We carried out a series of incubations with sediment from three different rivers and synthetic river water. Tests were carried out at an initial concentration of 100-200 µg L^{-1} for approx. 30 days; samples were filtered and subsequently analyzed by UPLC-qTOF-MS. The high-resolution mass spectrometric data were processed with a workflow combining the tools mzMine (http://mzmine.sourceforge.net/) and enviMass (http://www.eawag.ch/forschung/uchem/software/enviMass1). By comparing incubations containing pharmaceuticals to control samples without pharmaceuticals, this yields a list of peaks identified by exact mass and retention time for each time step of the incubation experiment. Using these time series data, peaks showing a temporal trend expected for transformation products (e.g., not present at the beginning of the incubation, increasing concentrations with time) can be located and processed further. Through application of this time series approach, the number of peaks to be processed further is substantially reduced.
The first results obtained by this approach are promising and provide a solid basis for the evaluation of the workflow, but also for scrutinizing its precision and robustness in detecting unknown peaks at low concentrations. This is necessary to increase confidence in the applied analytical and *in silico* methods for the specific aims of our study. We will present results of this evaluation, and we will discuss the tentatively identified transformation products with respect to their formation/elimination kinetics and their applicability as indicators for *in situ* micropollutant transformation.

MO 203
Evaluation of the contamination of aquatic micro-organisms by micro-QuEChERS-nano-LC-MS/MS
M.T. Tournier[1], J. Camilleri[2], R.B. Baudot[1], L.W. Wiest[1], A.B. Buleté[1], E.V. Emmanuelle[1], J.G. Garric[3], C.C. Cren-Olivé[1]
[1]CNRS UMR 5280 ISA, Villeurbanne, France
[2]SCA, Solaize, France
[3]CEMAGREF, Lyon, France
It is currently accepted that the main route for pharmaceuticals and Endocrine Disruptors Chemicals (EDCs) to the aquatic environment is via sewage treatment plants receiving wastewater from households, industries and hospitals.
In a concern to follow their fates and their impacts in the environment, we developed analytical methods to quantify endogen and synthetic hormones, pharmaceuticals and chemicals in benthic species. We established a molecule list in accordance with prioritisation lists [1] and identification of contamination sources around the wastewater treatment plant (industries, hospital, villages): estrone, 17α-ethinyl-estradiol, lorazepam, oxazepam, acetaminophen, carbamazepine, ibuprofen, 4-methylbenzylidene camphor, fluoroquinolones and sulfonamides for example.
We decided to evaluate the contamination of three different species which are well-known bio indicators of water quality. More precisely, invertebrates like gastropods (Potamopyrgus antipodarum), amphipods (Gammarus) and chironomidae larvae (bloodworms) are exposed to effluents from treatment plants..
In the interests of handling a few milligrams of biological matrices and of being accurate, we chose an adequate analytical technique: the innovative nano-LC coupled with tandem mass spectrometer. After cryo-grinding, we extracted samples with a salting-out assisted LLE followed by a purifying dSPE. The extract was evaporated then reconstituted in a proper mobile phase. Only a 1-µl injection is done on the pre-concentration cartridge and the capillary column. Thus, we can reach limits of detection of a few injected femtograms.
In conclusion, the comprehensive method was applied to the study of the fate and bio-accumulation of preoccupying micro-pollutants in aquatic micro-organisms.

MO 204
Occurrence and seasonal variations of preservatives and UV filters used in cosmetic products in Japanese rivers
K.K. Kimura[1], K.Y. Kameda[2], W.S. Watanabe[3], M.S. Masunaga[1]
[1]Yokohama National University, Yokohama, Japan
[2]Center for Environmental Science in Saitama, Kazo, Japan
[3]Saitama City Institute of Health Science and Research, Saitama, Japan
Preservatives and UV filters are widely used in many cosmetics. These compounds may enter the aquatic environment from showering, wash-off, and so forth via wastewater treatment plants or sewage treatment tank. Most of these preservatives are included in order to suppress microorganisms growing. UV filters are used to prevent skin damage from UV radiation, however some of them are hormonally active to aquatic organisms. Their ecological adverse effect on aquatic organisms should be concerned after discharge. But there is little published data of their occurrence in aquatic environment.
In this study, we determined twelve preservatives (2-Phenoxyethanol, Resorcinol, Chroloxylenol, 4-Isopropyl-3-methylphenol, Chlorphenesin, Triclosan, Methylparaben, Ethylparaben, Propylparaben, Isopropylparaben, Butylparaben, Isobutylparaben) and four benzophenone-type UV filters (BP-1, BP-2, BP-3, BP-6) using solid phase extraction and GC/MS. Surface water samples were collected monthly at six sites in four Japanese rivers from December 2010. 2-Phenoxyethanol, Resorcinol, 4-Isopropyl-3-methylphenol and Triclosan were found in most of the samples in all seasons. 2-Phenoxyethanol was detected at much higher concentration in winter. Isopropylparaben, Isobutylparaben, BP-2 and BP-6 were not detected at any sampling sites. The highest concentration in all samples was for 2-Phenoxyethanol at 1µg/L level. Further investigation is necessary to evaluate the ecological effect of high concentration preservatives including 2-Phenoxyethanol.

MO 205
Solid phase extraction and LC-MS/MS analysis of pharmaceuticals in the Irish aquatic environment
G.L. Mceneff[1], W. Schmidt[2], B. Kelleher[3], L. Barron[4], B. Paull[5], B. Quinn[2]
[1]Irish Separations Science Cluster/Irish Centre for Environmental Toxicology, Dublin, Ireland
[2]Irish Centre for Environmental Toxicology, Galway-Mayo Institute of Technology, Galway, Ireland
[3]School of Chemical Sciences, Dublin City University, Glasnevin, Dublin, Ireland
[4]Analytical and Environmental Science Division, King's College London, London, United Kingdom
[5]Australian Centre for Research on Separation Science, University of Tasmania, Hobart, Australia
Pharmaceutical and personal care products (PPCP's) are resisting water remediation techniques carried out currently in wastewater treatment plants and are thus being released into receiving waters. In previous studies PPCP presence has been detected in Irish effluent1 and soils2 in measurable quantities. In the work presented herein, 24 hour composite effluent samples were collected from two large Irish Wastewater Treatment Plants and analysed for a total of six pharmaceuticals from a range of therapeutic classes including non-steroidal anti-inflammatories, anti-biotics, lipid regulators and anti-epileptics. The complexity of these sample matrices requires a clean up and extraction step (Phenomenex Strata-X cartridges - 200mg, 6ml) before chemical analysis. Samples were eluted with 50:50 v/v ethyl acetate/acetone and reconstituted in 0.5mls of starting mobile phase. Qualitative and quantitative analysis was carried out using reversed phase LC separation (Waters Sunfire C18 3.5 µm 2.1 x 150 mm column with a 45 minute mobile phase gradient of 20 % acetonitrile with 13 mM ammonium acetate, pH6.2, to 80 % acetonitrile) with UV detection followed by MS/MS detection. Analytes were identified by comparing their retention times and precursor and product ions to those of a known standard.
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MO 206
Use of LC-Orbitrap accurate mass spectrometry in risk assessment after a chemical incident.in the Netherlands
A.P. van Wezel, T. van Leerdam, L. Puijker
KWR Watercycle Research Institute, Nieuwegein, Nederland
Early 2011, a big incident took place in a chemical storage site in Moerdijk, the Netherlands. There was an extensive fire up to 500 meters high, with formation of soot. The column of smoke went in the northeastern direction within a large area. On the chemical storage site, many different inorganic, organic solid and liquid chemicals were stored. The fire extinguishing caused a vast volume of contaminated water.
Several Dutch water utilities have surface-water related raw drinking water in large storage reservoirs in the area under the plume. After storage, the raw water is treated by different treatment processes on the drinking water production location. These reservoirs were possibly influenced by the Moerdijk incident. For precautionary reasons, the reservoirs relatively close to Moerdijk were directly taken out of production and intake of possibly contaminated surface water was stopped. The quality of the drinking water produced by the utilities in the period during and after the incident has never come into play. Despite these precautionary measures, it was relevant to know if the storage reservoirs were negatively influenced by this Moerdijk incident. Therefore, several drinking-water related surface waters were sampled and analyzed using broad-screening analytical-chemical GC-MS and LC-MS accurate mass screening. The high sensitivity, the high resolving power and accurate mass measurement make this a valuable technique for the screening of trace levels of organic contaminants. In contrast to most current environmental monitoring campaigns, this approach does not target a predetermined set of (known) chemicals. Also, the developed approach does not aim at the detection of all organic chemical compounds present in a sample as in general unknown screening approaches. Instead the data was screened for the presence of 249 known chemicals and 386 unidentified chemicals. The list of 386 unidentified compounds was the result of broad screening campaigns in our laboratory in several Dutch water samples for the last 5 years.
In most of the storage reservoirs, no different compounds were found than normal. An exemption was a storage reservoir that was located 15 km from the incident.

MO 207
Polybrominated diphenyl ethers, alternate brominated flame retardants and Dechloranes in sediments from German Bight and Laizhou Bay, China
S. Quade[1], Z. Zhao[1], J. Tang[2], G. Zhong[1], R. Sturm[1], A. Möller[1], Z. Xie[1], G. Zhang[3], R. Ebinghaus[1]
[1]Helmholtz-Zentrum Geesthacht, Geesthacht, Germany
[2]Yantai Institute of Coastal Zone Research, Yantai, China
[3]Guangzhou Institute of Geochemistry, Guangzhou, China
Brominated flame retardants (BFRs) have been commercially used since the 1970s.
Since then more and more polymeric materials have been introduced for textiles, electronic equipment, upholstery, automobiles and building materials. Equally the production and usage of chemical additives for fire resistance of the mostly easy inflammable products have been increasing as well.
Due to their physicochemical properties i.e. low volatility, low water solubility and high Kow-values the BFRs tend to adsorb on particles. Therefore they were detected preferably in sediment samples. Benthic organisms and other contaminated sediment consuming animals can be the first step for bioaccumulation in the marine food web.