Horizon 2020 MSCA-ITN Cluster event “Clean Water”

Institut Català de Recerca de l’Aigua, Girona

22 October 2019
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<tr>
<td>TreatRec 642904</td>
<td>EID-2014</td>
<td>Interdisciplinary concepts for municipal wastewater treatment and resource recovery. Tackling future challenges</td>
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<td>HypoTRAIN 641939</td>
<td>ETN-2014</td>
<td>Hyporheic Zone Processes - A training network for enhancing the understanding of complex physical, chemical and biological process interactions</td>
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<td>RELIEF 641459</td>
<td>EID-2014</td>
<td>RELIability of product Environmental Footprints</td>
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<td>ANSWER 675530</td>
<td>ETN-2015</td>
<td>ANtibioticS and mobile resistance elements in WastEWater Reuse applications: risks and innovative solutions</td>
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<tr>
<td>SuPER-W 676070</td>
<td>EJD-2015</td>
<td>Sustainable Product, Energy and Resource Recovery from Wastewater</td>
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<tr>
<td>ENIGMA 722028</td>
<td>ETN-2016</td>
<td>European training Network for In situ imaGing of dynamiC processes in heterogeneous subsurfAce environments</td>
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<tr>
<td>PROTECTED 722634</td>
<td>ETN-2016</td>
<td>PROTECTion against Endocrine Disruptors. Detection, mixtures, health effects, risk assessment and communication.</td>
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<tr>
<td>NaToxAq 722493</td>
<td>ETN-2016</td>
<td>Natural Toxins and Drinking Water Quality - From Source to Tap</td>
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<tr>
<td>AQUAlity 765860</td>
<td>ETN-2017</td>
<td>Interdisciplinar cross-sectoral approach to effectively address the removal of contaminants of emerging concern from water</td>
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<tr>
<td>P-TRAP 813438</td>
<td>ETN-2018</td>
<td>P-oSTER Diffuse phosphorus input to surface waters - new concepts in removal, recycling and management</td>
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<tr>
<td>AQUASENSE 813680</td>
<td>ETN-2018</td>
<td>P-oSTER Innovative Network for Training in wAter and Food QUality monitoring using Autonomous SENSors and IntelligEnt Data Gathering and Analysis</td>
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<tr>
<td>NOWELTIES 812880</td>
<td>EJD-2018</td>
<td>P-oSTER Joint PhD Laboratory for New Materials and Inventive Water Treatment Technologies. Harnessing resources effectively through innovation</td>
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<td>08:30 – 08:45</td>
<td>Arrival of participants</td>
<td>Emanuela Galeazzi - REA A.1 Sergi Sabater, ICRA’s Deputy Director</td>
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<tr>
<td>08:45 – 09:10</td>
<td>Welcome and Introduction</td>
<td>Sergi Sabater, ICRA’s Deputy Director</td>
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<tr>
<td>09:10 – 09:30</td>
<td>Career development opportunities in MSCA</td>
<td>Barbara Mester, Head of Sector REA A.1</td>
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<td>09:30 – 09:50</td>
<td>“Clean Water”: EU water policy development</td>
<td>Daniela Buzica &amp; Anna Marczak, DG ENV C.1 &amp; DG ENV C.2</td>
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<tr>
<td>09:50 – 10:05</td>
<td>The TreatRec project</td>
<td>Mira Petrovic, ICRA - Coordinator</td>
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<tr>
<td>10:05 – 10:15</td>
<td>Taking advantage of autotrophic biomass: Potassium and phosphorus recovery from municipal wastewater</td>
<td>Sara Johansson, Project TreatRec, ESR at Universitat de Girona</td>
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<tr>
<td>10:25 – 10:40</td>
<td>The ANSWER project</td>
<td>Irene Michael-Kordatou, University of Cyprus - Scientific Manager</td>
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<td>10:40 – 10:50</td>
<td>Investigating the potential of transformation products of antibiotics formed during advanced wastewater treatment to induce biological adverse effects and antibiotic resistance</td>
<td>Vasiliki Beretsou, Project ANSWER, ESR at University of Cyprus</td>
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<td>10:50 – 11:10</td>
<td>Coffee break</td>
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<td>11:10 – 11:25</td>
<td>The SuPER-W project</td>
<td>Gijs Du Laing, Ghent - Coordinator</td>
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<tr>
<td>11:25 – 11:35</td>
<td>Application of microalgae for wastewater treatment and recovery of bioenergy and high-value bioproducts</td>
<td>Larissa Terumi Arashiro, Project SuPER-W, ESR at Universitat Politecnica de Catalunya</td>
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<td>11:35 – 11:45</td>
<td>Tackling bottlenecks for water reclamation and reuse from municipal wastewater treatment plants</td>
<td>Philipp Kehrein, Project SuPER-W, ESR at Technische Universiteit Delft</td>
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<td>11:45 – 12:00</td>
<td>The AQUAlity project</td>
<td>Paola Calza&lt;br&gt;University of Torino - Coordinator</td>
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<tr>
<td>12:00 – 12:10</td>
<td>Evaluation of CECs in drinking water including toxicological assessment of their degradation by-products</td>
<td>Dimitra Papagiannaki&lt;br&gt;Project AQUAlity&lt;br&gt;ESR at Società Metropolitana Acque Torino S.p.A.</td>
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<td>12:10 – 12:20</td>
<td>Photolysis vs. (photo)-Fenton: a comparison for the fluoroquinolones degradation and its by-product study employing EEM-PARAFAC</td>
<td>Iván Matías Sciscenko&lt;br&gt;Project AQUAlity&lt;br&gt;ESR at Universitat Politècnica de Valencia</td>
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<td>12:20 – 13:50</td>
<td>Lunch</td>
<td>Jörg Lewandowski&lt;br&gt;IGB Berlin - Coordinator</td>
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<td>13:50 – 14:05</td>
<td>The HypoTRAIN project</td>
<td>Anna Jäger&lt;br&gt;Project HypoTRAIN&lt;br&gt;ESR at Forschungsverbund Berlin EV</td>
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<td>14:05 – 14:15</td>
<td>What happens to micropollutants in the hyporheic zone? – findings of an interdisciplinary joint mesocosm experiment</td>
<td>Damien Jougnot&lt;br&gt;UPMC-CNRS - Deputy Coordinator</td>
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<td>14:15 – 14:30</td>
<td>The ENIGMA project</td>
<td>Anne-Karin Cooke&lt;br&gt;Project ENIGMA&lt;br&gt;ESR at µQuans</td>
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<td>14:30 – 14:40</td>
<td>Can vertical gravity gradients monitor seasonal soil moisture dynamics in karst? - Improvements from a new portable absolute quantum gravimeter and coupled hydro-gravimetrical modelling</td>
<td>Guilherme Nogueira&lt;br&gt;Project ENIGMA&lt;br&gt;ESR at Helmholtz-Zentrum für Umweltforschung UFZ</td>
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<tr>
<td>14:40 – 14:50</td>
<td>Flow and reactions in stream-riparian zone systems, a multi-method space and time patterns characterization</td>
<td>Lisa Connolly&lt;br&gt;Queen’s University Belfast - Coordinator</td>
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<td>15:05 – 15:15</td>
<td>Fifty shades of cyanobacterial green</td>
<td>Vittoria Mallia&lt;br&gt;Project PROTECTED&lt;br&gt;ESR at Norwegian Veterinary Institute</td>
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<td>15:15 – 15:25</td>
<td>Are chemicals in water potential endocrine disruptors?</td>
<td>Elizabeth Goya Jorge&lt;br&gt;Project PROTECTED&lt;br&gt;ESR at ProtoQSAR</td>
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<td>15:25 – 15:40</td>
<td>The RELIEF project</td>
<td>Rosalie van Zelm&lt;br&gt;Radboud University - Coordinator</td>
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<td>15:40 – 15:50</td>
<td>Reliability in chemical footprint modelling of consumer products</td>
<td>Mélanie Douziech&lt;br&gt;Project RELIEF&lt;br&gt;ESR at Radboud University</td>
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| 15:50 – 16:05 | The **NaToxAq project**                               | Hans Chr. Bruun Hansen  
*Kobenhavns Universitet - Coordinator* |
| 16:05 – 16:15 | Natural Toxin Mobility from Source to Tap             | Carina Schönhsee  
*Project NaToxAq  
ESR at Agroscope* |
| 16:15 – 16:25 | Production Dynamics and Degradation of Emerging Cyanopeptides | Regiane Sanches Natumi  
*Project NaToxAq  
ESR at EAWAG* |
| 16:25 – 16:40 | Break                                                  |                                                                         |
| 16:40 – 16:55 | Next Generation of SiC Membranes                      | Haris Kadrispahic  
*LiqTech (DK)  
*Industrial partner of the AQUALity project* |
*ProtoQSAR (ES)  
*Industrial partner of the PROTECTED project* |
| 17:10 – 17:30 | Discussion                                             | All                                                                     |
| 17:30 – 17:55 | **Feedback and considerations**                       | Expert – Guy Duke                                                      |
| 17:55 – 18:00 | Closing word & end of meeting                         |                                                                         |
Set the scene

I. Cluster events: an added value for Policy Feedback
   *(Emanuela Galeazzi)*

Besides showing the high scientific value of Marie Skłodowska-Curie (MSC) Innovative Training Networks (ITN) and their contribution to the relevant scientific fields, cluster events are fantastic opportunities for the project to network and to enhance synergies among them.

Moreover, in recent years, an increasing need for concrete scientific evidence to support policy decisions and policymaking has been commonly acknowledged. Cluster events promote discussion and collect policy relevant information and data on specific policy areas to provide coordinated input to the relevant EU policy-making level, thus enhancing links between societal goals and policies.

Interaction with project coordinators and MSC-supported researchers will contribute to gather additional insights on the implementation of MSCA-ITN.

II. Career development opportunities in MSCA
    *(Barbara Mester)*

Every year the EU funded Marie Skłodowska-Curie Actions (MSCA) offer work and study opportunities to researchers in different stages of their career.

Besides funding research careers and excellent research, MSCA stimulates cooperation among networks of European Universities and industry, sectors and disciplines.
The Cluster Event is an occasion to learn about the MSCA actions, to meet top scientists, universities and industry in the field of waste-water. Background information and future developments (currently under discussion) will be presented at the event.

**III. “CLEAN WATER”: EU water policy development (Daniela Buzica & Anna Marczak)**

Water protection is one of the cornerstones of environmental protection in Europe. An overview of the latest developments on water at the European level is given in this session. This includes the Fitness Check of the Water Framework Directive, Groundwater Directive and Environmental Quality Standards Directive, the Evaluation of the Urban Waste Water Treatment Directive, the recently adopted Strategic Approach to Pharmaceuticals in the environment, the proposal for a regulation on minimum requirements for water reuse and also the proposal for the Drinking Water Directive. Some future research questions and/or topics that came up from all of these developments are also presented.
The H2020-MSCA-ITN projects

642904 - TREATREC

I. The TreatRec Project (Mira Petrovic)

Interdisciplinary concepts for municipal wastewater treatment and resource recovery. Tackling future challenges

Recent developments in the area of wastewater treatment and resource recovery technologies provide a fantastic opportunity to develop improved and more efficient treatment of wastewaters, to reduce discharges of microcontaminants in the aquatic environment and ultimately secure a healthier environment for humans. The application of technologies, developed and studied within TreatRec, could help meet the ever-increasing regulatory demands that are being placed on water agencies around the world. For these technologies and methods to be effectively adopted, the business and regulatory policy sectors will require professionals who not only have knowledge of processes and technologies, but also of monitoring, environmental contamination, modeling and social science. Important progress in research is frequently associated with interdisciplinary initiatives and insights. This is particularly true in addressing problems of wastewater treatment, which are always interdisciplinary in nature and the information and competence needed to progress research in the field often resides in different sectors.

The TreatRec project offered an innovative training programme in the technology, chemistry, process engineering, modeling and decision support systems, as well as business and entrepreneurial skills, provided by leading experts from academia and industry. Network-wide training was complemented by research training through an individual scientifically ambitious research project generating young professionals that:
• Have an understanding of science, policy drivers, technological solutions and the social science aspects associated with the monitoring and treatment of wastewater;

• Have experience of working on and delivering a research project that is aimed to meet the real needs of industrial sector;

• Have formal training in business skills (including project management, IPR, commercial exploitation of research results).

With their multi-sectoral insight, the TreatRec fellows are able to readily access that information and competence, and hence better progress research. In addition, their training in employing an entrepreneurial approach to research, supported by their training in transferable skills, equip them to progress research in a directed and efficient fashion.

The project contributed to fill in several technological gaps and knowledge needs such as (i) evaluation of state-of-the-art technologies for wastewater treatment upgrade for successful removal of emerging microcontaminants, (ii) getting better insight into transformations of organic matter occurring during wastewater treatment, (iii) identification of the best combination of anaerobic ammonium oxidation plus struvite precipitation to increase the phosphate recovery and to minimize ammonium recycles to the water line, (iv) provision of means to risk assess urban wastewater treatments response to current and future stressors in combination and (v) to provide a Decision support system (DSS) development within the wastewater treatment field by involving from the very beginning industrial partners.

II. Taking advantage of autotrophic biomass: Potassium and phosphorus recovery from municipal wastewater (Sara Johansson)

The Individual Research Project was aiming to identify synergies between two novel technologies for the removal and recovery of nutrients from municipal wastewater: anammox-based processes for nitrogen removal and mineral precipitation for phosphorus recovery. More specific; the project investigated the possibility to recover potassium in the form of potassium struvite by using anammox as a pre-treatment before struvite
precipitation. Precipitation of calcium phosphate biologically induced by partial nitritation-anammox (PNA) granules was also investigated.

The thesis was developed within the framework of the Urban Waste Water Treatment Directive, which regulates nutrient discharge limits for municipal wastewater treatment plants. During the time the thesis was developed, the EU fertilizer regulation was revised and ultimately updated to include recovered nutrient products that now can circulate on the internal market. The new regulation also sets limits on heavy metal content for all European fertilizers.

The thesis proved that anammox can remove sufficient nitrogen to allow for the formation of potassium struvite. A product consisting of one third potassium struvite and two thirds ammonium struvite could be recovered. PNA also proved to be efficient CO2 stripper which implies decreased need for alkali dosing for pH control during struvite precipitation.

The thesis further showed that PNA granular sludge can act as a biological crystallizer. Hydroxyapatite of high purity and the same phosphorus content as indigenous phosphate rock was confirmed within granules. The recovered product complied with the heavy metal limits in the revised EU fertilizer regulation.

The thesis resulted in contribution to a book chapter, two scientific articles published in peer reviewed journals and one technical article. The results were disseminated through oral presentations at four international conferences. The article on biologically induced precipitation has gained interest in the field and has 10+ citations.

III. Resilience of water resource recovery facilities: a framework for quantitative model-based assessment (Pau Juan Garcia)

It is believed that we are in a situation of high uncertainty regarding the forthcoming challenges for our water infrastructure and services. Government bodies, utilities, practitioners, and researchers have shown interest in the incorporation of resilience into the management and operation of water resource recovery facilities (WRRFs). Current practice is to ensure redundancy (or backup) for most critical equipment (e.g. pumps or blowers) but there is no objective manner on how to best allocate
resources for enhancing resilience. The research sector is progressing to support resilience implementation, but slowly in comparison with the increasing demand from industry and government. This thesis provided a model-based assessment approach for the quantitative evaluation of different strategies for enhancing resilience and properly allocating resources.

The first part of the thesis presented a review of studies that deal with resilience in the wastewater treatment sector, with a focus on understanding how these have addressed the key elements for assessing resilience, such as stressors, system properties, metrics and interventions to increase resilience. The review showed that only 17 peer reviewed papers and 6 relevant reports directly addressed resilience. The lack of consensus in the definition of resilience, and the elements of a resilience assessment, hinders the implementation of resilience in wastewater management. To date, there exists no framework for resilience assessment that is complete, comprehensive and directly applicable by practitioners.

The framework provides guidance on the overall modelling approach from data collection, model selection, model calibration and scenario analysis, while focusing on equipment failure and control strategies. A detailed mechanistic modelling of the air distribution system was used that enables understanding of the relationships between aeration equipment, control algorithms, process performance, and energy consumption, thus leading to a more realistic prediction of WRRF performance under stress conditions when properly calibrated. To illustrate this, a model-based energy audit has been performed for the Girona WRRF with the goal of assessing the ability of current models to provide an objective evaluation of energy reduction strategies. Results show that the implementation of an ammonia-based aeration controller, a redistribution of the diffusers, and the installation of a smaller blower might lead to energy savings between 12 and 21%, depending on wastewater temperature. The model supported the development of control strategies that counter the effects of current equipment limitations, such as tapered diffuser distribution, or over-sized blowers. The resilience of these strategies was tested against an ammonia peak.

In the fourth part of the thesis, the usefulness of the model-based framework for resilience assessment was illustrated by assessing the resilience of the WRRF of Girona against a storm event and a power outage. With regards to the WRRF of Girona, the model predicted that
stormwater events could cause sludge washout if the plant had to increase the volume of water treated, but the overall impact highly depends on the sludge settleability. It was also predicted that recirculation of activated sludge (RAS) flow manipulation can potentially increase resilience against stormwater. Limited energy back-up can cause non-compliance in case of blower power shutdown of around 6 h, and around 12 h in case of recirculation pumps shut-down. Another option to enhance resilience would be to increase the power back-up by 260 kW, which allows the plant to run with recirculation pumps and blowers at minimum capacity. In that case, resilience can be further enhanced by optimizing the trade-off between balancing oxygen needs in each reactor while lowering system pressure. Model-based assessment of resilience showed great potential to become a standard tool to assist on the decision making of future investment. However, before it is adopted by the industry, further work will be required in standardization and validation of the modelling approach.
675530 - ANSWER

I. The ANSWER project (Irene Michael-Kordatou)

ANTibioticS and mobile resistance elements in WastEwater Reuse applications: risks and innovative solutions

The main goal of the ANSWER project was to train fifteen ESRs to address the risks associated with chemical and biological contaminants of emerging concern, i.e. antibiotics, antibiotic-resistant bacteria and antibiotic resistance genes (A&ARB&ARGs) and urban wastewater reuse. ANSWER’s scientific conceptual framework, covered the entire wastewater reuse cycle, starting from the treatment of wastewater with conventional/advanced processes of varying technological level, utilising existing and developing new microbiological protocols and biodetection systems for monitoring ARB&ARGs in wastewater and understand their fate/transmission in soil, crops and water resources (groundwater, surface water), using advanced chemical analysis for the detection and identification of metabolites and transformation products (TPs) of A, testing new toxicological end-points for A/TPs, and processing all data necessary for the development of a web-database (using mathematical modelling and analytical data, synthesising the knowledge through data management) for prioritization and determination of emission limit values (ELVs) for A&ARB&ARGs for wastewater reuse.

The framework on which ANSWER was structured was the most suitable way for tackling the multi-faceted problem of wastewater reuse, being characterised by an interdisciplinary environment of high scientific level. To achieve its overall scientific goal, ANSWER was structured on a multidisciplinary consortium (10 Beneficiaries and 8 Partners from 9 countries) involving experienced researchers (academic/non-academic) from diverse disciplines. In addition, scientists with recognised expertise in the field were involved in the project (either as members of the Advisory Board or as Visiting Scientists) contributing to the training of the ESRs and providing expert opinions and experiences on the scientific aspects of the project. The ESRs have gained maximum exposure of the ANSWER multidisciplinary environment through secondments (41 in total) to the
partner organisations, embracing thus the value of interdisciplinary work. The scientific and training core of the project supported by advanced chemical, microbiological, toxicological, modelling, and process engineering tools, along with its strong network organisation and management structure, were essential elements for the successful achievement of its five scientific objectives. A Summer School and 8 Training Events were organised in the framework of the project, which included 10 Specialized Scientific Training Courses on specific issues including practical exercises and 11 complementary/soft skills courses.

ANSWER has been able to produce an excellent scientific knowledge around the main five directions of its technical Work Packages. The main scientific outputs were the (i) understanding of the fate and transmission of A&ARB&ARGs within urban wastewater, soil, ground/surface water, and crops (determination of A&ARB&ARGs with highest risk of transfer from wastewater to soils-crops, assessment of the physicochemical factors favoring the persistence of A&ARB&ARGs in soils-crops, determination of the environmental/public health risk factors related with A&ARB&ARGs in soils-crops), (ii) validation of a suitable battery of bioassays for A&ARB&ARGs effects evaluation and hazard identification (development and application of protocols for advanced bioassays for A and their TPs, assessment of the effects of A and of their TPs and relation to antibiotic resistance), (iii) development of a modelling framework capable of predicting the fate and assessing the risks associated with A&ARB&ARGs in activated sludge, soil, waters and crops (development of models on ARB&ARGs passage in soil/water resources affected by wastewater reuse schemes, development of models to assess the impact of conventional/advanced technologies on ARB&ARGs), (iv) assessment of the efficiency of innovative technologies to minimize A&ARB&ARGs (evaluation of the efficiency of innovative technologies to minimize A&ARB&ARGs, development and assessment of the efficacy of new photocatalytic reactors and cost analysis), and (v) development of a web-based database for A, TPs, ARB&ARGs in environmental matrices and development of guidelines for the determination of ELVs of A and their TPs, ARB&ARGs in urban wastewater used for irrigation.

Along with its scientific goals, ANSWER ensured via a number of dissemination/communication activities that its outcomes and impacts were widely shared with the respective research and innovation community, including industry, stakeholders, scientists, general public, as well as with EU/national policy makers setting the research agendas of the future. One of the main dissemination/communication outcomes of
ANSWER was the development of an educational children's book titled “The Secret Handbook of the Blue Circle”, which was produced by the PAPADOPOULOS Publishing in Greek and by the IWA Publishing in English language.

II. Investigating the potential of transformation products of antibiotics formed during advanced wastewater treatment to induce biological adverse effects and antibiotic resistance (Vasiliki Beretsou)

Antibiotics are now well-acknowledged contaminants of emerging concern. Advanced Oxidation Processes (AOPs) have exhibited enhanced removal capacity of such microcontaminants from urban wastewater treatment plants (UWTP) effluents. At the same time, the available scientific literature has extensively dealt with the optimization of these technologies for the removal of individual microcontaminants, and to a lesser extent with the identification and structural elucidation of their transformation products (TPs) and their biological potency.

Identification of TPs is a challenging task and represents a higher grade of difficulty than the analysis of target chemical microcontaminants, due to their unknown nature, the absence of analytical standards to confirm their identity, the complexity and diversity of the matrices and the broad range of concentrations at which these TPs are produced. Therefore, their monitoring in environmental matrices requires the use of high-resolution mass spectrometric (HR-MS) systems and appropriate analysis strategies providing high selectivity, high sensitivity and, in particular, high capability for structure elucidation. In this regard, hydrophilic interaction liquid chromatography (HILIC) is becoming an attractive alternative (or complementary technique) for the commonly used reversed phase liquid chromatography (RPLC), due to its ability to separate polar compounds which are poorly retained on RPLC columns.

However, chemical analytical data does not provide information on the cumulative biological effects of complex compound mixtures in wastewater or on possible environmental- or health-related effects. Thus, in order to get a more holistic view of the hazards posed by UWTP effluents, effect-based monitoring approaches are required to provide important complementary information to chemical analysis.
Within this context, the aim of this study was the investigation of the fate and transformation of selected antibiotics (i.e. azithromycin, ofloxacin, sulfamethoxazole and trimethoprim) during UV-C and UV-C/H₂O₂ oxidation in ultrapure and secondary-treated wastewater effluents as well as the identification of their TPs by applying suspect and non-target strategies based on liquid chromatography quadrupole-time-of-flight mass spectrometry (LC-QTOF-MS). The complementary use of RPLC and HILIC for the identification of polar TPs was also investigated. Finally, Chemically Activated Luciferase eXpression (CALUX®) bioassays; (BioDetection Systems BV, Amsterdam, the Netherlands) were applied covering multiple toxicological endpoints, such as cytotoxicity, genotoxicity and oxidative stress.
I. The SuPER-W project (Gijs Du Laing)

Sustainable Product, Energy and Resource Recovery from Wastewater

In many cases energy, water and resources contained in wastewater may have significant value if recovered. Therefore, the EU is currently confronted with a paradigm shift from wastewater treatment to resource recovery. To facilitate this shift, the SuPER-W European Joint Doctorate programme trains early-stage researchers (ESRs) in developing technologies for water, energy, nutrient and metal reuse, and bioproduction from (waste)water. The ESRs obtain knowledge and skills needed to turn environmental problems into economic opportunities. SuPER-W focuses not only on technology development through research, but the ESRs are also trained in translating research into policy, creative problem-solving, identification of bottlenecks for effective implementation of resource recovery technologies, development of business cases and urban/industrial ecosystems, and assessment of sustainability and the role of public perception and policy in innovation. Furthermore, they acquire a set of commercial, entrepreneurial and managerial skills that prepare them as future leaders. All ESRs are supervised by at least 2 promoters from 2 universities and co-supervised by a researcher from a non-academic partner organisation. Moreover, they conduct a mandatory internship in the non-academic sector, contributing to more effective dissemination and exploitation of their research results. All ESRs also should contribute to an outreach activity as a mandatory component of their doctoral training programme. This includes e.g. the setup of an open online course (MOOC) on resource recovery from wastewater and contribution to the setup of workshops for school children on resource recovery from wastewater within and outside Europe. To organise the training, SuPER-W brings together leading researchers from 5 renowned universities and 12 associated non-academic partner organisations, including industrial partners involved in technology development, SMEs focused on consultancy/engineering, a service provider, a government agency, and professional network organisations. ESRs who successfully defend the PhD thesis and finish the doctoral training programme receive a
double or joint PhD degree, jointly awarded by the universities of his/her promoters, as well as a joint doctoral training certificate of SuPER-W.

II. Application of microalgae for wastewater treatment and recovery of bioenergy and high-value bioproducts (Larissa Terumi Arashiro)

Optimization of algae-based wastewater treatment systems towards enhanced water reuse and recovery of microalgae for biogas and high value compounds production.

The use of microalgae-based technologies has been proved to be an effective alternative to recover resources from wastewater. These microorganisms can, not only reduce the energy requirement from wastewater treatment process, but also be used as a source of energy through biomass valorisation techniques (e.g. biofuels), showing their great potential to address the water-energy nexus in a sustainable way. The algae biomass can also be used as a source of valuable compounds of high relevance for industrial processes, such as carotenoids and pigments. The several applications of microalgae biomass help to re-conceptualize wastewater treatment facilities as resource recovery opportunities. However, there is still a need for a better understanding on the upstream and downstream processes related to algal technologies in a circular economy context. For this reason, further research has to be encouraged in this field to prove its feasibility for large scale in the future.

This PhD project addresses the following objectives: a) Investigating the performance of high rate algal ponds (HRAPs) under different operational conditions, more specifically assessing the effect of removing one step (primary treatment) from the conventional configuration of HRAPs systems, in order to reduce cost and area requirements; b) Assessing the potential to recover high-value phycochemicals from microalgae biomass grown in wastewater; c) Assessing the potential to recover energy through anaerobic digestion of algae biomass grown in wastewater, with and without extraction of high-value compounds; d) Investigation of sustainability of algae-based wastewater treatment and further valorization of biomass, through life cycle assessment (LCA).

The main tasks and activities proposed for this project have been successfully performed. The results achieved throughout this PhD have
been published as scientific articles, listed below. Most recent results are now being documented and planned to be published in the near future.

**III. Tackling bottlenecks for water reclamation and reuse from municipal wastewater treatment plants**

*(Philipp Kehrein)*

Implementing resource recovery from waste streams is a complex task and requires multidimensional planning and a whole-system perspective that takes into account technical, economic, environmental and societal aspects. Domestic wastewater cannot any longer be considered as “waste”, because it is a resource containing clean water, energy and valuable materials including nutrients. Academia has widely recognized that a sustainable wastewater treatment plant (WWTP) recovers resources from the wastewater stream and feeds into the circular economy. The term WWTP has therefore been changed into water resource recovery facility (WRRF) to emphasise the need for a paradigm shift in the wastewater sector. If existing WWTPs approach the end of their expected service life, a unique window of opportunity exists to replace the aging infrastructure with innovative WRRFs that reduce stress on water resources, provide renewable energy, decrease air and water pollution, and contribute to local economic activity by implementing successful resource recovery pathways. However, the emphasis on economic and treatment performance criteria in WWTP design still excludes resource recovery as a relevant factor for sustainability. Due to increasing available treatment and recovery technologies, WRRF design is gaining complexity and little attention has yet been given to how to plan and assess a WWTP from a resource recovery perspective instead of merely focusing on treatment and economic criteria. The point of departure for this project is to provide insights on (1) which technologies are available, (2) what are technical and non-technical bottlenecks hindering their implementation, (3) how energy and mass flows in innovative process designs, (4) how to support water utilities to strategically design WRRFs in the future? To achieve that, a critical literature review has been conducted that reveals the potentials of certain wastewater resource recovery technologies to supply national resource demands, the vast technological options available or currently developed, and existing bottlenecks for implementation mentioned in literature. Secondly, the innovative aerobic granular sludge (AGS) treatment process has been modelled in a case study using mass and
energy balances. The study explores different opportunities to integrate technologies that recover organic carbon (as energy or bio-polymers) and phosphorous (as struvite or ash-P) and quantifies these recoverable resources. Thirdly, advanced treatment processes to recover water from WWTP effluents are investigated to reveal the different energy requirements needed to recover water of different qualities for various reuse purposes, like irrigation or drinking water resource augmentation. Finally, a strategical planning framework is elaborated that supports decision making in WRRF design. It includes economic, environmental, and social assessment criteria that allow the comparison of processes at a very early design stage. It has been found that resource recovery technology implementation is mainly hindered by economic bottlenecks like e.g. process costs, market values, or resource quality. Therefore it has been recommended to water utilities to increase efforts in value chain development for recovered recourses. This requires to make decisions beyond the traditional scope of treatment process costs and effluent quality but to become a market actor. In addition it has been shown, that resource recovery technology integration into WWTPs may lead to trade-offs because a resource can only be recovered as a product once. For, example it is required to make decisions on the form that organic carbon should be recovered by a process. If it is recovered as biogas for subsequent electricity generation it cannot be recovered as biopolymer anymore. Therefore, careful analysis of which resources are preferably recovered by a process and why, is necessary. To support this decision making procedure at an early process design stage, a strategical planning tool is helpful that includes in addition to techno-economic and environmental criterial also marketability criteria to assess recovery options. However, water is the most precious resource in wastewater and should be reclaimed in places that may face scarcity problems. Since energy plays an important role as a major cost factor of reclamation processes, it is useful to consider or emphasize energy recovery in combination with water reclamation.
I. The AQUAlity Project (Paola Calza)

Interdisciplinary cross-sectoral approach to effectively address the removal of contaminants of emerging concern from water

AQUAlity is a multidisciplinary and cross-sectoral European Training Network aiming to generate and promote highly skilled scientists with the potential to face the present and future challenges concerning the protection of water resources from Contaminants of Emerging Concern (CECs). It enrolled fifteen early-stage researchers (ESRs) to conduct cutting-edge research on multidisciplinary aspects of novel hybrid technologies for the removal of CECs from aqueous systems. Moreover, these fifteen ESRs are trained to develop their creativity, critical and autonomous thinking, and entrepreneurial skills, thus boosting their scientific skills and innovation capacity in the field of water treatment technologies. This goal is attained via a structured training-through-research programme, consisting of original individual research projects (performed both at the beneficiary organization and through intersectoral secondments) and education on technical and transferable skills (performed both at local level and with network-wide events).

We develop advanced analytical tools for the determination of CECs in water bodies and for assessing their environmental fate. Firstly, we applied a simplified version of the NORMAN approach to select the proper pollutants; the substances were ranked using a score calculated from key indicators such as exposure, hazard, persistency, bioaccumulation and mobility. The selected chemicals were combined with those agreed within the consortium to provide a list of 25 CECs worth to be investigated. Several extraction protocols were developed or optimized for the analysis of the above substances, their transformation products have been identified and the elucidation of the photochemical processes is in progress. Contemporaneously, a sampling campaign was performed in spring 2019 to collect surface waters and wastewaters that were subjected to untarget analysis with the aim to search for new potentially hazardous compounds to be added in the NORMAN database.
We also developed sun-driven Advanced Oxidation Processes (AOPs) for the enhanced removal of CECs. AOPs are based on the generation of hydroxyl radicals, which can oxidize toxic and refractory pollutants yielding their mineralization to CO₂ and water. The phenomenon can be activated by solar light, a source of renewable and clean energy, which makes AOPs an environmentally friendly technology for CECs abatement. For such, we are studying the mechanisms and the potential in CECs abatement for three innovative solar Advanced Oxidation Processes, involving hybrid organic-inorganic photooxidation agents, namely: (i) organic photocatalysts immobilized on inorganic nanostructured materials, (ii) dye-sensitized TiO₂/ZnO photocatalysts, (iii) photo-Fenton at quasi-neutral pH. These AOPs will be coupled with membrane nanofiltration (NF), resulting in highly innovative hybrid nanofiltration/advanced oxidation systems. A great effort is in progress to explore new fabrication methods for developing NF membranes able to: (i) combine high water fluxes with high retention towards CECs, (ii) be recalcitrant to fouling, and (iii) be easily cleaned. These novel membranes will be used to both concentrate CECs during their degradation and recover the photooxidizing agents, making the overall process more effective and compact than AOP only.

II. Evaluation of CECs in drinking water including toxicological assessment of their degradation by-products (Dimitra Papagiannaki)

The individual project of ESR Dimitra Papagiannaki within AQUAlity focuses on the development of new analytical methods using LC-MS-MS-MS technique for CECs determination and assessment in a variety of water matrices -such as surface water, drinking water, treated water, wastewater etc.-, including evaluation of CECs’ fate after treatment by solar photochemical processes and hybrid membrane advanced oxidation processes (NF/AOP), identification of potential transformation products and evaluation of their toxicity. Moreover, as stated in the AQUAlity agreement, secondment periods in other academic institutes and industries for the ESR have been planned, in order to assure better knowledge transfer, training and integration of the network. The contaminant object of the ESR’s research includes a wide variety of molecules ranging from congeners such as PFAS to molecules belonging to different classes with different chemical characteristics such as
Pharmaceuticals, Personal Care Products, Pesticides, as well as their degradation products that may occur in a variety of water matrices.

The ESR till now has worked on developing a new “green” analytical method for determining trace level concentrations of 16 different perfluoroalkyl substances in drinking water samples using UHPLC-MS/MS. The key characteristic of this method is the absence of a pretreatment or preconcentration step. The method has been validated according to the requirements of ISO 17025 and Accredia (Italian National System for the Accreditation of Laboratories) achieving good recovery results and really low Quantification Limits (5 ng L\(^{-1}\)) and applied for an estimation study of PFAS pollution rates in the Metropolitan Area of Turin. During this assessment, 930 samples were collected and analysed, including different water matrices (underground, surface and drinking water). Among the results, only four compounds were detected in the study area (PFBA, PFHxS, PFOA and PFOS) above the limit of Quantification and only in the 6% of the analysed samples. Despite the low detected pollution rates, a correlation study between the assessment findings and the industries in the area was carried out using statistical and spatial analysis tools in order to guide future choice of the sampling points presenting higher risk factor and support the surveillance and water quality control activities.

Furthermore, it is well known that PFAS host in their carbon chain one of the strongest chemical bonds (C-F) that makes them very stable towards heat, acids and oxidation. In order to achieve their degradation, different processes using single molecules -such as photocatalysis, adsorption and high voltage electrical discharge- were attempted, and only the last one provided promising results (approximately 45% reduction). The toxicity of PFAS compounds and their potential by-products obtained from the degradation processes was also tested using different types of microorganisms (*Aliivibrio fischeri* and *Thamnocephalus platyurus*) showing that a mix of molecules is significant more toxic than the single ones and after the degradation process the toxicity is lower. Moreover, toxicity bioassays using different microorganisms (*Bacillus subtilis*, *Raphidocelis subcapitata*, *Aliivirbio fischeri* and *Daphnia magna*) were developed and used to measure changes in the toxicity of pesticides before and after UV exposure as well. More specifically, solutions of glyphosate and glyphosate based herbicides were exposed to UVA, UVB and UVC light and the results showed 40-80% reduction of the toxicity. The ESR is currently working on the development of an analytical method for determining 16 pharmaceuticals in different water matrices. An assessment monitoring will be done after selecting the sampling points using the spatial analysis tool developed before.
III. Photolysis vs. (photo)-Fenton: a comparison for the fluoroquinolones degradation and its by-product study employing EEM-PARAFAC (Iván Matías Sciscenko)

The treatment of water containing contaminants of emerging concern (CECs) represents an important environmental issue as they were detected in the past few years, and their harmful effects have not been determined accurately and the conventional treatments are not enough to deal with them; hence, alternative methodologies should be developed. Advanced oxidation processes (AOPs) have been demonstrated to be efficient enough to degrade CECs due to the formation of highly-reactive species such as hydroxyl radical (•OH). A particular AOP case is Fenton process, which consists in the use of iron salts and hydrogen peroxide, improving the effectiveness of the process with light irradiation (photo-Fenton). Although (photo)-Fenton have been widely studied, there are still aspects being not fully understood, as their applicability to salty waters or its implementation at mild pH conditions. These is of particular environmental relevance for the application of these processes in aquaculture facilities, where high concentration of antibiotics have been detected and which could be adsorbed within the marine sediments. On the other hand, actual procedures as HPLC-MS are complex, hard to interpret and expensive. Therefore, more simple methodologies based on fluorescence excitation-emission matrices (EEMs) followed by a mathematical analysis of the data are being under study in order to study in an easy way, the removal of pollutants present on water. As a case of commonly known CEC, family of broad-spectrum antibiotics, fluoroquinolones (FQs), are chemically stable compounds, extensively used in veterinary and human medicine. They present low metabolization percentages in many organisms and their degradation in wastewater treatment plants is incomplete. In this work, we report on the degradation of FQs in different conditions employing (photo)-Fenton and photolysis in order to compare the three processes. In all cases, FQs removals were followed by its signal decrease employing high-pressure liquid chromatography (HPLC) equipped with UV-visible detector, mineralization percentages were measured with total organic carbon (TOC) analysis, toxicity studies were performed with Aliviibrio fischeri and inhibition halo tests, and EEM-PARAFAC has been studied for the first time in order to study its applicability within the removal of these kind of compounds. Explored conditions were initial pH, being 2.8 (optimal for (photo)-Fenton processes), 5.0 and 7.0, and water matrix effect employing MilliQ water, tap water and salty water (30 g/L NaCl spiked in tap water).
Fast total FQ-removal by (photo)-Fenton treatment for pHs 2.8 and 5.0 has been observed, whereas in photolysis 40% removal was attained after 120 min in all cases. Chelation activity has been detected between FQs and iron, explaining the fast removals observed even at mild conditions as it was pH 5.0. However, TOC measurements showed that only photo-Fenton was able to produce significant mineralization (80% in 120 min, pH 2.8). The negligible mineralization observed in Fenton and photolysis indicates that FQ removal results in the release of important recalcitrant by-products. However, analysing EEM-PARAFAC results, a fast-total decay was observed for the components related to the FQ structure with (photo)-Fenton, whereas with photolysis they remained constant for the 120 min. These results have indicated that even though photolysis is able to remove FQs, it is not able to produce important changes on its structure; only under stronger oxidizing conditions the core of the FQ is attacked. As expected, antibacterial activity assays showed that the inhibition halo decays following the trend previously observed through EEM-PARAFAC. This might indicate that the destruction of the FQ structure is required to get rid of the antibiotic properties.

IV. Next Generation of SiC Membranes (Haris Kadrispahic)

Extremely durable, yet very porous membranes from LiqTech, are made of silicon carbide. They are used in water treatment and to clean the exhaust from diesel vehicles.

LiqTech International has existed since 1999 and have always been close part of the scientific community. We have kept close contact with leading European universities throughout.

Today we are manufacturers and system designers of our own product SiC membranes and turnkey solution providers, based on SiC UF water treatment systems.

Our group is working extensively on producing membranes with finer pores. The idea for this project is to be able to finally produce nanofiltration membranes.

Our development is working very closely with academia and currently have two European projects as well as Aquality project. We are pioneers within SiC membrane development, but we are more than that. We are pioneers
when it comes to innovation management as well. Nothing is ever done without universities and we are working with some of the best universities.
I. The HypoTRAIN Project (Jörg Lewandowski)

Hyporheic Zone Processes - A training network for enhancing the understanding of complex physical, chemical and biological process interactions

Hyporheic zones, i.e. the sediments in the river bed, are key compartments for the functioning of aquatic ecosystems. As dynamic and complex transition regions between rivers and aquifers, they are characterized by the simultaneous occurrence of multiple physical, biological and chemical processes. We are facing a significant knowledge gap in the understanding of how hyporheic processes are linked and how they impact on each other. This can be attributed to a lack of truly supra-disciplinary research. HypoTRAIN gathered a multi-disciplinary team from hydrology, ecology, microbiology, engineering, environmental physics, contaminant science, and modelling to generate new mechanistic insights into the functioning of hyporheic zones and enable a more holistic design of river management and restoration.

Rivers are important ecosystems under various anthropogenic pressures. Some of them are nutrients and contaminants that enter streams on different routes, e.g. by (treated) wastewater. Especially organic micropollutants such as pharmaceuticals and their daughter products are often neither degraded by the human metabolism nor the treatment processes in the wastewater treatment plant. Being discharged into rivers they might even be transported to the groundwater. Rivers and groundwater are important drinking water resources which is why attenuation or degradation of pollutants is relevant not only for ecosystems but also for human health. Rivers have some self-purification capacity which is assumed to result from the degradation of pollutants by (micro-) organisms and retention by sorption, both occurring in the hyporheic zone. Hyporheic zones are highly dynamic and productive river compartments. Surface water enters the river bed and travels through the sediment matrix. On its way it might mix with groundwater. Physical, biological and chemical processes occurring simultaneously in hyporheic
zones are assumed to stimulate retention and/or transformation of pollutants.

Key microbial taxa associated with degradation of several organic micropollutants of interest have been identified in HypoTRAIN using biological molecular techniques (qPCR, Next Generation Illumina sequencing). Their interaction with hyporheic geochemical parameters revealed that oxygen distribution directly influences the microbial guilds occupying particular compartments of the hyporheic zone. This in turn influences the degradation pathway of micropollutants reaching these microzones. Due to relatively low concentrations of micropollutants compared to other growth substrates, co-metabolism is predictably an important biodegradation process in the hyporheic zone, compounded by an inadequate enzyme catalogue to degrade the ever-dynamic generation of new anthropogenic compounds. The data on the microbial community structure and response to micropollutants form a basis for optimization of conventional wastewater treatment and/or manipulations of receiving rivers. We improved approaches to sample hyporheic water on extremely small vertical scales (e.g. mini-point samplers and an innovative passive sampling method). Analytical methods were advanced to quantify very low micropollutant concentrations. The development of “enantiomeric fractionation” enabled the differentiation of biodegradation processes from sorption and dilution. Furthermore, the performance of models describing and predicting hyporheic processes and the fate of pollutants was improved.

Turnover and degradation of nutrients and pollutants are among the prominent ecological services provided by the hyporheic zone. The removal or attenuation of pollutants strongly depends on hydrological fluxes transporting surface and groundwater into the river bed. Those fluxes enable the exposition of pollutants to the biogeochemical mechanisms driving their decrease in the hyporheic zone. It can be concluded that river restoration measures with a focus on reduction of pollutants should include features to increase hyporheic flow by creating physical barriers, e.g. woody deposits or rocks. These features will promote physico-chemical conditions favoring sorption and biodegradation in the hyporheic zone. At best, our results will facilitate the generation of better tools for assessing the effectiveness of restoration measures, river regulation, and the impact of climate change on hyporheic processes.
II. What happens to micropollutants in the hyporheic zone? – findings of an interdisciplinary joint mesocosm experiment (Anna Jäger)

Eight PhD candidates of the “HypoTrain” project came together at Birmingham University in 2017 to run an interdisciplinary joint mesocosm study. They sought to improve the understanding of the fate of wastewater-derived organic micropollutants in rivers, which is crucial to improve risk assessment, regulatory decision making and river management. Particularly, they were interested in the influence sediment bacterial diversity and hyporheic exchange have on micropollutant degradation and transformation. Although both factors gain increasing attention as drivers for micropollutant degradation, they are complex to study in field experiments and usually ignored in laboratory tests aimed to estimate environmental half-lives. Flume mesocosms are useful to investigate micropollutant degradation processes, bridging the gap between the field and batch experiments. Hence, the project team developed a novel experimental setup using 20 recirculating flumes and a response surface model to study the influence of hyporheic exchange and sediment bacterial diversity on half-lives of a range of micropollutants commonly found in rivers receiving treated wastewater. The effect of bedform-induced hyporheic exchange was tested by three treatment levels differing in number of bedforms (0, 3 and 6). Three levels of sediment bacterial diversity were obtained by diluting sediment from the River Erpe in Berlin, Germany, with commercial sand (1:10, 1:1000 and 1:100000). Their results show that the influence of sediment dilution and number of bedforms on micropollutant half-lives was compound specific. Half-lives of acesulfame, an artificial sweetener, for instance, were significantly influenced by both factors. However, the majority of compounds were primarily influenced by the sediment dilution treatment, showing that mostly higher bacterial diversity leads to higher degradation. In addition, various transformation products were identified. Their formation patterns were also in many cases strongly controlled by bacterial diversity, as for instance found for metoprolol acid deriving from the β-blocker metoprolol. Overall, the results of the experiment show that the flume-setup is a useful tool to study the fate of micropollutants in rivers, and that hyporheic exchange and bacterial diversity in the sediment are important factors driving the degradation of micropollutants in rivers.
I. The ENIGMA project (Damien Jougnot)

European training Network for In situ imaGing of dynaMic processes in heterogeneous subsurfAce environments

How to adapt subsurface imaging strategies to the processes of interest is an overarching question addressed in ENIGMA.

Most geophysical methods used by practitioners aim at improving our knowledge of subsurface structures. But field techniques for monitoring and imaging flow, transport, and reaction processes that evolve in space and time are still nascent. A new generation of scientists familiar with both emerging Earth observation technologies and detailed process upscaling and modelling is thus needed to respond to the increasing demand to understand and monitor subsurface processes at the scientific, public administration and industrial levels. To address this challenge, the ENIGMA training network is creating an innovative and entrepreneurial training environment for young scientists, which gathers 21 partners (15 academic and 6 industrial) from 8 European countries. It aims at training young researchers in the development of innovative methods for imaging process dynamics in subsurface hydro systems, in order to enhance understanding and predictive modelling capacities and to transfer these innovations to the economic sector. A key aspect of the ENIGMA network is the added-value that can be gained by enhancing exchanges between areas of excellence, which have developed relatively independently so far.

The term imaging, central within the ENIGMA network, refers herein to the spatial representation of subsurface heterogeneity, fluxes, chemical reactions and microbial activity, through the integration of data and approaches from geophysics, hydrology, soil physics, and biochemistry.

Achieved results (September 2019, Month 33)

- Training: most of training program established in the Grant Agreement has been completed, enabling the young researchers to
have a full grasp and to be innovative on their research projects. Especially, the Summer School (2018) was successful by opening perspectives beyond network research. Young researchers are leading the organization of the ENIGMA final conference, using previously learned life skills.

- Collaborations of young researchers across the network have led to multiple fruitful field experiments, such as tracer tests in India or in Ploeumeur (France)

- One peer-reviewed article was published so far by a young researcher, and others are currently in the reviewing process.

Young researchers are very active and regularly participate in European or international colloquiums and research seminars. List of communications is to be found on ENIGMA website.

II. Can vertical gravity gradients monitor seasonal soil moisture dynamics in karst? - Improvements from a new portable absolute quantum gravimeter and coupled hydro-gravimetical modelling (Anne-Karin Cooke)

Unlike point measurements such as borehole water levels, gravity measurements provide a valuable, depth-integrated constraint on the water storage dynamics of subsurface reservoirs. Gravity measurements integrate (water) mass changes across scales: gravity variations can be the effect of local up to continental scale soil moisture or aquifer storage changes. This technique can provide an estimation of the spatial variability of water storage at kilometer scale with an integration scale of about 100 m.

1) Validation of a new absolute quantum gravimeter (AQG)

μQuans is developing a new absolute quantum gravimeter (AQG), fast and transportable. The AQG is a real technological breakthrough compared to current portable gravimeters, which provide relative measurements. It will allow a more efficient and precise mapping of gravity in space and time. The objective of this thesis is the field validation of the first AQG against the most accurate gravimeters located at fixed stations at H+ Larzac and
other sites. The AQG will be used to estimate the contribution of different water storage reservoirs. The AQG A01 was delivered to RESIF and to the facilities of Geosciences Montpellier in 2018. Gravity time series of several weeks in different locations (Larzac, Geosciences Montpellier and LNE (Trappes)) with different ambient noise levels have been obtained. Analyses of stability and reproducibility are under still evaluation and their publication outlined.

2) Vertical gravity gradient monitoring

A precisely estimated vertical gravity gradient is necessary for the inter-comparison of absolute gravimeters that measure at different heights. Apart from this practical aspect, the method of vertical gravity gradient monitoring and its potential for the detection of soil moisture distributions are being investigated. The method aims at exploiting the complementary spatial sensitivities of gravity and gradient observations, respectively, to improve the localization of (water) mass changes in the subsurface. The following research questions are considered:

- What is the contribution of and how can gravity gradient time series be used for hydrological monitoring?

- How can they be effectively combined with gravity and other (hydro-)geophysical data and hydrological modelling to enhance temporal and spatial detection of mass changes caused by hydrological phenomena?

A year of monthly gravity measurements and vertical gradient estimations with a relative gravimeter has been completed at the geodetic observatory in karstic environments (GEK) on the Larzac plateau in France. Temporal variations have been observed. The repeatability of the gradient estimates as well as its uncertainty concerning different protocols and instruments have been evaluated. For gradients on a pillar, temporal differences exceed the estimated uncertainty of the method.

3) Hydro-gravimetrical modelling and inversion

A hydrological model – based on the 3D-modeling framework Pflotran – has been implemented for the Larzac site. The hydro-meteorological time series provided by the on-site instrumentation are used for calibration. The hydrological model has been coupled with a gravity forward routine, hence translating the simulated soil water content into an expected gravity signal and a vertical gravity gradient signal at the exact locations of the gravity
observations. The model is used to test hypotheses of probable causes of observed gravitational gradient variations. Firstly, an ‘umbrella effect’ of the building on the local water balance is well known in hydrogravimetry literature. Another hypothesis concerns sinkholes, weathered areas in the karst around the building, that appeared in previous seismic studies. These areas of higher porosity that are subject to wetting and drying. An optimization algorithm for nonlinear geophysical inversion was used to search the dimensions of this area, assuming that it was saturated and had an impact on the vertical gradient.

The umbrella effect does not yield gravity gradient changes of expected order of magnitude. The hypothesis of zones of modified porosity (sinkhole) is still under evaluation. The next step is to use the new instrument (AQG) for gradient estimations and provide an estimate on the precision of vertical gravity gradient estimations.

Further numerical and empirical studies on the application of the gravity-gradient method that go beyond the observation of natural mass changes are in development, aiming at hydrological experiments such as aquifer tests for aquifer characterization.

**III. Flow and reactions in stream-riparian zone systems, a multi-method space and time patterns characterization (Guilherme Nogueira)**

Safeguarding water quantity and quality for humankind is one of most important UN Sustainable Development Goals. The combination of high-resolution sensors with state-of-art modelling will allow the assessment and quantification of important local processes patterns that affect water quality and the watershed as a whole. Recognizing and understanding the important functional role of riparian zones in sustaining water quality will support a sound management of our water resources, which is crucial in the light of a global Contrary to a few decades ago, groundwater and surface water are now seen as one dynamically connected entity. Many biogeochemical turnover processes, which are important for shaping water quality, take place in riparian groundwater adjacent to streams and are linked to groundwater-surface water and hyporheic exchange. The exchange of waters with different chemical composition and temperature not only leads to mixing-related concentration changes, but also affects the biogeochemical and temperature regimes and may facilitate enhanced
reactive turnover, which in turn affects solute concentrations. This reactive potential of the riparian aquifer typically shows distinct patterns in space (hot spots) and time (hot moments), which are controlled by the hydrologic dynamics of exchange, seasonal temperature variations and heterogeneity of system (e.g., carbon content).

Some of the open questions to be answered are, for instance: what is the link between extreme discharge events and the aquifer’s reactive potential; or how is subsurface heterogeneity linked to reactivity in terms of hot spots and hot moments; how can reactive potential and turnover be effectively assessed; or how will climate change affect such reactivity?

The main objective of this thesis is to identify and characterize the space and time patterns of exchange between streams and their riparian zone and the resulting potential for solute turnover by jointly using novel and advanced tracing, imaging, and modelling techniques. For that, we make use of combined field techniques for aquifer characterization, high-resolution measurement sensors for capturing small and large events variations, and advanced numerical modelling to synthetize main observed and relevant processes of the system. Moving from a simplistic static view to a more realistic dynamic view and interpretation of the system is anticipated and expected.

The first publication is in preparation and comprises the collected high-resolution integrated data, analysed and compared with direct and indirect methods to assess groundwater travel-times under bank filtration processes to uncover solute turnover and its spatio-temporal variation. Using the identified patterns of water and solute fluxes and additional measurements of solutes in the stream and piezometers with varying distance to the stream will enable a mapping of the turnover capacity for reactive solutes in the riparian aquifer. A synthesis of the observations will be achieved using a reactive transport model to replicate flow and reactivity patterns. Further numerical modelling will allow us not only to reproduce and gain extra insights into system behaviour, but will also enable us to comprehend which dataset should be considered and acquired when planning bank filtration activities, or river restoration measures.
I. The PROTECTED project (Lisa Connolly)

**PROTECTion against Endocrine Disruptors.**
Detection, mixtures, health effects, risk assessment and communication

PROTECTED aims to develop expertise and protective capabilities against Endocrine Disruptors (EDs). EDs and their mixtures are a modern day health concern leading to failing ecological systems, poor agricultural production and health effects such as obesity, cancer and infertility. While analytical methods have advanced enormously, focus has been mainly on synthetic chemicals, overlooking emerging EDs and real-life multiple substance exposure. A new generation of creative, entrepreneurial and innovative early-stage researchers equipped with skills to assess and understand the real-life risk of complex mixtures of EDs and trained to convert resulting knowledge and ideas into accessible tools and services for the long-term control of potential ED risk is urgently needed. The PROTECTED Innovative Training Network [ITN] proposes a holistic approach by providing 15 individual, personalised research projects with exposure to scientific, innovative and entrepreneurial training mobility across the ITN. The intersectorial network is comprised of 12 training sites at academia, research centres, a bioassay technology SME, a QSAR technology SME, water provider, and animal feed supplier. Together they cover multiple disciplines including analytical science of food, feed, and environment, epidemiology, risk assessment, social science and toxicology. This combined expertise enables a highly focused program for developing novel tools and concepts and training for the detection, analysis and improved risk assessment of EDs, especially mixture effects. Methodology will include emerging technologies; multiplexed analysis, mixture modelling, mechanistic and exposure studies, explants and cell or whole organism bioassays. The project will provide a unique and high level of training for a new generation of specialists with transferable skills and enhanced career perspectives. These specialists will ultimately aid the efficient development of future control strategies for improved health.
II. Fifty shades of cyanobacterial green (*Vittoria Mallia*)

Cyanobacteria are cosmopolitan photosynthetic prokaryotes, also known as “blue-green algae” because of their appearance. They can form dense blooms (visible discoloration of the water due to their accumulation) in brackish, marine and fresh water environments. Cyanobacterial blooms can produce a large variety of active metabolites, including well-known cyanotoxins. Therefore, they may have negative effects on the water quality (drinking, bathing, fishing, recreational uses) and result in harm to invertebrates and vertebrates including humans.

The aim of the “Endocrine disrupting compounds in cyanobacteria” project is to investigate the potential role of cyanobacterial metabolites as endocrine disrupting compounds (EDCs), that is, compounds able to interfere with the hormonal system, using a multidisciplinary approach.

A collection of cyanobacterial strains (*Microcystis* and *Planktothrix* spp.), has been screened using liquid chromatography coupled to low-resolution and high-resolution mass spectrometry (LC-MS, LC-MS2, LC-HRMS(/MS)). Knowledge of chemical structures of cyanobacterial metabolites is still quite limited, but related to their potential effects and therefore fundamental for risk assessment. Microcystins (MCs) are the most known and studied family of cyanotoxins (hepatotoxins). However, even though more than 260 congeners have been reported, only for one of them (MC-LR) there are regulations on intake limits. Literature reports MC-LR as having estrogenic effects as well. Combining mass spectrometry analysis and derivatization techniques, we were able to report four putative structures of new MCs-congeners and several unusual conjugates in a *Planktothrix prolifica* strain.

There are several potential mechanisms for a compound to interfere with the endocrine system. We are testing cyanobacterial extracts, both MC-containing and non-MC-containing, as well as standard solutions of MCs, using different *in vitro* bioassays. We aim to assess their potential effects as EDCs, the possible role of MCs and their mechanisms of action. We were unable to detect interference with estrogen receptors caused by presence of MCs in the cyanobacterial extracts (Reporter Gene Assays, E-
screen). However, in studies of non-receptor mediated mechanisms; we tested a *Microcystis aeruginosa* strain and a pure MC-LR standard, on estradiol (natural estrogen hormone) metabolism, using human liver microsome assays. We detected an effect on estradiol metabolite ratios, suggesting important role of MCs. We are now studying the non-receptor mediated mechanisms using H295R steroidogenesis model to investigate potential activity of cyanobacterial extracts and MCs on the steroid production pathway.

Cyanobacterial blooms and EDCs represent two wide-spread and very current concerns. The variety of compounds released by cyanobacterial species combined with the variety of modes of action of EDCs create a complex and interesting research topic.

### III. Are chemicals in water potential endocrine disruptors? *(Elizabeth Goya Jorge)*

The PROTECTED Innovative Training Network (ITN) aims to develop new methods to control and assess the risk of substances and mixtures as endocrine disruptors (EDs). The contribution of the Early Stage Researcher in the company ProtoQSAR is expected to be the theoretical elucidation and analysis of EDs using computational tools combined with experimental in vitro bioassays. The combined expertise and results obtained from in silico and in vitro modelling can provide a better perspective leading to an efficient development of future control strategies for improved health of humans and reduce the environmental risks associated with the phenomenon of endocrine disruption.

Novel tools and concepts for the detection, analysis and to improve the risk assessment of EDs have been developed. Firstly, the construction of several databases of chemical structures with reported toxicity on several mechanisms of endocrine disruption have been accomplished. The mechanisms under study have included mainly estrogen receptors, androgen receptors and aryl hydrocarbon receptor. Computational tools have been used to predict the binding affinity to nuclear receptors and the agonistic/antagonistic activity of high concern substances.

Meanwhile, in vitro results profiling the chemical characteristics inducing endocrine disrupting activity have been used to model and to predict
untested chemicals. In that sense, Toxicophoric Ligand-Based Models have been designed. As an outcome of such methods, features and physicochemical properties were suggested as main contributors to the activity induced experimentally.

Quantitative Structure-Activity Relationship (QSAR) models have been obtained also where, through the parametrization using molecular descriptors, chemical substances were statistically associated with their biological effect upon endocrine receptors. Some emerging mechanisms as the disruption of coactivators have been studied using machine learning algorithms in QSAR modelling.

IV. ProtoQSAR: Contributions, Impact and Challenges in the PROTECTED Project Context (Stephen J. Barigye)

ProtoQSAR is a computational chemistry company, specialized in the development and optimization of chemical compounds for use in diverse areas such as therapeutics, agriculture, cosmetics or functional foods (neutraceutics). Our activity consists in the development and application of computational methods for the evaluation of physicochemical, biological and/or (eco)toxicological properties of chemicals, natural and/or synthetic origin.

Our computational approach allows us to work in a “virtual” environment, which has the following advantages over traditional laboratory tests: 1) Fast results: our methods reduce the time needed with in vitro and in vivo tests, thanks to its easy and immediate applicability to thousands of chemical structures, something impossible to perform experimentally; 2) Saving of material and financial resources, avoiding the costs associated with experimentation, both personal and laboratory equipment; 3) Limitation of animal testing (3Rs), which have to be performed only as a last resort, when no other scientifically reliable ways to demonstrate the impact of chemicals on humans and/or the ecosystem are available.

We present herein our experience in the context of “PROTECTED”, an EU project which aims to develop expertise and protective capabilities against Endocrine Disruptors (EDs), which are chemical pollutants capable of altering our hormonal balance. The EDs and their mixtures are currently a health problem of the first order, with adverse effects such as obesity,
cancer and infertility. They can also have a great impact on ecological systems, and for example be responsible for poor agricultural production.

In the specific case of ProtoQSAR, we have been involved in the development of computational predictive models to evaluate the effects of specific groups of chemical products (POPs, plasticizers, mycotoxins, etc.) and their mixtures as potential EDs. These predictions have been achieved through the use of advanced cheminformatics techniques, mainly mathematical quantitative structure-activity (QSAR) models.

PROTECTED has allowed us to work in close collaboration with representatives of an intersectoral network (comprised of 12 training sites at academia, research centres, other SMEs, water providers, etc). As a SME, this experience has enriched our knowledge in a relevant domain of research, and has increased our visibility as a company providing services in the computational area. Furthermore, the expertise acquired in EDs has allowed us to develop new internal lines of business to propose to our clients, and therefore to enlarge the typology of customers to whom we can address our business propositions.
I. The RELIEF project (Rosalie van Zelm)

*RELI*ability of product Environmental Footprints

Life cycle assessment is a tool to evaluate the environmental impacts of products or services throughout their entire life cycles. It is increasingly used to quantify environmental footprints, thought of as decision-support tools for consumers and companies to choose between products or ingredients. Environmental footprinting approaches are influenced by uncertainty and variability. Uncertainty because of an incomplete knowledge of the processes and properties influencing footprints and variability because of spatial, consumer-related, or technologically-induced differences.

The aim of the European Industrial Doctorate program entitled “RELI*ability of product Environmental Footprints“ (RELIEF) was to train early stage researchers (ESRs) to assess and improve the reliability of product environmental footprints. Four ESRs worked on different aspects of a product’s environmental footprints: land, energy, chemicals, and water, while the fifth focused on macro-scale environmental models to incorporate cross-cutting issues from the other four ESRs.

Sadegh Shahmohammadi quantified the variability in the greenhouse gas (GHG) footprints of 3 daily consumer activities i.e. laundry washing, showering and shopping for fast moving consumer goods. He further investigated the influence of different types of consumer behavior i.e. reasoned-actions and habits on the variability in the GHG footprints. Improvement potentials were also discussed in each study.

Valerio Barbarossa focused on improving global assessments of freshwater systems. Using machine learning techniques, he developed a dataset of global streamflow estimates from 1960 till 2015 at 1 km resolution. Further, he developed a species-specific modelling approach combined with high-resolution hydrology to assess global impacts of dams-driven fragmentation and climate change on the habitat of freshwater fish species.
Mélanie Douziech focused on improving the reliability of key factors determining the chemical footprint of consumer products released mostly down-the-drain after use. She developed a method to improve the reliability of chemical effect predictions. Further, she suggested ways to improve the prediction of removal efficiencies of chemicals in activated-sludge wastewater treatment plants.

Wan Yee Lam focused on understanding the drivers of variability of GHG footprints of global crop production. She developed a spatial approach to estimate land use change-induced GHG footprints of crops without exact farm location. Using a dataset of global production of 26 different crops, she found that GHG footprints of crops are mostly driven by fertilizer application and land use change, if any. Where land use change occurs, analysis at a high spatial resolution and consideration of peat lands are important to reflect the spatial variability of GHG footprints.

Sandra Marquardt is working on the assessment of biodiversity implications associated with current production, consumption, and trade dynamics. She calculated the biodiversity footprints of nations using three alpha-diversity and one gamma-diversity biodiversity indicators and concluded that biodiversity assessments should include at least two different types of indicators to capture the multifaceted nature of biodiversity. She also investigated the biodiversity impacts of forward-looking consumption scenarios.

Overall, the RELIEF ESRs enhanced the knowledge relevant for key global challenges such as deforestation, sustainable agriculture, freshwater availability, sustainable consumption, climate change, and chemical pollution. Besides their scientific achievements, the ESRs developed their project and team management skills, communication skills, creativity and entrepreneurship. Working with both academia and the private sector has provided them with the ability to develop and manage an integrated research project taking advantage of the complementarities and synergies between both environments. This will increase their ability to transfer between institutions and sectors in their careers.
II. Reliability in chemical footprint modelling of consumer products (Mélanie Douziech)

Chemical footprinting approaches quantify and evaluate the potential human and ecotoxicological impact of a product due to its constituting chemicals. Quantifying the chemical footprint of consumer products released mostly in wastewater after their use, requires a thorough understanding of the emission, fate, and effects of their constituting chemicals and the parameters influencing the variability and uncertainty of each step. The main aim of this project was to improve the reliability of key factors that determine the chemical footprint of down-the-drain consumer products.

First, a method was developed to estimate spatially-explicit chemical emissions from the use of down-the-drain consumer products. The approach combined consumer survey data with typical product formulations, wastewater removal efficiency (RE) predictions, and spatial distributions of populations and wastewater treatment plants (WWTPs). Emissions of three surfactants and two preservatives were estimated at national and WWTP level from the use of bodywash, shampoo, and conditioner for the Netherlands, France, the USA, and South Korea. Emissions varied up to two orders of magnitude between countries due to differences in population numbers connected to WWTPs. The uncertainty in WWTP specific emission estimates was smaller and mainly related to the uncertainty in the RE estimate.

In a second step, the focus was therefore to improve the prediction of RE from activated sludge WWTPs. A meta-analysis was conducted on RE (1539 data points) measured for 209 chemicals (fragrances, surfactants, and pharmaceuticals). A linear mixed-effects model (LMM) was fitted to understand which physico-chemical properties and WWTP operational parameters influenced the RE. Overall, the LMM confirmed that readily biodegradable chemicals and increased sludge retention times increase RE. Further, the LMM showed an unexpected decrease in RE with increasing organic carbon partitioning coefficient. This calls for a better understanding of electrochemical interactions between chemicals and sludge. The LMM performed slightly better than the widely used process-based model SimpleTreat but the predictive performance stayed low. The poor understanding of the chemicals undergoing deconjugation can explain the limited predictive power of both models.
In a third step, a systematic quantification of the influence of uncertain and variable parameters on the calculation of the potential ecotoxicological impact (PEI) of the use of a down-the-drain products was carried out (54 shampoos). The influence of the statistical uncertainty in the prediction of physicochemical properties and freshwater toxicity and various sources of variability relating to consumer habits and geo-spatial aspects (e.g., wastewater treatment technology and coverage) were separately quantified via a 2D Monte Carlo simulation. Shampoo formulation composition was the most influential source of variability, while the overall uncertainty in the PEI was driven mainly by the limited number of toxicity data available (three species) to estimate the ecotoxicological impacts of the chemicals.

This result shows the need for methods to more reliably predict ecotoxicological effects. An ecotoxicological modelling approach combining two in silico methods: quantitative structure-activity relationships (QSARs) and interspecies correlation estimation (ICE) models was therefore developed. Hazardous concentrations (HCs) of chemicals, at which a certain percentage of all species are exposed above the concentration causing acute effects, were estimated. The principle of this QSAR-ICE approach was illustrated for 51 chemicals by quantifying the representativeness of the estimated HCs compared to experimentally derived HCs and their statistical uncertainty. Overall, combining at least two QSAR-based ecotoxicity values with the corresponding ICE, led to HCs with comparable bias and lower statistical uncertainty compared to using only three QSARs. This QSAR-ICE approach can be used to derive toxicity values for substances for which measured or estimated ecotoxicity data are lacking and thus help prioritize chemicals, as long as these chemicals are within the applicability domain of the QSARs used.

This thesis presented several techniques to better account for and, to some extent, increase the reliability of chemical footprints of consumer products.
The NaToxAq ITN started January 2017, with most ESRs on board by mid 2017. The consortium comprise 10 beneficiaries located in Denmark, UK, Germany, Spain, Switzerland, Czech Republic, Sweden and the US; in total 22 partners of which many are from the water sector. Sixteen ESRs are involved of which 2 are shorter term ESRs.

NaToxAq is about toxins produced by living organisms and their impact on drinking water reservoirs. Organisms produce a multitude of bioactive natural compounds that are toxic, "warfare" chemicals with the purpose to protect the organism against other species. Examples comprise cyanotoxins in algal blooms, coniin from poison hemlock, ricin from Castor oil plant, aflatoxins from molds, or just something as common as solanin in potatoes. Natural toxins are produced in vast amounts, they are widely distributed, many are highly mobile and persistent. There are more than 25,000 natural toxins distributed over all known natural product classes, of which some are well known from food and feed poisoning, but with very little data on environmental fate and the potential of the toxins to affect water resources. Certain cyanotoxins are well known to affect water quality, while less is known about plant toxins.

In NaToxAq we dig deeper into the many unknowns. Work packages comprise i) analysis of natural toxins by specific, non-target and effect-directed analysis, ii) natural toxin production, distribution and release, iii) Experimental and QSAR estimation of phys-chem properties of toxins incl. abiotic and microbial degradation and opportunities for toxin removal at water works, iv) human toxicity of mainly cyanotoxins, and v) databases of natural toxins, geographical mapping of toxin loads, transport modelling, and risk scenario analysis.

Many new analytical methods have been developed for sensitive detection and for screening. New toxins have been discovered in soils and water. Natural toxin concentrations in natural waters are highly fluctuating with
pulses appearing during storm events when toxins are washed off from plants. A substantial fraction (> 30 %) of natural toxins is estimated (QSAR) to constitute persistent, mobile and toxic compounds (PMT), with alkaloids as the dominating class. In fact alkaloids appear in many of the monitoring programs performed by the ESRs. Many natural toxins are quickly degraded mainly by microbiota, but some toxins are unexpectedly resistant to both hydrolysis, photolysis and enzymatic degradation. Invasive species and climate change adds a new dimension as both factors introduce new toxins at high loads in environments not previously exposed to those toxins.

NaToxAq aims to train a first generation of ESRs prepared to handle natural toxins covering all aspects from analysis via fate to biological impact, health issues, mapping, risks and regulation. We have had 4 training events, each of 7 - 10 days duration, in Denmark, UK, Spain, and Germany. Nine specialist PhD courses and 7 complementary skills courses have been taught. News are published via the homepage https://natoxaq.ku.dk, that also includes a newsletter. All ESRs are involved in outreach activities. A final international conference open to all interested will be held in Brno, 10 - 12 June 2020.

II. Natural Toxin Mobility from Source to Tap (Carina Schönsee)

Natural toxins are not yet commonly regarded as environmental contaminants of concern for water quality. However, over 34% of plant secondary metabolites (phytotoxins) fulfil the criteria for aquatic persistency, mobility and toxicity based on predicted property data (Günthardt, et al., 2018, doi/10.1021/acs.jafc.8b01639). Hardly any experimental data describing natural toxin aquatic mobility are available. In silico prediction tools additionally show limited applicability for complex ionizable compounds. Hence, effective environmental exposure/risk assessment of natural toxins is difficult and systematic research on environmental distribution processes is urgently needed. Only then, we are able to reliably determine whether natural toxins are mobile enough to end up in potential drinking water abstraction sites.

Within this context, our ongoing project focusses on the experimental determination of intrinsic physicochemical properties affecting environmental mobility of natural toxins. We established HPLC-based high-
throughput methods for the systematic evaluation of model phase partitioning coefficients under changing environmental conditions. Generated data is subsequently used in exposure/risk assessment of natural toxins. Moreover, as model compounds for complex ionizable organics, experimental data will additionally allow valuable insights into environmental behavior of this highly important class of compounds.

As an indicator for the partitioning of natural toxins from aqueous media to organic matrices, the octanol-water partition coefficient Kow can be seen as first proxy estimating natural toxin mobility in the aquatic environment. We derived pH-dependent octanol-water partition coefficients (Dow) for a diverse set of 45 largely ionizable natural toxins in the environmentally relevant pH range from pH 4 to 10. The chosen method allowed the reliable determination of log Dow < 4, the relevant range for potential aquatic contaminants. Analyzed natural toxins comprised phytotoxins and mycotoxins from several compound classes (alkaloids, polyketides, steroids, terpenoids). Results show that all analyzed toxins are highly polar, independent of compound ionization. A publication of the generated dataset is currently in preparation.

Additionally, a column chromatography system has been set up to systematically study sorption of natural toxins to different geosorbents. For this purpose, HPLC columns were manually packed with the sorbents of interests. Using Pahokee Peat as a first sorbent, organic carbon-water partitioning coefficients (Koc) were derived as primary toxin mobility indicator. Firstly, results show that column chromatography can be reliably applied in sorption studies of large diverse sets of polar, complex compounds. Secondly, all considered natural toxins are highly mobile. The analyzed set comprises over 100 natural toxins from 30 different subclasses of which more than half are ionizable. Advantages of the method are the very short analysis time and little material requirements that easily allow systematic investigations of differing influences on sorption. By changing experimental settings (pH, eluent composition), charge effects as well as ion competition on natural toxin sorption are evaluated. Thus, detailed mechanistic insights are gained that are of great value for understanding transport and fate processes in the environment. Applying the method to other different sorbents in the future (minerals, activated carbon) will help to determine their individual contribution to the natural toxins’ overall mobility on their path from source to tap (drinking water).
In close collaboration with other researchers from the NaToxAq network, generated natural toxin property data is used to critically evaluate the applicability of commonly used prediction models. Additionally, our data is valuable input in prioritization for monitoring campaigns as well as environmental fate studies and models. Ultimately, natural toxin mobility data will support reliable exposure/risk assessment with regards to protecting the quality of our drinking water resources.

III. Production Dynamics and Degradation of Emerging Cyanopeptides (Regiane Sanches Natumi)

Cyanobacterial blooms are a growing public health concern due to the production of a wide range of bioactive compounds including a hundreds of cyanopeptides beyond the famous hepatotoxic class of microcystins. Hardly any information is available regarding the occurrence, production dynamics, environmental fate and toxic mode of action for the majority of cyanopeptides. To improve our understanding of the exposure site of the risk equation for cyanobacterial bloom events our project evaluates a) production dynamics of the potentially toxic cyanobacterial peptides, and b) the stability and fate processes of emerging cyanopeptides in surface waters.

We developed culturing, harvesting and extraction protocols to study the occurrence of cyanopeptides and we further purify peptides to study their fate processes as these compounds cannot be obtained commercially or by chemical synthesis. We build an in-house database of more than 700 structurally known cyanopeptides including cyclamides, cyanopeptolins, anabaenopeptins, microginins, aeruginosins and microcystins. This database in combination with a vigorous data analysis workflow allows us to perform suspect screening with liquid chromatography high resolution tandem mass spectrometry to identify toxins in our samples. Our cyanopeptide suspect list will be made publicly available to assist other researchers and water suppliers for the identification of emerging cyanopeptides and to assess their global occurrence.

With this analytical methods, we first analyzed the production dynamics of various bloom-forming cyanobacteria. We verify that one species can produce more than one family of cyanopeptides and one cyanopeptide can be produced by more than one species. We demonstrate that these emerging cyanopeptides can be just as abundant or even dominating over
the well-known microcystins. The production is maintained during different growth-phases and total production can be affected by a change in nutrient availability. These production dynamics have thus far only been reported for few microcystins and we demonstrate similar trends for the emerging peptides. Consequently, monitoring only single microcystin variants greatly underestimates exposure to other potentially toxic cyanopeptides during cyanobacterial bloom events.

Next, we investigate the persistence of cyanopeptides to improve our estimates of exposure during bloom events. Since cyanobacterial blooms are dominant in sunlit surface water, we first focus on phototransformation processes. We demonstrate that out of 50 abundant cyanopeptides tested, most are transformed in sunlight but some half-lives are too long to expect significant removal. Currently we investigate the dependence of pH and presence of different lake matrices on the direct and indirect photochemical transformation pathways and establish bimolecular reaction rate constants with photochemically produced reactive oxygen species that can later be applied in predictive models. Knowing which cyanopeptides are persistent in surface waters will also indicate which compounds can reach drinking water treatment plants and thus need further attention.

The knowledge gained through this project provides necessary information regarding co-occurrence and stability of emerging cyanopeptides for risk assessment of cyanobacterial blooms for recreational use and their potential relevance in drinking water treatment.
The flux of phosphate (P) from agricultural areas to surface waters is wasting a resource which is becoming scarce and is in conflict with the principles of a circular economy. Enhanced loading of surface water with P is the main cause for eutrophication and presents a key challenge in meeting the objectives of the EU Water Framework Directive. P-TRAP targets both problems and develops new methods and approaches to trap P in drained agricultural areas and in the sediments of eutrophic lakes. Trapping of P involves the application of iron(Fe)-containing by-products from drinking water treatment. Ferric iron ((oxy)hydr)oxides have a high affinity for P. Therefore, the elemental cycles of P and Fe are strongly coupled in natural systems. The strategy of P-TRAP is to optimally benefit from this naturally strong association between P and Fe and the underlying processes in order to improve the quality of surface waters and to recycle immobilized P. P-TRAP targets two environmental systems in which understanding and managing interactions between Fe and P can lead to an effective removal of P from the water cycle: 1) drained agricultural areas and 2) lakes. The P-TRAP concept consists of three elements: i) Immobilizing P in drainage systems, including the application of new sorbents based on by-products from water treatment, and convert the P-containing Fe(III) oxides into marketable fertilizers ii) use Fe-containing by-products of water treatment to achieve long-term stabilization of P in lake sediments iii) provide fundamental understanding of Fe-mineral transformations to underpin the innovative approaches to trap and recycle P. P-TRAP aspires the ideas of a circular economy and aims at recovering the retained P in agricultural systems. Novel microbial technologies will be developed to convert P-loaded Fe-minerals into marketable fertilizers whose suitability will be evaluated. The new P-TRAP technologies have in common that they rely on the naturally strong connection between P and Fe and the innovative P-TRAP strategies will be underpinned by process-orientated investigations on the behavior of P during the transformation of Fe minerals. The latter are key in trapping and recycling of P in agricultural systems and lakes.
I. The AQUASENSE Project (Saoirse Dervin)¹

Innovative Network for Training in wAter and Food QUality monitoring using Autonomous SENSors and IntelligEnt Data Gathering and Analysis

The deterioration of water quality, caused by climatic and seasonal changes, global warming, or industrial waste etc. is a major global concern. Water quality has a direct impact on our lives as any drinks or food made from it affect human health. Over the last decade, water quality observing technology has risen to the challenge of scientists to identify and mitigate poor water quality by providing them with cost-effective tools that can take measurements of essential biogeochemical variables autonomously. Yet, despite these options becoming more readily available, there is a gap between the technology and the end-user (including the investigators and technicians that deploy these technologies) due to a collective lack of training, in-depth knowledge, and skilled workers who can meet new and emerging challenges.

There is also a disconnect between data quality, data gathering by autonomous sensors and data analysis, which is a major obstacle, as the sensors are already being deployed (e.g. through buoys, boats etc.) to broaden data coverage in space and time. AQUASENSE will resolve these challenges by providing 15 early stage researchers (ESRs) with unparalleled multidisciplinary training in the field of water quality through autonomous sensors and autonomous deployment. The ESRs trained through AQUASENSE programme will fill the skill-gap and contribute towards strengthening of Europe’s human resources and industry competitiveness in the strategic fields of aqua/agriculture and sensing technologies.

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I. The NOWELTIES Project (Mira Petrovic)

**Joint PhD Laboratory for New Materials and Inventive Water Treatment Technologies. Harnessing resources effectively through innovation**

Future challenges, including climate change and the resulting unpredictability of precipitation patterns and temporal or permanent water scarcity, generate a high diversity of demands on water treatment technologies obliging them to be able to cater towards a variety of source and target water qualities across multiple scales, depending on application. It is evident that this will generate a market pull towards the development of new water treatment technologies, employing new materials or improving the integration of existing technologies. However, the integration of research and innovation within the water sector needs to be supported by education of a new generation of interdisciplinary trained wastewater professionals able to face future challenges and implement wastewater-related directives in practice.

The primary objective of NOWELTIES is to organize a platform (European Joint Doctorate) that will provide cutting edge training opportunities for the education of tomorrow`s water treatment experts. The core activity is the research programme (composed of 14 individual research projects) aimed at development of inventive water treatment technologies (advanced biological treatments, innovative oxidation processes, hybrid systems) that allow catering for the varied treatment demands for a plethora of interconnected streams arising from recycling loops. These technologies will be able to control contamination by organic micropollutants (OMPs) and improve recovery of water across a diversity of scales enabling a smart combination of decentralized and centralized approaches.

The **specific research objectives** of NOWELTIES research programme are:

- To improve understanding of the mechanisms and controlling factors affecting elimination of OMPs in wastewater treatment
- To synthesize a range of novel nanomaterials and nanocomposites followed by detailed characterization of their composition, structure and photocatalytic/sorption properties

- To develop and test novel high performance hybrid systems combining innovative biological and physico-chemical processes

- To optimize operational parameters and evaluate efficiency of a range of innovative concepts based on advanced biological treatments, AOPs, electrochemical processes, and hybrid systems while minimizing energy demands and generation of residuals

- To translate findings into new treatment concepts and applications.

Besides a holistic training in the field of wastewater treatment dealing with state-of-the-art technologies, experimental techniques and knowledge management methodologies, NOWELTIES will provide a unique training approach to learning complex complementary skills leading to independent and critical thinking which seeks for originality and innovation.
Short CV of the speakers

SERGI SABATER

Professor of Ecology at the University of Girona (UdG). His research career has been focused on the ecology of fluvial ecosystems, particularly regarding the role of biofilms, the metabolism and functioning of fluvial systems, and the effects of global change on fluvial systems.

He is the Deputy Director of ICRA.

EMANUELA GALEAZZI

I graduated in Biology at the University of Torino (Italy) in 1987 and I worked for 12 years in medical and biological research on head and neck tumors at the University of Torino (Italy) being (co-)author of more than 30 scientific publications.

In 2008, I joined the European Commission. Between 2011 and 2015 I held a position of Policy Officer at the Unit "Research and the European Innovation Partnership" of DG Agriculture and rural development.

In November 2015 I joined the Research Executive Agency as Project Adviser in the Unit in charge of Innovative Training Networks (ITN) of Marie Skłodowska-Curie Actions.
I am the Panel Coordinator of ITN European Joint Doctorates and in charge of some horizontal tasks in the Unit, the Policy Feedback being one of them.

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**BARBARA MESTER**

I graduated at the Catholic University of Milano in Business, economics and finance.

Between 1998 and 2002 I have worked in Frankfurt in the finance sector followed by a period of ca 5 years in the marketing sector.

Since 2007 I dedicated myself to the management of EU funded scientific projects, working for the European Commission first and then for the Research Executive Agency.

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**DANIELA BUZICA**

Daniela Buzica is Policy Officer at Unit C.1 - Clean water of DG Environment. She is in charge of water-related research and of reporting on the Water Framework Directive. She is also following the International Commission for the Protection of the Danube River.
ANNA MARCZAK

Anna Marczak is Policy Officer at Unit C.2 - Marine Environment & Water Industry of DG Environment. Beyond coordinating tasks with other Directorate-Generals on operational and research programmes, she follows files related to the Water Industry, Drinking water and urban waste water Implementation and Information Framework (SIIF).

GUY DUKE

Guy Duke is founding Director, GD NatCap Ltd, consulting on natural capital markets, policy, research, innovation and knowledge exchange, for government, business and not-for-profit clients. Current work includes PI for the H2020 project We Value Nature, and Business Champion for the UK Valuing Nature Programme.

Guy was previously (2010-17) Director Europe & Research for The Environment Bank Ltd (EBL), a company at the forefront of emerging UK and EU ecosystems markets.

Guy held a Public Appointment (appointed by UK Secretary of State for Environment, Food and Rural Affairs) as Deputy Chair (2015-17) and Independent Member (2009-17) of the Joint Nature Conservation Committee (statutory adviser to UK Government on UK and international nature conservation).

Guy is an Honorary Research Associate, Environmental Change Institute, University of Oxford (2011-ongoing) and a Fellow (2018-ongoing) of the Centre for Ecology & Hydrology (CEH). He Chairs the COST Action ‘European Raptor Biomonitoring Facility’ (2017-2021).

Guy acts frequently as Chair/Vice-Chair for evaluation of EU H2020 large-scale research and innovation proposals (SC5 Climate Action &
Environment, SC2 Sustainable Agriculture & Forestry, SC3 Energy) and Marie Skłodowska-Curie Action proposals (International Training Networks, Individual Fellowships) and as a Monitor of MSCA-ITN projects.

From 2002-07, Guy was Principle Administrator Biodiversity Policy, DG Environment, European Commission. He authored the 2006 EU biodiversity and ecosystem services policy, which introduced the concept of ecosystem services to the EU acquis, played a key role in commissioning 'The Economics of Ecosystems and Biodiversity' (TEEB) (a precursor to the Natural Capital Coalition) and commissioned € multi-million research to policy projects.

From 1998-2002, Guy was Technical Director in the International Development Services division of Environment Resources Management (ERM), creating a net €1 million p.a. natural resources and biodiversity business with donor clients (World Bank, EC, UK DFID, etc).

During his career, Guy has authored numerous successful tenders and grant proposals.

MIRA PETROVIC

ICREA Research professor, Water Quality Area, ICRA – Catalan Institute for Water Research, Girona, Spain

ICREA Research Professor since December 2005. PhD in Chemistry (1995), Faculty of Chemical Engineering and Technology, University of Zagreb, Croatia. From 1999-2011 research scientist at the Department of Environmental Chemistry, Institute for Environmental Assessment and Water Studies (IDAEA-CSIC), Barcelona. Since July 2011 senior researcher at the Catalan Institute for Water Research (ICRA), Girona, Spain. At ICRA she is the head of Water Quality Area and responsible for the research line Contaminants in water treatment processes. She has participated in over 20 EU projects since 1999; published 220 papers in SCI journals (Hirsch Index 64); edited 8
books and published 36 book chapters. She is Highly Cited Researcher 2018 (ranked in the top 1% by citations) in the field of Environment/Ecology according to Clarivate Analytics.

Her main expertise is in the field of analytical environmental chemistry, specifically analysis of trace organic contaminants, such as pharmaceuticals, endocrine disrupting compounds and surfactants by advanced mass spectrometric techniques (liquid chromatography-tandem and hybrid MS) and the study of their fate and behaviour in the aquatic environment and during wastewater and drinking water treatment. Specific research lines are: (i) non-target analysis and fingerprinting of organic substances in wastewater and receiving environment, (ii) the study of biotic and abiotic transformation of emerging contaminants, identification of transformation products, elucidation of transformation pathways; (iii) the study of occurrence and distribution of emerging contaminants in aquatic environment and environmental risk assessment and (iv) sustainable wastewater management; application of innovative wastewater treatment technologies; innovative practices for reuse of reclaimed waters.

**SARA JOHANSSON**

Sara Johansson has several years of experience in the field of innovative wastewater treatment. She is recently graduated from the University of Girona where she obtained her PhD in Water Science & Technology with a thesis on the topic of nutrient removal and recovery from municipal wastewater. As part of her PhD she conducted an 18-months research stay with Aquafin in Belgium.

Her interest in wastewater treatment started at R&D company AnoxKaldnes where she was affiliated at the biopolymer research group. She also worked with AnoxKaldnes as an employee of the French branch of Veolia Water in the setting up of a pilot plant for biopolymer production from municipal wastewater in Brussels, Belgium.
She obtained her M.Sc. in Environmental Engineering from Lund University, Sweden. She spent one semester at the Technical University of Denmark in the bioenergy group at the Department of Environmental engineering and developed her master thesis on anaerobic wastewater treatment coupled with membrane filtration at the Universidad Nacional Autónoma de México.

Before starting her PhD she was affiliated at the Department of Chemical Engineering at Lund University.

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**PAU JUAN GARCIA**

Pau is a research scientist in the Strategic Advisory Services (SAS) Research team in the Water Management Consultancy group at Atkins UK. His areas of expertise include wastewater process modelling and resilience, water quality modelling, data analysis and GIS programming. He is particularly interested in operations research to support decision making in water management. His background is in environmental science with a Masters in environmental engineering. Pau doctoral studies focused on resilience assessment of sewage treatment works through process modelling. He has been in the scientific committee of various international conferences and authored several peer reviewed publications on wastewater resilience.

He has key experience in water science and technology, environmental modelling, wastewater process engineering (including modelling and optimization, data analysis and statistics, programming (Python, Bash, C#), resilience of water and wastewater treatment and geospatial analysis.
Dr. Irene Michael-Kordatou is a Chemical Engineer graduated from the School of Chemical Engineering of the National Technical University of Athens in July 2008. She has received her Ph.D. in Environmental Engineering from the University of Cyprus in May 2012. She is currently a senior researcher at the Nireas-International Water Research Center of the University of Cyprus. The overlying goal of her research is the understanding of the fate and behaviour of contaminants of emerging concern (CECs) during advanced wastewater processes, the application of analytical methods and diagnostic tools for their identification and monitoring, and the assessment of their potential environmental effects. Her research activity of the last ten years included among others, the (i) development, application and optimization of advanced wastewater treatment processes (e.g. membrane filtration and separation processes, adsorption on activated carbon, advanced chemical oxidation processes) for the removal of CECs in urban wastewater, (ii) elucidation of the major transformation products (TPs) of CECs formed during advanced treatment, (iii) assessment of the biological potency of CECs and of their TPs through the application of bioassays, and (iv) assessment of the efficiency of wastewater treatment technologies (individual and/or combined) to inactivate antibiotic-resistant bacteria and to remove antibiotic resistance genes. She has participated as a guest researcher at the Plataforma Solar de Almería funded by the European Commission (EC) (SFERA project), wherein she acquired extensive experience in the development/operation of solar-driven pilot plants for the removal of CECs and dissolved effluent organic matter present in urban wastewater effluents.

She has participated (or she is currently involved) either as Principle Investigator or as Scientific Manager, in a number of collaborative water-related research projects (more than 24) funded by the EC. She is the Scientific Manager of the ANSWER project (H2020-MSCA-ITN-2015/675530) and she participated in the NEREUS COST Action ES1403, in which she was a Management Committee Substitute and the Grand Holder Administrator. She has (co)authored more than 25 refereed journal papers in high-impact international scientific journals (h index: 20, citations:
3121; Google Scholar: October 2019) and 8 book chapters, and she presented her work in high-level scientific conferences (more than 30). She serves as Guest Editor of special volumes of scientific journals, and on various Scientific/Evaluation Committees.

### VASILIKI BERETSOU

Ms. Vasiliki Beretsou is a Chemist graduated from the School of Chemistry of the National and Kapodistrian University of Athens (Greece) in July 2013 and she received her M.Sc. in Analytical Chemistry from the same university in October 2015. She is currently a Ph.D. Candidate in Environmental Engineering at the University of Cyprus and an Early Stage Researcher (ESR) of the ANSWER project (H2020-MSCA-ITN-2015/675530) at Nireas-International Water Research Center of the University of Cyprus.

Her research focuses on the (a) occurrence and fate of contaminants of emerging concern (CECs) in engineered and natural environments, with emphasis on the identification of transformation products (TPs) of antibiotics by applying state-of-the-art analytical techniques (LC-QTOFMS), and suspect and non-target screening approaches, (b) assessment of the biological potency of CECs and of their TPs through the application of bioassays, (c) assessment of the efficiency of wastewater treatment technologies to remove antibiotic-related microcontaminants including antibiotic-resistant bacteria and antibiotic resistance genes, and (d) accumulation of CECs in soil irrigated by treated wastewater and their subsequent uptake by crops.

She has gained working experience at the academic and non-academic sector; as an intern, at the Pesticide Residues Laboratory of the General Chemical State Laboratory (Greece) in 2013, as an analytical chemist, at the Laboratory of Analytical Chemistry of the National and Kapodistrian University of Athens (Greece) in 2015 and as an ESR at the private sector and at renowned research centers in the framework of the ANSWER
project during her secondments at Biodetection Systems b.v. (The Netherlands), Environmental Institute s.r.o. (Slovakia), HighChem (Slovakia), Agricultural Research Organization, Volcani Center (Israel) and Istituto Superiore di Sanità (Italy) from 2016 to 2019.

She has participated (or she is currently involved), in several collaborative water-related research projects funded by the European Commission, the Cyprus Research Promotion Foundation and Greek national funds. She has (co)authored 3 refereed journal papers in high-impact international scientific journals (h index: 3, citations: 49; Google Scholar: October 2019), and she presented her work in high-level scientific conferences.

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GIJS DU LAING

Gijs Du Laing was appointed associate professor at the Laboratory of Analytical Chemistry and Applied Ecochemistry of Ghent University (Belgium) in 2009, where he also received his MSc degree in Bioscience Engineering in 2000 and a PhD in Applied Biological Sciences in 2007. His research focuses on the chemistry of trace elements in the environment and human health, with a particular focus on trace element speciation. Particular attention goes to the development of more effective and more sustainable technologies for the removal of toxic trace elements from wastewater and groundwater to be used as drinking water, and novel technologies for selective recovery of valuable metals from industrial wastewaters. Gijs Du Laing currently coordinates the MSCA-ITN European Joint Doctorate Programme on Sustainable Product, Energy and Resource Recovery from Wastewater (SuPER-W, www.superw.ugent.be). Moreover, he is academic coordinator of the international joint master programme on Sustainable and Innovative Natural Resource Management SINReM (www.sinrem.eu), funded by EIT Raw Materials and Erasmus+, and actively involved in the setup of a modular toolbox for web-based professional education (MOTOPED) in EIT Raw Materials. Furthermore, he coordinates the setup of an open online course (MOOC) on resource recovery from wastewater, to be launched on EduNext in early 2020.
LARISSA TERUMI ARASHIRO

Larissa is an Environmental Engineer graduated from São Paulo State University. During her bachelor studies, she carried out a research on water quality by applying mathematical tools to develop an enhanced water quality index for public supply purposes. Just after obtaining her Bachelor degree, Larissa worked in industry for three years, where she acquired relevant experience in organizational Quality, Environmental, Health and Safety (QEHS) management systems, suppliers qualification process and management, as well as product certifications according to international standards. Afterwards, she was granted the Erasmus Mundus scholarship for the International Master of Science in Environmental Technology and Engineering, which was a great experience to expand her knowledge on several fields within the broad scope of environmental science. Her master thesis, which was carried out in UNESCO-IHE (Delft, Netherlands) and University of South Florida (Tampa, FL, USA), involved experimental and modeling studies on wastewater treatment, with focus on water and energy recovery.

Following that, Larissa did an internship at the International Water Association (IWA), where she worked on projects to improve global water and sanitation safety in collaboration with the World Health Organization (WHO).

Larissa is currently a MSCA-ITN fellow of the joint PhD programme SuPER-W, investigating potential wastewater treatment and resources recovery technologies using microalgae.

She is very interested in expanding her knowledge and contributing to the water sector, as well as interacting with inspiring people who also want to create positive impacts in the world.
PHILIPP KEHREIN

After a B.Sc. in Environmental Management at the Justus Liebig University Giessen focussing on waste treatment facilities, landfill management, waste water treatment, circular economy, waste management legislation and renewable energy, Philipp has been awarded a European Double Degree M.Sc. in Environmental Science – Soil, Water, Biodiversity by the University of Copenhagen & the University of Hohenheim. His thesis’ title was “Global Warming Potential of Sewage Sludge Thermal Conversion Technologies – A comparative life cycle assessment”.

Subjects studied include nutrient recycling, sewage sludge energy recovery, life cycle assessment, soil science, ISO 14001, and optimal resource utilisation.

Philipp attended an education as Waste Management Officer and is currently certified according to the German circular economy law.

In 2014-2015, he has worked as Research Assistant at the Department of Plant and Environmental Sciences of the University of Copenhagen (Faculty of Science).

He currently is a MSCA-ITN fellow of the joint PhD programme SuPER-W.

PAOLA CALZA

Paola Calza received her Master Degree in Chemistry on July 1994 at the University of Torino and her Ph.D in Chemistry in 1998 at the same University. She started her career as an Assistant Professor in January 1999 in the Department of Analytical Chemistry of the University of Torino and is Associate
Professor since October 2010 in the same Department.

Since 2015 she is President of the Master’s Degree in Environmental Chemistry. She supervised several fellowship and PhD students and over 70 final dissertations for Chemistry degree, is member of the board of the PhD program on “Innovation in the Circular Economy” at the University of Torino and member of the Scientific Committee of the International PhD School in Advanced Oxidation Processes.

Her research interests are on the study of photocatalytic processes and photoinduced transformations occurring in aquatic systems and on the development of processes for soil remediation. Particular attention has been devoted to the identification and characterization of transformation products formed during pollutant degradation, and the effect of inorganic ions on xenobiotic transformations.

Co-editor of the book “Surface water photochemistry”, co-author of over 120 papers on high impact factor journals and of seven book chapters, she attended over 120 conferences, also with keynote talks.

She was visiting professor at the McGill University (Montreal, Canada) in 2013, 2014 and 2017, at La Plata University (Argentina) in 2015 and at the Stellenbosch University (South Africa) in 2018.

Recently, she coordinated or was involved in several projects focus on the development of processes/materials for water treatment (i.e. FP7-PEOPLE-2012-IRSES PHOTOMAT, MOTREM-WATERJPI2013 –Water Challenges for a Changing World Joint Programming Initiative project, H2020-MSCA-RISE-645551 Mat4Treat and H2020-MSCA-ITN-765860 AQUAlity) or for soil remediation (i.e. ReHorti-Torino University and Compagnia di San Paolo 2017-2020 and SCC-02-2016-2017 776528 ProGiReg).
DIMITRA PAPAGIANNAKI

Dimitra Papagiannaki studied Chemistry at the University of Ioannina in Greece. Soon after, she started her master studies in Analytical and Environmental Chemistry at the same department, working on the determination of organic compounds in several environmental matrices using different extraction methods and hyphenated chromatographic techniques. She received her Master Degree on 2017 after working for her thesis on untargeted analysis of biological matrices using High Performance Liquid Chromatography tandem with Mass Spectrometry and chemometric analysis tools.

Afterwards, she has been selected from the AQUAlity ITN project as an ESR for an industrial PhD position with the main activities carried out at SMAT Research Centre Laboratories (Turin, Italy). Moreover, she is enrolled in a PhD program for Innovation for Circular Economy, since water management is one of the key issues within the implementation of European Circular Economy Policy. Within AQUAlity her research interests focus on the development and validation of new analytical methods for evaluating the presence of Contaminants of Emerging Concern (CECs) at trace level concentrations in a variety of water matrices using advanced analytical techniques (UHPLC-MS/MS and LC-HRMS/MS) and statistical tools. Furthermore, evaluation of contaminants’ removal with traditional and new photochemical treatments identifying possible transformation products, including toxicological screening are enclosed. As planned from the AQUAlity agreement she has already carried out her research activities for a short time period (secondment) in different working sectors – specifically in Aalborg University – boosting her scientific skills and bridging the gap between different working environments. Since now, her work has already been published through poster and oral presentations in conferences and a summer school and with a publication titled ‘Perfluoroalkyl Substance Assessment in Turin Metropolitan Area and Correlation with Potential Sources of Pollution according to the Water Safety Plan Risk Management Approach’.
IVÁN MATÍAS SCISCENKO

Iván M. Sciscenko is a PhD student at Universitat Politècnica de València (Alcoy campus). His main interest within AQUAlity project is the design and optimization of novel Fenton-based photochemical methods for the degradation of contaminants of emerging concern from water, their integration with other processes and assessment of their real applicability for wastewater treatment.

Regarding professional education, he has studied Chemistry at Faculty of Exact and Natural Sciences of UBA (Universidad de Buenos Aires), Argentina. While doing his university career, he gained experience in scientific field as a volunteer researcher at the Materials Physical-Chemistry, Environment and Energy Institute (INQUIMAE) with projects related to electrochemistry, and afterwards as a research scholar at the Argentinian Atomic Energy Commission (CNEA) within projects related to the removal of metals of environmental relevance from water, such as uranium, arsenic or chromium, employing zerovalent iron nanoparticles.

JÖRG LEWANDOSKI

PD Dr. rer. nat. Dipl.-Ing. Jörg Lewandowski (ORCID: 0000-0001-5278-129X, ResearcherID: E-9028-2012), Senior scientist and group leader “Groundwater-surface water interfaces”, Leibniz-Institute of Freshwater Ecology and Inland Fisheries (IGB), Department Ecohydrology, Berlin, Germany

Jörg studied Environmental Engineering at TU Berlin and Environmental Sciences at ETH Zürich. He defended his thesis on contaminants in soil at TU Berlin.
Before joining the University of Hohenheim as Senior scientist, he did his PhD and 3-year PostDoc at the Biogeochemistry group at the IGB.

Since 2006, Jörg is Senior scientist at IGB, Department 1 and, in 2015, he has completed his habilitation at HU Berlin.

Research Topics

- Hydrodynamic transport and biogeochemical turnover processes in floodplain aquifers and hyporheic zones (groundwater-stream interface)
- Hydrodynamic transport and biogeochemical turnover processes at aquifer-lake interfaces (lacustrine groundwater discharge)
- Impacts of macrozoobenthos activities on hydrodynamic transport and biogeochemical turnover processes in lake sediments and on adjacent compartments
- Phosphorus retention in limnetic sediments, early diagenetic processes and phosphorus turnover in lake ecosystems
- Lake restoration

ANNA JÄGER

Anna Jaeger is an Environmental Scientist with main interests in biogeochemistry, environmental chemistry, pollutant fate and water and soil protection. Since 2015 she is a PhD candidate in the EU Marie Skłodowska-Curie ITN project “HypoTrain” at the Leibniz Institute for Freshwater Ecology and Inland Fisheries, Berlin, Germany. The project’s research focuses on hyporheic zone processes promoting a particular international and interdisciplinary approach to the topic. In the course of the project work, Anna Jaeger went for research stays at Stockholm University, Stockholm, Sweden and Birmingham University, Birmingham, UK. Her PhD Thesis
deals with “Environmental controls on fate of organic micropollutants in urban rivers and their hyporheic zones”. Her most recent publications concern in particular the reach-scale degradation of organic micropollutants and associated formation of transformation products in the surface water of an urban lowland stream, as well as the influence of sediment bacterial diversity and hyporheic exchange on this kind of degradation processes.

In 2014 she received her Master of Science double-degree in European Environmental sciences from the University of Copenhagen, Copenhagen, Denmark and the University of Natural Resources and Life Sciences, Vienna, Austria. The base of her academic education is a Bachelor of Science degree in Molecular Life Sciences earned in 2010 at the Friedrich-Alexander University Erlangen-Nuremberg, Erlangen, Germany.

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**DAMIEN JUGNOT**

Born and raised in Dijon, France, Damien Jougnot received a Bachelor in Environmental Geo-engineering from the University of Bordeaux in 2004 and a Master of Hydrogeology from the University of Avignon in 2006. Over the course of his PhD thesis at University of Savoie, Damien developed several petrophysical models to determine the transfer properties of a potential host rock for nuclear waste storage from geophysical measurements. This work was funded by the French Nuclear Waste Agency and supervised by André Revil. During this period, he spent 15 months as a visiting scholar at the Colorado School of Mines and obtained a PhD degree in Geosciences in 2009. From 2009 to 2014, Damien was a Junior Lecturer working in the group of Niklas Linde at University of Lausanne, Switzerland.

Since 2015, Damien is Associate Scientist at CNRS, in UMR 7619 METIS, Sorbonne University (previously University Pierre and Marie Curie), Paris, France. His current research activities mainly focus on how geo-electrical
measurements can be used to better understand, quantify, and predict processes in the critical zone from the laboratory to the field scale. He is a specialist of self-potential, induced polarization and seismoelectrics. More recently, he has broaden his expertise to other geophysical methods and aims at better taking into account the effect of mesoscale heterogeneities (fracturation and partial saturation) and biogeochemical processes on the signal generation. His objective is to develop hydrogeophysical tools and use them as proxy to describe the various processes happening in the critical zone.

Author of 34+ scientific paper and 2 book chapters, Damien is the leader of the transdisciplinary team GeoProcess (6 permanent researchers) since 2018 and actively co-supervise 6 PhD students. He is also Associate Editor of Geophysical Prospecting (EAGE) since 2015 and deputy coordinator of the ENIGMA ITN since 2017.

https://sites.google.com/site/damienjougnot.

ANNE-KARIN COOKE

Anne-Karin Cooke is an environmental scientist, specialized in hydrological sciences, currently exploring the potential of new hydrogeophysical monitoring methods for groundwater storage changes.

She obtained her Bsc in Geo-Ecology from Potsdam University, Germany, and her MSc in Earth and Environment from Wageningen in the University, the Netherlands, specialization Hydrology. Her Master thesis was a collaboration with the University of Sydney, Australia, on ecohydrological modelling of saline groundwater rise. During her studies she was volunteering in students chapters and environmental groups as well as politics on university and county level concerning sustainability.
Her PhD topic within the ITN Enigma is entitled “Monitoring water storage changes with a new portable absolute quantum gravimeter”. Anne-Karin is currently based at Geosciences Montpellier (University of Montpellier 2), France. Extended parts of her PhD she worked at the facilities of MuQuans, a quantum technology company specialised in the field of quantum inertial sensing, high performance time & frequency applications, and advanced laser solutions. She hence gained insight into the process of instrument development and working in an industrial company, complementing her experience in working in an academic setting in Montpellier.

Her interest in hydrogravimetry stems from its unique feature of being a non-invasive monitoring method that provides depth-integrated constraints on water mass changes. Her vision is to improve the method in order to provide valuable contributions to hydrological monitoring and modelling. She aims at gaining deeper insight into the dynamics of subsurface water resources in heterogeneous environments.

She wants to look at the bigger picture: With the livelihood of millions worldwide increasingly dependent on groundwater extraction, innovative solutions to achieve the UN Water Sustainable Development Goals need to be implemented. Accurate water balance estimates of aquifers and catchments play a crucial role for integrated sustainable water management. Gravimetry – in combination with other geophysical and classical hydraulic and meteorological methods as well as state-of-the-art modelling and inversion techniques – has shown to be effective in scientific settings. Its potential contribution to societal challenges and resource management is promising and many aspects remain to be explored.

GUILHERME NOGUEIRA

Guilherme Nogueira is a geologist, with specialization in hydrogeology and water sciences. He currently studies the link between flow dynamics and reactivity potential of riparian aquifers using high-resolution imaging-sensor
methods and state-of-the-art modelling techniques.

He received his BSc in Geology from Sao Paulo State University (UNESP Rio Claro), Brazil, and his MSc in Water Science and Engineering from IHE-Delft, the Netherlands, with specialization in “Groundwater: global change and adaptation”. The MSc was achieved in collaboration with IST-Lisbon, Portugal, and TU-Dresden, Germany, under the Erasmus Mundus + Joint Programme “Groundwater and Global Change – Impacts and Adaptations” (acronym GroundwatCH). In his MSc thesis, he worked locally with UEM-Maputo staff, Mozambique, on understanding and revealing salinization mechanisms behind high salinities on both surface and groundwater in a coastal aquifer-system using hydrogeochemical and water isotope data.

His PhD topic within the ENIGMA-ITN is entitled “Imaging flow dynamics and resulting reactivity in the transition zone between streams and riparian aquifers”. Guilherme is based at UFZ-Leipzig (Helmholtz Centre for Environmental Research), Germany. In his first secondment, he worked partially in the University of Neuchâtel (UNINE), Switzerland, where he attended courses and gained experience in numerical modelling and calibration/optimization procedures. During his final secondment, he was in Copenhagen University (KU), Denmark, where he attended courses in ‘geostatistics for stochastic modelling of heterogeneous environments’, as well as in ‘groundwater-surface water exchange processes and monitoring techniques’. In his secondments he could expand and sharpen his skills in specific field-monitoring and modelling techniques needed for his research as well as discuss his work with more experienced researchers in his field of study.

Safeguarding water quantity and quality for humankind is one of most important UN Sustainable Development Goals. The combination of high-resolution sensors with state-of-art modelling will allow the assessment and quantification of important local processes patterns that affect water quality and the watershed as a whole. Recognizing and understanding the important functional role of riparian zones in sustaining water quality will support a sound management of our water resources, which is crucial in the light of a global change.
Dr Lisa Connolly is a Reader in Toxin Food Safety within the Institute for Global Food Security at Queen’s University Belfast, Northern Ireland. She is currently leading a vital research programme focusing on endocrine disrupting environmental and food based toxins resulting from modern day industrial, agricultural or natural sources and assessing the effects that these contaminants may have on health. Dr Connolly and her team primarily develop and utilise in vitro bioassays for the screening of endocrine disruptors and assessing their adverse biological effects. This work also covers horizon scanning for emerging endocrine disruptors, assessing their mode of action and mixture effects.

See publications at:  
https://www.researchgate.net/profile/Lisa_Connolly/research

Dr Connolly is coordinator of a 4.1 million euro international project on endocrine disruptors, PROTECTED (PROTECTion against Endocrine Disruptors; detection, mixtures, health effects, risk assessment and communication (PROTECTED)) which is funded through the Marie Skłodowska-Curie Actions (MSCA), specifically within the “Innovative Training Networks” (ITN) program, an initiative of the European Commission (EC) to promote academic-industrial collaboration and the training and mobility of PhD students. PROTECTED aims to develop specialized knowledge and protection capabilities against endocrine disruptors, which are chemical pollutants capable of altering our hormonal balance.

Endocrine disruptors and their mixtures are currently a health problem of the first order, contributing to adverse effects such as obesity, cancer and infertility. They can also have a great impact on ecological systems, and for example be responsible for poor agricultural production. Endocrine disruptors can be found in pesticides, plastics, cosmetics, paints, etc., and given their widespread presence there is a high risk of transfer to the food chain.

Her coordination of this project involves 9 countries (UK, Scotland, France, Spain, The Netherlands, Belgium, Chile, India, Canada) and 4 SMEs. This global network facilitates the innovative research and training of 17 early stage researchers in this worldwide issue.
She is also a key partner of the 6.1 million euro H2020 FREIA project – an international collaboration exploring the impact of endocrine disrupting chemicals on women’s fertility. This project provides dedicated, human-relevant, test methods to identify EDCs that cause female reproductive toxicity.

VITTORIA MALLIA

Vittoria Mallia is an Italian PhD student, based at the Norwegian Veterinary Institute of Oslo and University of Oslo (Norway). Her project, entitled “Endocrine Disrupting compounds in Cyanobacteria”, is part of the ProtectED (Protection against Endocrine Disruptors) ITN (Marie Skłodowska-Curie Innovative Training Network), where Vittoria is involved as Early Stage Researcher.

She has previously obtained two bachelor degrees (“Technology for conservation and restoration of cultural heritage” and “Chemistry”) and one master degree in “Organic Chemistry” (drug-discovery field), all from the University of Perugia (Italy). After graduation, she spent five months in France for a European traineeship (Eurodyssey) at the University of Reims (Champagne-Ardenne, France), working in the environmental chemistry field. She also passed the Qualifying State Examination to Chemists Register in Perugia (Italy).

Alongside her education, Vittoria has experienced different jobs while she was a student/intern, including private teacher of Math, Physics and Chemistry, photographer and journalist for a website and for some football teams, animator for children.

She speaks Italian (mother tongue), English and French.
ELIZABETH GOYA JORGE

Elizabeth Goya-Jorge is a Ph.D. Student in Chemistry since 2017 at the Universitat de València. As an Early Stage Researcher of the Marie-Curie Innovative Training Network from the European Commission named **PROTECTED Protection against endocrine disruptors**, she is developing her research work in a computational chemistry and bioinformatics company called ProtoQSAR.

As previous experiences, she graduated with honors as a pharmacist in her home country Cuba, where she also obtained a master’s degree in Pharmaceutical Sciences in 2016. Her postgraduate research projects focused on *in vitro* and *in silico* modeling of antioxidant activity of individual compounds and natural mixtures extracted from plants. Moreover, she was training as a graduated university teaching assistant in the field of pharmacology and pharmacotherapy prior to access to Ph.D. level studies two years ago.

Elizabeth has received training to work with animal models, although her research is based on alternative methods *in vitro* using cell culture methods combined with *in silico* modeling approaches. The main interest of her research is the identification of chemical compounds modulating the endocrine system by different mechanisms to assess their toxicological and/or pharmacological importance. Theoretical elucidations of modes of action of endocrine-disrupting compounds using computational methods are the main goals hoping to accomplish as part of PROTECTED project.

She speaks Spanish as her mother tongue, and she is able to use English for scientific purposes.
Rosalie van Zelm is assistant professor at the Environmental Science department at Radboud University. In 2005 she graduated from the University of Twente as an environmental engineer. Rosalie wrote a PhD thesis on the development of renewed life cycle impact assessment methods and impact indicators on an endpoint level. The focus was on ozone and particulate matter formation causing human health damage, and terrestrial acidification, groundwater extraction, and freshwater ecotoxicity causing ecosystem damage. After completing her PhD she continued with a PostDoc related to land use impacts, and since 2011 as an assistant professor. Her current research focuses on the advancement of methods to quantify ecosystem and human health impacts from anthropogenic inputs to and outputs from the environment, related to the life cycle of products and technologies. Uncertainty and variability in these methods are an important pillar, as well as a circular economy context and application in sustainability assessments. Also, technology assessment and developing methods to aid in the quantification of environmental impacts of technologies, such as wastewater treatment technologies and carbon capture, utilization, and storage, are of interest to her. She has been supervising over 10 PhD and 25 MSc students and (co-)wrote over 50 peer-reviewed articles. Her work falls within several EU- and Dutch funded projects and she has been involved in various initiatives to harmonize and improve life cycle impact assessment methods. She was involved in the development of the life cycle impact assessment methodologies ReCiPe2016 and LC-IMPACT. Within the Marie Curie ITN RELIEF she supervised two PhD students on method development related to chemical and land footprints. Also, she was the training coordinator.
I was born on the 6th of August 1992 in Clermont-Ferrand, France. My parents and I then moved to Niger for four years before settling in Switzerland until I was 11. We then spent a few years in Rwanda and came back to Switzerland in 2007. I finished high school in Bern in May 2010 and started my studies in Environmental Engineering at the ETH in Zürich in September. After finishing my Bachelor thesis on “Climate Change and Flood Hazards in Switzerland” in 2013, I started with the consecutive Environmental Engineering Master at the ETH. My major subjects were water resources management and ecological systems design and waste management. During my Master, I spent five months at the National Institute of Water and Atmospheric Research (NIWA) in Christchurch, New Zealand, working on comparing the precipitation predictions made by various climatic models. In August 2015, I handed in my Master thesis, a life cycle assessment of wave and tidal energy plants, which I wrote at the Department of Energy and Process Engineering at the Norwegian University of Science and Technology (NTNU) in Trondheim, Norway. In October 2015, I then joined the RELIEF project, a collaboration between the Radboud University and Unilever, as an Early Stage Researcher of the Marie Sklodowska-Curie Innovative Training Network program. My aim was to identify the sources of uncertainty and variability in the ecotoxicological impact assessment of chemicals and propose strategies to increase its reliability. Besides the time spent at the Radboud University, I also spent 21 months of my PhD at the Safety and Environmental Assurance Centre (SEAC) of Unilever in Colworth, United Kingdom. There, I received the SEAC PhD award for Science and Communication in 2018 for my work on the modelling of removal efficiencies of pharmaceuticals, fragrances, and surfactants. I also had the chance to spend 2.5 months as a visiting PhD candidate in Østfoldforskning, Fredrikstad, Norway, where I worked on the chemical migration from packaging into food. I will defend my thesis titled “Reliability in chemical footprint modelling of consumer products” on the 4th of December 2019 in Nijmegen, the Netherlands. In January 2020, I plan to start a tenure track position as assistant professor in the environmental impact of energy pathways at the Centre for Observation Impact Energy of MINES ParisTech in France.
Hans Christian Bruun Hansen, Professor, Department of Plant and Environmental Sciences, Faculty of Science, University of Copenhagen.

Hans Chr. B. Hansen (HCBH) is head of the research group in Environmental Chemistry at University of Copenhagen. He is coordinating the ITN project "NaToxAq" comprising 16 ESRs focusing on contamination of drinking water with natural toxins produced by plants and by cyanobacteria. HCBH started research on natural toxins in plants in 2003 initially looking at toxin extraction, analysis and occurrence in soils and since then extended to environmental fate of natural toxins in soil and water. More than 50 papers have been published on the topic covering a range of toxins in crop and non-crop plants such as illudane glycosides in bracken, glucosinolates in Brassicaceae, cyanogenic glycosides clover and other plants, glycoalkaloids in potato, and terpenoids and troplones in thuja trees. Research has demonstrated that many natural toxins are highly mobile in the environment, that toxicities are similar or higher than for many xenobiotics, and that environmental fate of these compounds including degradation pathways are very poorly known and needs much more attention. Production and release patterns are specific to the toxins and climate driven.

HCBH has been professor at University of Copenhagen since 2000 and in addition to the field of natural toxins his research focus on solid-solution processes in soils and sediments with focus on iron geochemistry, redox interactions, hydrolysis and sorption processes. Current research projects comprise, in addition to the NaToxAq ITN project, reductive dehalogenation of chlorinated solvents using a novel iron-organic material, and phosphate retention and recycling in agriculture. He is head of studies for MSc in Environmental Science and teaches MSc and PhD courses in soil and water pollution. He has been the supervisor of 95 MSc students and 40 PhD students. He has 206 papers in international peer reviewed journals.
CARINA SCHÖNSEE

Carina’s research within NaToxAg focuses on the intrinsic physicochemical properties affecting environmental mobility of natural toxins. Experimentally determined property data will support reliable exposure/risk assessment of natural toxins with regards to protecting the quality of our drinking water resources.

Carina works in the research group Environmental Analytics at Agroscope (https://www.agroscope.admin.ch/agroscope/en/home.html) and is enrolled as a doctoral student at ETH Zürich in Switzerland since 2017. She holds a BSc and MSc degree in Water Science from the University of Duisburg-Essen (UDE, Germany, https://www.uni-due.de/water-science/index_en.php). Since starting her studies in 2011, Carina gained diverse international experience in environmental science and analytics as a research assistant for INEOS Köln and UDE (both Germany) as well as during research stays at AgResearch (New Zealand), the University of Vienna (Austria), the University of Copenhagen (Denmark) and the University of Stockholm (Sweden).

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REGIANE SANCHES NATUMI

Regiane attained her BSc degree in Environmental Chemistry at the University of São Paulo. During her studies she did several years of practical work both at her University as a student research assistant and at the Industry as an intern. Her work experience ranges from life cycle assessment of solid waste incineration plants to analysis and purification of bioactive natural products. After her bachelor, Regiane moved to
Germany to pursue a Master degree in Environmental Sciences at the University of Trier. She did her Master’s Thesis at the Fraunhofer Institute IGB-Biocat, focusing on the enzymatic synthesis of novel biosurfactant using renewable resources as raw material. Since April 2017, Regiane is working at the Swiss Federal Institute of Aquatic Science and Technology (EAWAG) as a PhD student under the supervision of Dr. Elisabeth Janssen and she is attending the PhD program in Biogeochemistry and Pollutant Dynamics at the ETH Zürich under the co-supervision of Prof Dr. Kristopher McNeil. Her current work is focused on the co-production and environmental fate of novel cyanopeptides in surface waters to help improve risk assessment of cyanobacterial bloom events. The aim of the project is to investigate the stability and possible transformation processes of emerging cyanopeptides by determination of photochemical transformation mechanisms and biodegradation processes.

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**HARIS KADRISPAHIC**

I am Danish and I hold a MSc in Management of Innovation and Business Development, CBS.

I have 10 years’ experience from Ministry of Food, Agriculture and Fisheries of Denmark (among others), where I have been directly involved in a number of EU funded projects. I currently serve as an internal project manager of two European projects: ROMEO (Horizon2020) and NexTower (Horizon 2020) as well as being member of steering committee of the project FYMAFY (Udvikling af filtreringsteknologi til mikroalger og bæredygtigt højkvalitetsfoder til fiskehynge). R&D Lead at LiqTec International since 2018. Initiator of several funded development projects: Cryptosporidium retention Membrane (MUDP), RETROMAX (GUDP), DRIP (Innovationsfonden), Sulfate removal membrane for water reinjection systems (EUROSTARS), Fimafy (GUDP).

I have experience in application and management of funded project from funds such as Innovationsfonden (Danish Advanced Technology Foundation), Fornyelsesfonden, GUDP/EUDP/MUDP, Eurostars and 7th framework program and Horizon 2020.
I have hands on experiences in product development with industrial partners and SMEs, public private co-creation and innovation. Broad experience in filtration technology and the ability to define business strategy based on novel technology.

My key qualifications are in water treatment technologies, project management, management of innovation and business development, national & international funding, SiC material processing.

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**STEPHEN J. BARIGYE**

Stephen J. Barigye, is a Senior Research Scientist at ProtoQSAR SL, Valencia, Spain. He received his PhD in Chemistry from the Central University of Las Villas (Santa Clara, Cuba) in 2013 and posteriorly carried out postdoctoral research at Federal University of Lavras, Brazil (2014 - 2016) and McGill University, Canada (2016-2018).

Dr. Barigye is an author of over 50 peer-reviewed research papers and 2 book chapters. His research interests include: Structure and Ligand-based Drug Design, QSAR/QSPR/QSTR Studies, ADME/Tox Predictions, Docking and Molecular Dynamics Simulations, Statistical Data Analysis, Feature Selection Methods and Machine Learning Algorithms, Quantum and Computational Chemistry, Chemoinformatics, Mathematical and Theoretical Chemistry.
STEFAN PEIFFER

Stefan Peiffer is Chair of Hydrology at the University of Bayreuth.

He is member of the Research Commission/Forschungskommission of the University of Bayreuth, of the Board of the Division of Hydrogeology of the German Society for Geosciences and of the Board of the German Water Science Alliance. Since 2016 Stefan is External Expert in DFG Review Board (“Fachkolleg”) 318, Water Research and Associate Editor “Chemical Geology”.

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SAOIRSE DERVIN

Saoirse Dervin is an Aquasense Marie Curie Early Stage Researcher in the Bendable Electronics and Sensing Technologies (BEST) group at the University of Glasgow. She graduated with a BSc. (Hons) in Forensic Investigation and Analysis from the Institute of Technology Sligo, Ireland in 2014. While studying for her undergraduate degree, Saoirse
undertook a number of research projects in functional materials and chemical analysis. Saoirse is currently working towards the submission of her PhD thesis entitled, “In Vitro activity of graphene and low-dimensional nanomaterials.” Throughout the course of her PhD studies Saoirse acquired extensive experience in the areas of nano-fabrication and nano-characterization and has successfully authored/co-authored 9 publications, including research papers, a review paper and book chapters and contributed in 4 international/national conferences. Her research interests include the synthesis and characterization of 0, 1 and 2D nanomaterials, biomaterials and their interactions with living organisms, their safety profiles and their potential to contribute towards safeguarding environmental sustainability. She is also interested in the application of these materials as nanotherapeutics, drug delivery systems, biosensors, smart wearable technologies and technologies for environmental monitoring and remediation.
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