expected outcome are suggestions to minimize the chemical burden of water by lining materials.

Young Scientist Event at the 95th Anniversary Celebrations of the Masaryk University

Masaryk University celebrates its 95th anniversary in 2014 and is organizing cycles of seminars, exhibitions and events to showcase various disciplines. One of the first events was dedicated to the interactive science exhibition "Touch the Science", which takes place on the Brno-Bohunice campus from March 26 to June 26, 2014, and is accompanied by four Saturday workshops. The RECETOX Centre participated in the first workshop on March 29, 2014. Our event, "Young Scientist – Discovering Nature", was prepared for parents with children aged 8–15 years as a short program of tasks by Jaroslava Daňsová, Petr Masner, and Dr. Jaromír Literák. The children observed zebrafish embryos and midge fetuses and divided plant pigments by thin layer chromatography. Upon completion of all tasks they were given small prizes. Our booth was always very busy as there were about two hundred children eager to become young scientists that afternoon.

Photo: © Zuzana Hanzelková, RMU

N-trophy 4th Contest

For a fourth year, six young RECETOX researchers, biologists and chemists, spent part of their free time as lecturers and organizers of the interdisciplinary competition course N-trophy (biology, chemistry, physics and logic) for talented high school students. The main organizer is the South Moravian Centre for International Mobility (JCMM) with partners and the contest runs January–end of April, 2014. The first round involved 150 three-person teams from four regions – South Moravia and North Moravia from the Czech Republic and Trnava and Žilina regions in Slovakia. The grand finale took place April 25–27, 2014, at Masaryk University in Brno and the winner of this cross-border contest was the team SPOŽÚS from Gymnázium Brno-Řečkovice.

We thank our science communicators for their dedication to spread science among the young generation. Congratulations to the winners and we hope to welcome some among our students in near future.

More information about the contest is on www.ntrophy.cz (Czech only).











RECETOX News



Professor Jiří Damborský, Head of the Research Programme Protein Engineering in the RECETOX Centre extended his involvement as a member of the Editorial Board of Biotechnology Journal and was nominated a Senior Editor. This international journal with an impact factor of 3.4 publishes only peer-reviewed articles and focuses on various aspects of biotechnology and related fields. Professor Damborský will be overseeing the peer-review of manuscripts on biocatalysis. We congratulate him on this achievement and wish him further success in his work!

Use of the RECETOX Research Infrastructure in 2014

Approximately 20% of the capacity of the RECETOX research infrastructure has been made available to external users. They are from institutions cooperating with the RECE-TOX Centre over a longer term in the implementation of international research projects, but also from new institutions, industry partners, and national or regional authorities. A total of 28 requests for open-access to RECETOX research in-

Brno - city of science, research and innovation

A two month long exhibition showcasing Brno as city of science, research and innovation took place in Urban Centrum, Brno from February 18 to April 10, 2014. It introduced the best research institutions in fundamental and applied research in South Moravia Region on large panels to allow visitors discover their work, location, equipment and many photographs. The RECETOX Centre was one of the ten research centres presented on large panels (together with ALISI, the Central European Institute of Technology (CEITEC), Czech-Globe, the Centre of New Technologies for Mechanical Engineering (NETME), the International Clinical Research Center (ICRC), the National Supercomputing Center (IT4Innovations), the Regional Centre for Applied Molecular Oncology (RECAMO), and the Centre of Sensor, Information and Communication Systems (SIX).



frastructure were submitted in 2014. Consequently, the RECETOX research infrastructure hosted 11 researchers (seven international ones) who have already spent 253 working days in the Centre between January and April 2014. All interested in using the RECETOX research infrastructure please visit www.recetox.muni.cz/RI for more details and contact us by e-mail.

Article in Nature Chemical Biology

Understanding the functioning of biological catalysts is one of the important milestones in biological and biochemical research. The molecular basis of enzyme catalysis is not yet fully explained even 120 years since the publication of the first model of enzyme catalysis by Dr. Emil Fischer, Nobel Prize winner in Chemistry. The role of protein dynamics on the course of the enzymatic reaction is one of the controversial issues.

Researchers from the Protein Engineering research programme in RECETOX have just published a joint article in the renowned international journal Nature Chemical Biology on April 13, 2014, that increases our knowledge on the above issue. The scientists from Masaryk University, two institutes of the Academy of Sciences of the Czech Republic (Institute of Physical Chemistry J. Heyrovsky and Institute of Nanobiology and Structural Biology), and the University of South Bohemia transplanted the active site in the protein molecules and found that the dynamics is essential for its proper functioning.

Our heartfelt congratulations to all authors for this great achievement (Sykora, J., Brezovsky, J., Koudelakova, T., Lahoda, M., Fortova, A., Chernovets, T., Chaloupkova, R., Stepankova, V., Prokop, Z., Kuta Smatanova, I., Hof, M., Damborsky, J., 2014: Dynamics and Hydration Explain Failed Functional Transformation in Dehalogenase Design. Nature Chemical Biology doi: 10.1038/nchembio.1502)!

Transplantation of the active site and the access tunnel in the protein







International Cooperation

RECETOX NETWORKING - Supporting Expertise and International Cooperation

A three year long project "RECETOX NETWORKING" (funded from the European Structural Fund and the state budget of the Czech Republic, Operational Programme Education for Competitiveness No. CZ.1.07/2.3.00/20.0053) provided over 1 million EUR to support various international networking activities of the RECETOX Centre during May 2011-2014. More than 25 top environmental experts from all around the world have been invited to Brno (including Prof. John P. Giesy, Prof. Alice Hontela, and Dr. Tom Harner (all from Canada), Prof. Martin Scheringer, Dr. Marc Suter, and Dr. Francesco Pomati (all from Switzerland)) to share their expertise with our researchers. The project also supported the International Summer School by inviting ten experts each year to lecture (2011-2013) and allowed for more than 42 exchange stays, study visits and courses of the researchers and PhD students from RECETOX abroad. Furthermore, newly established international partnerships were successfully used in several recently submitted project applications to European Horizon 2020 and Norwegian Funds project calls (2013 - 2014).

Moreover, the project also brought two top scientists to Brno and allowed them to establish their own research groups that would complement RECETOX portfolio with the expertise previously unavailable. Professor Gerhard Lammel (previously working at the Max Planck Institute in Germany) has built an interdisciplinary team composed of PhD students and postdoctoral fellows from Netherlands, Greece and Slovakia. His team develops global models for transport and fate of POPs in the atmosphere. These models help not only in



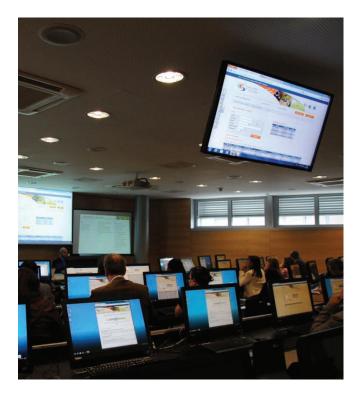
fundamental research but also in practical applications such as understanding the role of global change in chemical risks. The second research team, led by Dr. Branislav Vrana (previously working in Slovakia, UK and France) develops progressive methods in passive sampling and studies ultratrace levels of contaminants such as antibiotics, pharmaceuticals, pesticides and other chemicals in water in the Czech Republic and Europe. Activities of both groups have resulted in more than 25 high quality research publications published in international journals. Finally, both new groups were also successful in competing for external funds to support their future sustainability and further development of their expertise at RECETOX from the EU FP7 programme project calls and Czech Science Foundation (GAČR) grants. More detailed information about the project is available on the dedicated project website www.recetox-networking.cz.

10th International Summer School on Toxic Compounds in the Environment

The Research Centre for Toxic Compounds in the Environment will host the 10th annual International Summer School of Toxic Compounds at its premises from June 23 to 28, 2014. The Summer School is organized in collaboration with the Secretariat of the Stockholm Convention on Persistent Organic Pollutants, the Ministry of the Environment of the Czech Republic and the Stockholm Convention Regional Centre for Capacity Building and the Transfer of Technology in the Central and Eastern European countries.

The upcoming Summer School will focus on methods for analyses of toxic substances in the environment using isotopes. It will also open a parallel class, which will focus on the implementation of the Stockholm Convention and its Global Monitoring Plan. The participants will receive intensive hands-on training in using the electronic data warehouse of the Global Monitoring Plan, learn how work with available data, add new data and interpret results from the database. This training targets preparation for the upcoming 7th meeting of the Conference of the Parties of the Stockholm Convention on POPs in 2015.

Those interested in participating can apply on the website for vacant places: https://is.muni.cz/obchod/fakulta/ sci/?lang=en.







RECETOX activities abroad

RECETOX in Bosnia and Herzegovina

A three year long (end of 2012–end of 2015) project financed by the EU TEMPUS programme established a Training Network of experts (NETREL – Network for education and training for public environmental laboratories) to train researchers and experts in Serbia and Bosnia & Herzegovina to become trainers in environmental analytical techniques. This is required to meet the major challenges in monitoring, assessment and management of pollution, and emission of toxic compounds to water in Western Balkan countries. The project will also provide necessary sampling, laboratory and computer equipment to comply with requirements of the EU Water Framework 2000/60/EC and Drinking Water Directive 98/83/EC.

Experience gathered by EU project partners from Slovakia, Czech Republic and the UK is shared through a number of a week-long learning courses to train future trainers in Bosnia & Herzegovina and Serbia and ensure dissemination and implementation of state-of-the-art methodologies for moni-



toring emerging environmental pollutants, in line with EU legislation and priority substances list and available documentation. The training introduces courses in sampling, sample treatment, analytical methods, quality assurance and control, and data handling and processing.

Masaryk University, through RECETOX, is one of the project partners. Dr. Brano Vrana, one out of three key experts in this project, and Dr. Zdeněk Šimek share their expertise with researchers in Belgrade, Sarajevo and Novi Sad universities. So far, a sampling workshop took place in September 2013, a sample treatment learning workshop took place in February 2014 and additional training in analytical procedures/ methods, QA/QC, data handling and management are upcoming with the use of the new equipment in summer 2014. As a follow-up, the newly trained trainers will then organize their national courses under the supervision of our experts in late 2014 and throughout 2015.







Two Years in Turkey

Professor Ivan Holoubek from our Centre is currently spending two intensive years in Ankara, Turkey. He is working there as a key expert in the EU technical assistance project implemented by the NIRAS IC consortium since June, 2013. This project, "Technical Assistance for Implementation of the Persistent Organic Pollutants Regulation" (TR2010/0327.03-01/001), financed by the EU and Turkey, aims at eliminating the negative effects of POPs and POPs wastes on human health and environment in line with the implementation of EU legislation – Regulation No. 850/2004/EC on Persistent Organic Pollutants – and the decisions of the global environmental agreement: the Stockholm Convention on Persistent Organic Pollutants.

The project will establish and strengthen the institutional and technical capacity in the implementation of the POPs Regulation through a series of eight individual week-long intensive trainings on all aspects of sound management of POPs, including POP wastes, and two study visits for government officials, representatives of research institutions, academia and NGOs to experience infrastructure for POPs monitoring and reporting, and implementation of BAT/BEP. In addition, it aims to raise public awareness on POPs through dissemination of project information and results, including analyses of the current status of implementation of POPs-related requirements and measures in Turkey. Furthermore, one of the outputs will be an update of the National Implementation Plan for the Stockholm Convention, with the aim to determine national priorities and prepare regulatory and sectoral impact assessment.

For the above, two international study visits will take place. The Czech Republic will host the first study visit in 2014. The group of experts from Turkey will visit RECETOX to see its laboratories, monitoring devices, analytical tools developed for monitoring of POPs, as well as to meet our experts.









RECETOX Broke the Record

The RECETOX team composed of staff, students, and family members successfully represented at the official attempt to set a new Czech record in PET bottles placed into a yellow container for recycled plastics. The event took place at SITA Logistics Centre in Brno Slatina on April 25, 2014 and its outcome is officially certified by the Czech Agency Dobrý Den that collects all Czech records. All five competing teams surpassed the former Czech record of 1,333 PET bottles. RECETOX team succeeded to increase it to 2,131 pieces but finished on a second place. The new Czech record was set by the team SITA Ostrava division, which managed to place over 2400 PET bottles into their container.



RECETOX: Laboratories of the Trace Analyses

Accredited Laboratories Offer the Following Services:

- QA/QC system, validated analytical methods
- Modern equipment for extractions, fractionations and purification of samples
- State of the art instrumentation for analyses of endocrine disrupting chemicals, persistent organic pollutants, and heavy metals
- Speciation analyses of toxic and essential elements in the environment and biota
- · Long term monitoring air, precipitation, soil, water, sediments, needles, mosses and lichens
- Air monitoring networks MONET in Europe, Africa and Asia
- Sampling by active and passive samplers
- Sampling of precipitation and surface waters, sediments, soils and biotic materials



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Publication of this eRECETOX newsletter has been supported by the CETOCOEN project and by Ministry of Environment of the Czech Republic

