

relationships. The multidimensional word-embedding vectors of concepts were used to train a prediction model with MIE concepts as input and AO concepts as output. We present promising results for the validation performance of our deep learning model and demonstrate its capabilities to predict AOs based on the external data from AOP-Wiki. Predicted key events and relationships might help with development and evaluation of new putative AOPs in future.

7.01.4

Development of Adverse Outcome Pathway based on ToxCast™ and deep learning models combined approach

J. Jeong, University of Seoul / School of Environmental Engineering; J. Choi, University of Seoul / Environmental Engineering
Adverse outcome pathway (AOP) is a framework that organizes existing knowledge about linkage between molecular-level perturbation and an adverse outcome. The AOP framework allows the use of molecular level experimental data for hazard assessment. ToxCast™ project was launched in 2006 by the US EPA to generate toxicity information on large number of environmental chemicals at the molecular level. Deep learning has attracted researchers' attention due to its efficient feature extraction and prediction properties. Deep learning may be particularly well-suited for toxicology because the approach deals with complex pattern and "big data". It integrates information and data from a variety of sources to develop mathematical and computer-based models to better understand and predict adverse health effects caused by environmental chemicals. In this study, development of AOP was attempted based on molecular mechanism data obtained from ToxCast and Deep learning combined approach. The hit call data were collected from the selected 339 assays with intended target information in the ToxCast database. The intended targets belonged to 17 intended target families, mainly nuclear receptors, cytokines, DNA binding, GPCR, cell adhesion molecules, etc. We built 339 chemical activity classification models for the assays. The accuracy of the models ranged from 48.82 to 99.85. In order to improve the reliability of the analysis results, the models with accuracy less than 90 were excluded. As a result, 218 models were selected. Assay activities of chemicals were classified using ToxCast and deep learning models. Through this analysis, we have provided potential insights into the toxicity mechanism of environmental chemicals. By incorporating toxicity pathways information from ToxCast and deep learning models and in vivo toxicity data, we tried to develop the AOP relevant to environmental chemicals. In this study, we proposed an integrated approach using ToxCast database and deep learning models for mechanism-based screening and development of AOP. Since the coverage of experimental data is limited in ToxCast database, it is possible to use deep learning technique for prediction of missing data. This could be used as the screening step in enabling mechanistic-based assessment and could also be used in development of AOP. Acknowledgement - This work was supported by a grant from the Korean Ministry of Environment through 'Environmental Health R&D Program' (2017001370001).

7.01.5

Automated feature recognition in zebrafish embryos

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The zebrafish embryo represents a small scale model used to measure diverse endpoints for research and to identify hazards in ecotoxicology and human toxicology. The assessment of morphological alterations provoked by chemicals or environmental samples is one of the most often used endpoints typically conducted by visual assessment by an experienced observer using a microscope. Visual assessment can be biased by the experience and potential fatigue of the observer. Furthermore, subtle changes may not be recognised. Particularly if the data would be used for subsequent pattern analysis and a diagnostic purpose a more quantitative approach for the assessment would be required. Using an automated assessment based on the FishInspector software (Teixido et al. 2019, *Tox. Sci.*, 167, 438–449.) we obtained EC50 patterns of morphological alterations for 26 different test compounds. Similarity was observed between compounds that shared similar mode of actions such as interference with retinoic acid metabolism or ACCase inhibition. However, variable responses were observed within the same MoA group as well. The variability may be explained by discrepancies between the pharmacological mode of action used for grouping of chemicals and the MoA provoking the developmental phenotype. Initially the morphological feature recognition was based on standard image segmentation approaches. The detection occasionally required user correction and the number of features that could be detected was limited. Therefore, the previously detected features were used to train feature-specific models using Matlab Computer Vision Toolbox and the VGG-19 pretrained Convolutional Neural Network. Some features such as body contour or yolk revealed very high recognition superior to the previously used segmentation based approach. Given the versatility of the model-based approach new features can be trained in step wise approach using initially a small number of manually labeled image with subsequent rounds of automated

recognition and gradually reduced the need for user interaction. This approach allows to train images from various orientation of embryos and is more flexible regarding different image characteristics.

7.01.6

Poster spotlight: Recent updates to the MechoA scheme, a tool to support mechanistically-driven read-across approaches.

F. Bauer, KREATiS

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7.01.7

Poster spotlight: The development of a Molecular Initiating Event (MIE) based profiler for chemical classification and read-across

D. Ebbrell, Liverpool John Moores University / School of Pharmacy and Biomolecular Sciences

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7.01.8

Poster spotlight: Training a molecular dissimilarity measure for target specific activities

C. Garcia-Hernandez, Universitat Rovira i Virgili / Departamento de Ingeniería Química

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Exploring the Potential of Wastewater-based Epidemiology to Monitor Human Exposure to Pollutants and Public Health

7.02.1

Do we know how to best develop new wastewater-based epidemiology applications?

S. Castiglioni, Mario Negri Inst. / Environmental Health Sciences; E. Zuccato, Istituto Mario Negri / Environmental Health Sciences; B. Kasprzyk-Hordern, University of Bath / Department of Chemistry
Wastewater-based epidemiology (WBE) is an innovative methodology enabling the retrieval of epidemiological information from urban wastewater via the chemical analysis of specific human metabolic excretion products (biomarkers). The first WBE application was developed to estimate illicit drugs use, and it is now recognised as an additional drug use indicator among the existing epidemiological indicators. When WBE started to be applied by several groups in different countries, it was very soon clear that improving, coordinating and harmonising its application was necessary. A cross-sectoral and transdisciplinary network (Sewage analysis CORE group – SCORE; <https://score-cost.eu/>) was established in 2010 with the aim to develop a common protocol of action and perform international studies. The first best practice protocol established covered the main critical steps to perform WBE studies: i.e. wastewater sampling, biomarkers selection, chemical analysis, back-calculation of drug use and data normalization. More recently, several studies have focused on optimising the specific steps necessary to apply reliably a WBE approach. These findings go beyond the estimation of drug use are nowadays particularly valuable for developing novel WBE applications. The SCORE network is currently working to update the protocol of best practice previously developed, and this presentation will give an overview of the main essential requirements as highlighted by the recent literature. For instance, technical guidelines are now available on how to perform sampling of wastewater and select suitable biomarkers. Since WBE is based on the chemical analysis of specific substances, it is also essential to develop and validate proper analytical methods, and interlaboratory exercises may help to check the quality of measurements among different laboratories. Finally, ethical issues has to be carefully considered when dealing with small communities (i.e. workplaces, schools, prisons, city districts, entertainment venues) in order to avoid any kind of stigmatization of a specific group of persons. WBE is a very promising new approach to obtain a wide range of information on the health status of a population, but it is essential to follow common and standardised guidelines in order to allow comparisons among different studies and obtain reliable complementary information to epidemiological studies.

7.02.2

Assessment of the Spanish population exposure to phthalate plasticizers as obtained by wastewater-based epidemiology

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Virgili; M. Miró, Universitat de les Illes Balears / Department of Chemistry; Y. Pico, University of Valencia / Environmental Quality and Soil; E. Pocurull, Universitat Rovira i Virgili; C. Postigo, IDAEA, CID-CSIC / Environmental Chemistry; A. Rico, IMDEA Water Institute; Y. Valcárcel, Universidad Rey Juan Carlos / Department of Medical Specialties and Public Health.; J. Quintana, University of Santiago de Compostela

Phthalate diesters are high-production-volume chemicals that have been widely used in the manufacturing and processing of plastics for more than 80 years. Recently, they have been included in the priority lists of dangerous substances in most of the industrialized countries. Ingestion is considered the major route of exposure to phthalates, either by consuming contaminated food, accidental ingestion of contaminated dust and soil, or licking of products in which they are contained. Once in the human body, phthalates are hydrolysed to their corresponding monoesters and further oxidized or conjugated into glucuronide complexes and, finally, excreted. Wastewater-based epidemiology (WBE) is a complementary approach to human biomonitoring to estimate the level of exposure to a substance through the analysis of its metabolic residues in urban wastewater [1], considering that raw wastewater is a highly diluted urine sample representing an entire community. The objectives of this study were to analyse [2] the metabolites of 6 phthalate diesters in wastewaters from different locations in Spain and to assess the exposure to phthalate diesters in the investigated cities. Raw wastewater samples from 17 wastewater treatment plants, serving a total population of ca. 6 million inhabitants (13% of the Spanish population), were analysed. The results show that the highest population-weighted exposure loads were obtained for diethyl phthalate, followed by dimethyl phthalate and the isomers di-*i*-butyl phthalate and di-*n*-butyl phthalate. *Acknowledgements* - The authors acknowledge support by Xunta de Galicia (refs. ED431C2017/36 and IGM postdoctoral contract, Plan Galego I2C-Modalidade B, ED481D 2017/003), the Spanish Research Agency-AEI (ref. CTM2016-81935-REDT/AEI and CTM2017-84763-C3-R-2) and FEDER/ERDF. References [1] Zuccato, E.; Chiabrando, C.; Castiglioni, S.; Bagnati, R.; Fanelli, R. *Environ. Health Perspect.* 2008, 116 (8) 1027–32 [2] I. González-Mariño, R. Rodil, I. Barrio, R. Cela, J. B. Quintana. *Environ. Sci. Technol.* 2017, 51, 3902–3910

7.02.3

Estimation of community-wide exposure to chemicals via water fingerprinting and high resolution tandem quadrupole time-of-flight mass spectrometry

B. Kasprzyk-Hordern, University of Bath / Department of Chemistry
Timely and comprehensive assessment of community-wide public exposure to harmful and toxic chemicals is essential for the prevention, control or mitigation of exposure risks and for improving health. There is growing evidence of association between man-made chemicals present in industrial and household products and public health outcomes. Current human monitoring approaches are associated with high cost, are the restricted size of study groups and inability to gather comprehensive information on combined spatiotemporal exposure to mixtures of stressors, and their effects. More efficient approaches are critically needed to identify cause-effect linkages between harmful chemicals and human health. Wastewater-based epidemiology (WBE) via water fingerprinting provides a timely alternative to traditional approaches. This presentation will discuss the development and application of WBE for spatiotemporal estimation of community-wide exposure to several industrial and household derived chemicals including endocrine disruptors such as bisphenol A, and pesticides (e.g. atrazine) or biocides (e.g. triclosan).

From Ecology to Land Management via Regulation to Protect Biodiversity in Agricultural Landscapes

8.01.1

FAO's Engagement in the Post-2020 Global Biodiversity Framework: Mainstreaming Biodiversity Across Agricultural Sector
P. Lourenço Dias Nunes, FAO

8.01.4

Measuring biodiversity status – national action taken to protect biodiversity in the agricultural landscape in Switzerland
K. Knauer, Federal Office for Agriculture / WBF

8.01.5

A farmer's perspective on biodiversity
A. Bergin, Andrew Bergin - Regenerative Farmer

8.01.6

Case study on pesticides: generating data to assess effects and risks to biodiversity through a risk assessment
V. Ducrot, Bayer Ag / Environmental Safety Ecotoxicology; M. Miles, Bayer

CropScience UK / Environmental Safety; E. Pilling, Corteva Agriscience / REgulatory Sciences; A. Alix, Corteva Agrisciences / Risk Management

8.01.7

Case study on pesticides: Risk mitigation measures to protect biodiversity from side effects of pesticides

A. Alix, Corteva Agrisciences / Risk Management; E. Pilling, Corteva Agriscience / REgulatory Sciences; M. Miles, Bayer CropScience UK / Environmental Safety; V. Ducrot, Bayer Ag / Environmental Safety Ecotoxicology

In the context of EC Regulation No. 1107/2009 on the placing on the market of Plant Protection Products (pesticides) in the agricultural area, risk mitigation measures may be defined to ensure that the “high level of protection” goal to human health and the environment, including biodiversity, is reached. These measures are defined at country level and are tailored based on the outcome of the risk assessment. They were inventoried in the proceedings of the SETAC workshop MAGPIE. The MAGPIE toolbox complements the set of farm management measures listed in the Common Agriculture Policy (CAP) that include field margins, hedges, trees, buffer strips, or conservation areas. Although the two sets of measures may take different forms, they are aiming at bringing a common benefit on biodiversity. This benefit could be assessed in a number of studies dedicated to the evaluation of the efficacy of farmland management plans at improving biodiversity in cultivated areas. This presentation will illustrate the effect of risk mitigation measures derived from both the MAGPIE and CAP toolboxes, as measured in field and monitoring studies, on metrics to evaluated biodiversity in cultivated areas.

8.01.8

Ecosystem services and biodiversity; towards a holistic approach to risk assessment

L. Maltby, The University of Sheffield / Dpt. of Animal & Plant Sciences

Gender and other Forms of Bias. How Do We Achieve Diversity and Equal Opportunity in Scientific Research?

8.02.3

The SETAC award for scientists returning to research after a maternity break
M. Bloor, Scotlands Rural College

Open Science in Regulatory Environmental Risk Assessment

8.03.1

Introduction

T. Broek, Wageningen Environmental Research / Environmental Risk Assessment Team; Y. Devos, EFSA; P. Dohmen, BASF SE / Environmental and Consumer Safety, Ecotoxicology

8.03.2

Open Science in Regulatory Environmental Risk Assessment: An Overview

K. Elliott, Michigan State University / Lyman Briggs College
This talk will introduce the session on “Open Science in Regulatory Environmental Risk Assessment” by providing an overview of key objectives, initiatives, barriers, and opportunities. First, it will discuss the major goals associated with the open science movement as a whole, including efforts to generate more rapid innovation, promote more reproducible science, and make information available to a wide array of stakeholders. Second, it will highlight the range of initiatives currently being implemented or considered as part of the open science movement, including open access publications, data repositories, registries of study results, guidelines such as the FAIR and TOP principles, open peer review processes, sharing of materials and computer code, and strategies for reporting study results in “real time.” Third, it will discuss barriers to achieving full transparency in regulatory science, such as the privacy concerns that have complicated the U.S. Environmental Protection Agency’s recently proposed policy associated with data availability. Finally, it will discuss major opportunities for achieving greater levels of openness in regulatory environmental risk assessment, including strategies for reaching a wider range of stakeholders with the forms of information that are most relevant to them.

8.03.3

SETAC perspectives to Open Science - past, current and future activities to make it an integral part of environmental research

T. Seiler, RWTH Aachen University / Ecosystem Analysis
Open Science is more than simply making our findings accessible to everyone. It