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### 1) A schematic sampling protocol for contaminant monitoring in raptors

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Birds of prey, owls and falcons are widely used as sentinel species in raptor biomonitoring programmes. A major current challenge is to facilitate large-scale biomonitoring by coordinating contaminant monitoring activities and by building capacity across countries. This requiressharing, dissemination and adoption of best practices addressed by theNetworking Programme Research and Monitoring for and with Raptors in Europe (EURAPMON) and now being advanced by the ongoing international COST Action European Raptor Biomonitoring Facility. The present perspective introduces a schematic sampling protocol for contaminant monitoring in raptors. We provide guidance on sample collection with a view to increasing sampling capacity across countries, ensuring appropriate quality of samples and facilitating harmonization of procedures to maximize the reliability, comparability and interoperability of data. The here presented protocol can be used by professionals and volunteers as a standard guide to ensure harmonised sampling methods for contaminant monitoring in raptors.

### 2) Receptor-based in vitro activities to assess human exposure to chemical mixtures and related health impacts

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Humans are exposed to a large number of chemicals from sources such as the environment, food, and consumer products. There is growing concern that human exposure to chemical mixtures, especially during critical periods of development, increases the risk of adverse health effects in newborns or later in life. Historically, the one-chemical-at-a-time approach has been applied both for exposure assessment and hazard characterisation, leading to insufficient knowledge about human health effects caused by exposure to mixtures of chemicals that have the same target. To circumvent this challenge researchers can apply in vitro assays to analyse both exposure to and human health effects of chemical mixtures in biological samples. The advantages of using in vitro assays are: (i) that an integrated effect is measured, taking combined mixture effects into account and (ii) that in vitro assays can reduce complexity in identification of Chemicals of Emerging Concern (CECs) in human tissues. We have reviewed the state-of-the-art on the use of receptor-based in vitro assays to assess human exposure to chemical mixtures and related health impacts. A total of 43 studies were identified, in which endpoints for the arylhydrocarbon receptor (AhR), the estrogen receptor (ER), and the androgen receptor (AR) were used. The majority of studies reported biological activities that could be associated with breast cancer incidence, male reproductive health effects, developmental toxicities, human demographic characteristics or lifestyle factors such as dietary patterns. A few studies used the bioactivities to check the coverage of the chemical analyses of the human samples, whereas in vitro assays have so far not regularly been used for identifying CECs in human samples, but rather in environmental matrices or food packaging materials. A huge field of novel applications using receptor-based in vitro assays for mixture toxicity assessment on human samples and effect-directed analysis (EDA) using high resolution mass spectrometry (HRMS) for identification of toxic compounds waits for exploration. In the future this could lead to a paradigm shift in the way we unravel adverse human health effects caused by chemical mixtures.

### 3) Asymmetrical flow field-flow fractionation to probe the dynamic association equilibria of β-D-galactosidase

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Protein dynamics play a significant role in many aspects of enzyme activity. Monitoring of structural changes and aggregation of biotechnological enzymes under native conditions is important to safeguard their properties and function. In this work, the potential of asymmetrical flow field-flow fractionation (AF4) to study the dynamic association equilibria of the enzyme β-D-galactosidase (β-D-Gal) was evaluated. Three commercial products of β-D-Gal were investigated using carrier liquids containing sodium chloride or ammonium acetate, and the effect of adding magnesium (II) chloride to the carrier liquid was assessed. Preservation of protein structural integrity during AF4 analysis was essential and the influence of several parameters, such as the focusing step (including use of frit-inlet), cross flow, and injected amount, was studied. Size-exclusion chromatography (SEC) and dynamic light scattering (DLS) were used to corroborate the in-solution enzyme oligomerization observed with AF4. In contrast to SEC, AF4 provided sufficiently mild separation conditions to monitor protein conformations without disturbing the dynamic association equilibria. AF4 analysis showed that ammonium acetate concentrations above 40 mM led to further association of the dimers (“tetramerization”) of β-D-Gal. Magnesium ions, which are needed to activate β-D-Gal, appeared to induce dimer association, raising justifiable questions about the role of divalent metal ions in protein oligomerization and on whether tetramers or dimers are the most active form of β-D-Gal.

### 4) Rapid Screening α-Glucosidase Inhibitors from Natural Products by At-Line Nanofractionation with Parallel Mass Spectrometry and Bioactivity Assessment

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In this study, a novel at-line nanofractionation screening platform was successfully developed for the rapid screening and identification of α-glucosidase inhibitors from natural products. A time-course bioassay based on high density well-plates was performed in parallel with high resolution mass spectrometry (MS), providing a straightforward and rapid procedure to simultaneously obtain chemical and biological information of active compounds. Through multiple nanofractionations into the same well-plate and comparisons of the orthogonal separation results of hydrophilic interaction liquid chromatography (HILIC) and reversed-phase liquid chromatography (RPLC), the α-glucosidase inhibitors can be accurately identified from co-eluates. The screening platform was comprehensively evaluated and validated, and was applied to the screenings of green tea polyphenols and Ginkgo folium flavonoids. After accurate peak shape and retention time matching between the bioactivity chromatograms and MS chromatograms, ten α-glucosidase inhibitors were successfully screened out and identified. The proposed screening method is rapid, effective and can avoid ignoring low abundant/active inhibitors.

### 5) Reducing the influence of geometry-induced gradient deformation in liquid chromatographic retention modelling

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Rapid optimization of gradient liquid chromatographic (LC) separations often utilizes analyte retention modelling to predict retention times as function of eluent composition. However, due to the dwell volume and technical imperfections, the actual gradient may deviate from the set gradient in a fashion unique to the employed instrument. This makes accurate retention modelling for gradient LC challenging, in particular when very fast separations are pursued. Although gradient deformation has been addressed in method-transfer situations, it is rarely taken into account when reporting analyte retention parameters obtained from gradient LC data, hampering the comparison of data from various sources. In this study, a response-function-based algorithm was developed to determine analyte retention parameters corrected for geometry-induced deformations by specific LC instruments. Out of a number of mathematical distributions investigated as response-functions, the so-called “stable function” was found to describe the formed gradient most accurately. The four parameters describing the model resemble the statistical moments of the distribution and are related to chromatographic parameters, such as dwell volume and flow rate. The instrument-specific response function can then be used to predict the actual shape of any other gradient programmed on that instrument. To incorporate the predicted gradient in the retention modelling of the analytes, the model was extended to facilitate an unlimited number of linear gradient steps to solve the equations numerically. The significance and impact of distinct gradient deformation for fast gradients was demonstrated using three different LC instruments. As a proof of principle, the algorithm and retention parameters obtained on a specific instrument were used to predict the retention times on different instruments. The relative error in the predicted retention times went down from an average of 9.8% and 12.2% on the two other instruments when using only a dwell-volume correction to 2.1% and 6.5%, respectively, when using the proposed algorithm. The corrected retention parameters are less dependent on geometry-induced instrument effects.

### 6) Influence maximization in the presence of vulnerable nodes: A ratio perspective

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Influence maximization is a key problem seeking to identify users who will diffuse information to influence the largest number of other users in a social network. A drawback of the influence maximization problem is that it could be socially irresponsible to influence users many of whom would be harmed, due to their demographics, health conditions, or socioeconomic characteristics (e.g., predominantly overweight people influenced to buy junk food). Motivated by this drawback and by the fact that some of these vulnerable users will be influenced inadvertently, we introduce the problem of finding a set of users (seeds) that limits the influence to vulnerable users while maximizing the influence to the non-vulnerable users. We define a measure that captures the quality of a set of seeds as an additively smoothed ratio (ASR) between the expected number of influenced non-vulnerable users and the expected number of influenced vulnerable users. Then, we develop methods which aim to find a set of seeds that maximizes the measure: greedy heuristics, an approximation algorithm, as well as several variations of the approximation algorithm. We evaluate our methods on synthetic and real-world datasets and demonstrate they substantially outperform a state-of-the-art competitor in terms of both effectiveness and efficiency. We also demonstrate that the variations of our approximation algorithm offer different trade-offs between effectiveness and efficiency.