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BUILDING A BETTER FUTURE: RESPONSABLE INNOVATION AND ENVIRONMENTAL PROTECTION

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zone, the impact on the quality of settling particles is noticeable for locations relatively far from the Tillet mouth, PCBs sorbed to the particles are bioavailable for aquatic invertebrates and fishes in river Tillet as well as in the lake, some ecotoxicological effects are noticeable during *in vitro* exposure of organisms, the macroinvertebrate communities of river Tillet are highly impaired by chemical and physical (substrate clogging) damages, PCBs and PAHs quantities lead to different bacterial community structures and abundances in the sediments and the epilithic biofilms. The study will continue after restoration of the river, including the assessment of the effects of an *in situ* treatment of sediments using granular activated carbon applied on a particular section of river Tillet in spring 2013. These effects will concern the fluxes of PCBs and PAHs towards the lake, the bioavailability of PCBs, the microbial communities and the recovery of biodiversity following restoration of river Tillet.

WE289
Replicability of marine outdoor mesocosm to assess toxicity at ecosystem level
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Mesocosms have been used in aquatic ecotoxicology over 30 years and were sometimes claimed to be essential tools, especially for regulatory purposes. The use of mesocosms refines the classical methods of ecotoxicological risk assessment because mesocosms provide conditions for a better understanding of environmentally relevant effects of chemicals. Ecological realism, representativity, and replicability of mesocosms are critical for evaluating their usefulness. Considering the objectives of most studies carried out in mesocosms, replicability is the most important point. Each natural ecosystem is unique because its structure and function mainly depend on local factors. Therefore, there is a conceptual opposition between realism and replicability when applied to mesocosms. Considering the objectives of most mesocosm studies, replicability should be preferred to realism. Replicability of outdoor marine closed mesocosm (MCM) was assessed to validate an ecotoxicological research at ecosystem level for one year. Chemical and biological variability was investigated between mesocosm sizes and light availability. Microcosm was designed by four size groups (200, 400, 600, 1000L) using cylindrical plastic water tanks (opaque or semitransparent) with five replicates. Each tank was filled with 5cm gravel layer on the bottom and another 5cm natural sediment layer with overlying natural seawater collected in Ganghwa tidal flat in west coast of Korea. Seawater in mesocosm was circulated vertically through outside vertical pipe by air injection from bottom to top. Water quality was measured daily (salinity, water temperature, pH and dissolved oxygen) and sediment quality by weekly. Phytoplankton, zooplankton and meiobenthic community were also analyzed by 10 day interval to identify the difference in community structure and variation within replicates. The results were analyzed by 2-way ANOVA. Important issues related to using mesocosms include: (1) the need to establish/maintain realistic communities; (2) need to establish replicate ecosystem; (3) variability that increases directly with realism; (4) problems associated with down scaling of physical systems; and (5) the cost of construction and operation. All of the above issues were discussed and evaluated through this preliminary microcosm experiment. This work was supported by Ministry of Land, Transport and Maritimes Affairs of Korea (MLTM).

WE290
INCLUSION OF TROPHIC NETWORK VARIABILITY IN REGULATORY ENVIRONMENTAL RISK ASSESSMENT
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Ecosystems can be defined as complex networks implying trophic relationships between species but also as functions to maintain ecosystem equilibrium. The basic paradigm in REACH or Biocides regulations or in the Water framework Directive assumed that the protection of the most sensitive species protect the structure and thus the function of the ecosystem. As the concept of the most sensitive does not take into account bioaccumulation mechanisms, this has to be completed (for bioaccumulative substances only) by the study of the predator compartment, which is assumed to reach the maximum concentration. Classical method described in the ECHA guidelines targets an undefined bird or mammal as predator feeding from their usual prey: fishes and/or worms. This unspecific scenario can be perceived as very simple and the exposure of the top predator in complex ecosystem may insufficiently be captured in case of biomagnification of chemical substances. In the plant protection product area, the assessment is slightly different when considering the initial hypotheses since the risk is basically evaluated independently for each trophic levels, and the assessment of secondary poisoning is linked to the crop under consideration: including type and age of crops to identify specific targets: bird, small mammalian, of various trophic regimen. Yet, industrial chemical following sludge applications (from Sewage Treatment Plant) ends up the very same agricultural field receiving plant protection products. The present work includes a case study comparing the two assessment frameworks for a selection of substances with different bioaccumulation potential. Nevertheless, the approaches used in these regulations remain overall linked to a generic environment. They do not consider the surrounding habitats and the impact of anthropic activities on landscape modeling. In other contexts, such exposure tools that could be adapted to specific or local trophic networks are developed, including a selection of target species, its habitats and diet. These models such as Terrasys™ or BERISP™ have the option to supply information on the top predators or modify the presence of specific habitat and thus the trophic network. We propose to confront the classical non specific exposure assessment with a much more elaborated scenario, including human intervention and management measures on ecosystem exposition in a fictional case study involving terrestrial compartment.

WE291
A Spatial Eco-epidemiological Approach for Identifying and Ranking Potential Stressors in Aquatic Ecosystems of England and Wales
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Spatial analysis of existing monitoring data and other environmental data resources provides a cost-effective means of enhancing more traditional approaches to ecological risk assessment. In this study, a probabilistic spatial data modeling approach employing weights-of-evidence and logistic regression was used to attempt to explain riverine macrofaunal community condition in terms of a range of potential stressors such as water chemistry, metal and pesticide toxicity, waste water effluent, flow regime and land use variables (as surrogates of diffuse pollution). Various monitoring and modeled data resources were used in a study area comprising 307 catchments in England and Wales. The analysis generated quantitative screening-level hypotheses related to ecological risk, based on relating spatial patterns of environmental data to delineate significant spatial associations between biological response (macrofaunal community condition) and environmental variables. Associations between biological response and environmental variables were compared between environmental stressors associated with land use, measured water chemistry and modeled wastewater effluent contributions, as well as modeled seasonal pesticide exposure and associated mixture toxicity. Analysis performed using seasonal data (spring and autumn) allowed for the delineation of other seasonal differences in stressor-response relationships, such as increased influence of biological oxygen demand and nitrate in the autumn season. This study demonstrated the potential of this type of spatial eco-epidemiological analysis for screening-level assessments, which can be used for river basin management or to help identify further diagnostic assessment needs. It has also shown that improvements in model explanatory power can be achieved as new data sources and methods become available.

Alternative Methods for Evaluating Toxicity: Methods, Endpoints, and New Testing Strategies (P)

TH001
Effects of a mixture of herbicides on non-target organism
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Herbicides are widely used in agriculture and are known as a diffuse source of water pollution. The impact of herbicides use on non-target organisms is not well known although negative effects have already been observed. Sugarcane is the predominant culture of São Paulo State, Brazil, with arround 6 million hectares of land cultivated. Acute and chronic toxicity tests with juvenile tilapia (*Oreochromis niloticus*) were undertaken to determine if the combination of herbicides commonly applied on sugarcane crops (ametryn, tebuthiuron and a commercial mixture of diuron and hexazinone) affect hematological and enzymatic parameters. The $LC_{50\text{-}96h}$ determined to fish exposed to herbicides was: ametryn 4.41 (3.63 - 5.26) mg L^{-1}; mixture of diuron+hexazinone 18.62 (14.79 – 24.45) mg L^{-1} and tebuthiuron 223.04 (199 - 250) mg L^{-1}. When fish were exposed to the mixture of these herbicides the $LC_{50\text{-}96h}$ was 11.09 (9.25 – 15.85) mg L^{-1}, showing antagonism between components of the mixture (Additive Index = -0,129). During the prolonged toxicity (14 days) test, fish were exposed to the following concentrations of herbicides mixture: 0 (control), 0.119 e 1.190 mg L^{-1} a.i.; corresponding to 1/100 e 1/10 of $LC_{50\text{-}96h}$. Fish (Ls = 9.90 ± 0.125 cm; Wt = 32.35 ± 1,33 g) (n=36) were fed *ad libitum* and maintained in tanks of 115L with aeration, in a density around 3.8 g L^{-1}, in room with temperature (26.0 ± 2 ºC) and photoperiod (16:8h, light: dark) control. At seven and 14 days of expositon, fish were sacrificed (benzocaine solution 8%) and blood and liver were collected. Blood was drawn by caudal puncture, with the help of a needle and syringe previously heparinized. The blood specimens were assayed for: number of erythrocytes (RBC); hematocrit (Ht) and hemoglobin level (Hb). After these procedures, the following RBC indices were calculated: MCV (mean corpuscular volume) and MCHC (mean corpuscular hemoglobin concentration). Assays were performed to analyze enzymatic activities (GST, CAT, GPx and SOD) in fish liver. These samples were stored at - 80 ºC until enzymatic analysis. With regard to hematological analyses, it did not show any significant differences between control and other treatments ($P > 0.05$). This study presented complementary tools available for pesticide risk assessment in tropical ecosystems, helping to establish maximum environmental concentrations of herbicides mixtures in aquatic ecosystems.

TH002
Innovation of 3Rs in ecotoxicology
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For over 10 years Brixham Environmental Laboratory has had a strong input into the development and validation of alternative assessment methodologies and the 3Rs (reduction, replacement and refinement), in ecotoxicology. In this poster we describe some of the key achievements and various initiatives that have been undertaken to address this issue. For example: REDUCTION: Fish full life-cycle tests are considered the "gold standard" for assessing chronic effects of chemicals and use hundreds of animals. However, by utilizing all available information (e.g. preclinical data), it is possible to focus testing on sensitive life-stages and endpoints. This strategy was employed to design a 'targeted' chronic study, for an endocrine disrupting chemical, that used fewer fish than the standard test[1]. REFINEMENT: There is pressure to improve environmental enrichment for fish, although, most current approaches are based on mammalian research. Consequently, we aimed to identify enrichments that are suitable for fish and compatible with prescriptive regulatory protocols[2]. In addition, little information is available on pain alleviation in fish and alternative procedures are being developed that are both scientifically and ethically preferable to existing approaches to anaesthesia and analgesia[3]. REPLACEMENT: Cell culture is a promising alternative to fish use, although questions remain around *in vivo* translation. The use of fish hepatocytes and spheroids have been assessed to understand metabolic functionality and to develop alternatives to *in vivo* screens for assessing bioconcentration[4]. We have also evaluated algae and crustaceans, as surrogates for fish genotoxicity assessment, with the data generated suggesting effective metabolic activation and measurable induction of DNA damage[5]. [1]Panter et al., 2012. Aquatic Toxicol, 114-115, 31-38. [2]Wilkes et al., 2012. Appl Anim Behav Sci, 139: 143-150. [3]Readman, 2012. Platform presentation at BJZH, UCL, 17th May. [4]Baron et al., 2012. Ecotoxicology, 21, 2419-2429. [5]David et al., 2012. Chemosphere, 88, 912-927.

TH003
Consensus Model for Predicting the Acute Fish Toxicity of Organic Compounds
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According to REACH, in-te-grated testing strategies (ITS) are recommended to reduc-ing animal test-ing as far as possible. Since different non-animal methods may differ substantially in their reliability, a way forward is to combine the out-comes of several methds through a consensus model approach. This holds in particular for in silico ITS components such as QSARs, struc-tural alert models, and read-across approaches, because all of them can be applied with-out undertaking laboratory experiments. A consensus model approach is presented for combining QSAR, structural alert and read-across predictions of the acute fish toxicity into a consensus outcome, taking into account both the ap-pli-ca-tion domains of the individual models and their variation in scope (quan-ti-ta-tive vs. categorical prediction). To this end, 692 96-h LC_{50} values (acute toxicity to-ward fat-head minnow) have been taken from lite-rature. The new approach is organised in a hierarchical manner, and yields either a quan-ti-tative or a categorical (narcosis level vs. excess toxicity) estimate for the acute fish to-xicity of the com-pound of interest. The latter is triggered by a computerized as-sess-ment of the individual model domains through appli-cation of the ACF (atom-cen-tered frag-ment) approach.[1] In addition to an extended version of the recently intro-duced quan-ti-ta-tive read-across,[2] the consensus model includes a classification of the compound of in-terest as exerting narcosis-level vs. ex-cess toxicity, and ECOSAR-model[3] predictions that in turn are based on class-spe-ci-fic linear regression equa-tions employing log K_{ow} (octanol/water partition coefficient) as only molecular des-crip-tor. The fully automatized model ap-proach has been implemented in the OSIRIS[4] edition of the ChemProp software[5] that is available free of charge due to a license agreement. [1] Kühne R, Ebert R-U, Schüürmann G 2009. *J. Chem. Inf. Model.*49: 2660-2669. [2] Schüürmann G, Ebert R-U, Kühne R 2011. *Environ. Sci. Technol.*45: 4616-4622. [3] U.S. Environmental Protection Agency 2012. ECOSAR v.1.11. [4] OSIRIS. EU Project, contract no. GOCE-CT-2007-037017, 2007-2011. http://www.osiris-reach.eu/. Web-tool: http://osiris.simpple.com/OSIRIS-ITS. [5] ChemProp 5.2.8, 2012. UFZ Dep. Ecological Chemistry, http://www.ufz.de/index.php?en=6738.

TH004
Evaluation of CADASTER QSAR models for aquatic toxicity of (benzo-)triazoles and prioritization by consensus.
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The REACH regulation encourages the use of alternative *in vitro* and *in silico* methods in order to minimize animal testing, costs and time. Among these, Quantitative Structure-Activity Relationships (QSARs) represent a useful tool to predict unknown activities/properties for existing or even not yet synthesized chemicals. Triazoles and benzo-triazoles ((B)TAZs), which are a class of synthetic molecules studied in theeuropean project FP7 CADASTER (CAse studies on the Development and Application of in-Silico Techniques for Environmental hazard and Risk assessment), have different industrial and pharmaceutical uses, i.e pesticides, antimycotic and antidepressants medicines, UV-light stabilizers for plastics, anti-corrosives, dishwashing additives, and components of liquid aircraft de-icing agents and for airport runways. (B)TAZs have been found distributed throughout the environment, mainly in water compartments, and are cause of concern due to their possible effects mainly on aquatic organisms. Several QSAR models for toxicity of triazoles and benzo-triazoles to algae (*Pseudokirchneriella subcapitata*), *Daphnia magna* and fish (*Onchorhynchus mykiss*), the three key species which are usually considered to perform risk assessment of chemicals in water, were developed by five partners in the CADASTER project. The models were developed by different methods (Ordinary Least Squares (OLS), Partial Least Squares (PLS), Bayesian regularized regression and ASsociative Neural Network (ASNN)), using various molecular descriptors (calculated from DRAGON, PaDEL-Descriptor and QSPR-THESAURUS online platform), and different procedures for variable selection, validation and Applicability Domain inspection. The predictions of the developed models, as well as those obtained in a consensus approach by averaging the data predicted from each model, were compared with the results of experimental tests that were performed within the CADASTER partners. The individual and the consensus models are able to correctly predict the chemicals tested in CADASTER according to their toxicity class, confirming the utility of the QSAR approach. The models were also applied to predict the aquatic toxicity for over 300 (B)TAZs without experimental data, many of which are included in the REACH pre-registration list. This work highlights the importance of QSAR for screening and prioritization of untested chemicals, in order to reduce and focus the experimental tests.

TH005
Read-across Approach to Predict Acute Daphnid Toxicity
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REACH requires the assessment of daphnid toxicity for industrial chemicals with market volumes of at least 1 t/a. A hierarchical read-across approach allows predicting the 48-h LC_{50} toward the *Daphnia magna* from experimental data [1]. Dependent on the similarity of the actual compound to the training set chemicals, the method yields quantitative, qualitative, or screening level qualitative predictions. An identification of the applicability domain is integrated. The model alternatively exploits the octanol/water partition coefficient K_{ow} or an Abraham type LSER equation to calculate the baseline toxicity. Since the latter is the more promising approach for further refinements, the current study focuses on the LSER version. The reliability of this version with regard to particular compound classes is examined, and the dependence of the performance on different sources of LSER parameters is investigated. The presented model can be applied in a fully automated manner in the OSIRIS edition of the software system ChemProp [2]. It is publicly available free of charge due to a bilateral license agreement. [1] Kühne R, Ebert R-U, von der Ohe PC, Ulrich N, Brack W, Schüürmann G 2013. Read-across prediction of the acute toxicity of organic compounds toward the water flea Daphnia magna. *Mol. Inf.*, accepted November 2012. [2] Chemical Proper-ties Estimation Software System (ChemProp) 5.2.8, 2012. UFZ Department of Ecological Chemistry, http://www.ufz.de/index.php?en=6738.

TH006
Why the NOEC is not a NOEC but a function of power: Finding alternatives
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In toxicity tests and in ecotoxicological risk assessments the NOEC is one standard measure to address the risk of pesticides or other substances. It is used routinely for example to address the chronic risk in aquatic organisms or in birds