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CHEMICAL EFFECTS

Emerging investigator series: the role of chemical properties in human exposure to environmental chemicals

2021-09-20

One of the ultimate goals of environmental exposure science is to mechanistically understand how chemical properties and human behavior interactively determine human exposure to the wide spectrum of chemicals present in the environment. This comprehensive review assembles state-of-the-art knowledge of the role of partitioning, dissociation, mass transfer, and reactive properties in human contact with and absorption of organic chemicals via oral, dermal, and respiratory routes. Existing studies have revealed that chemicals with different properties vary greatly in mass distribution and occurrence among multiple exposure media, resulting in distinct patterns of human intake from the environment. On the other hand, these chemicals encounter different levels of resistance in the passage of intestinal, dermal, and pulmonary absorption barriers and demonstrate different levels of bioavailability, due to the selectivity of biochemical, anatomical and physiological structures of these absorption barriers. Moving forward, the research community needs to gain more in-depth mechanistic insights into the complex processes in human exposure, advance the technique to better characterize and predict chemical properties, generate and leverage experimental data for a more diverse range of chemicals, and describe better the interactions between chemical properties and human behavior.

Authors: Zhizhen Zhang, Shenghong Wang, Li Li

Full Source: Environmental science. Processes & impacts 2021 Sep 20. doi: 10.1039/d1em00252j.

Filling the knowledge gap: A suspect screening study for 1310 potentially persistent and mobile chemicals with SFC- and HILIC-HRMS in two German river systems

2021-09-10

Persistent and mobile chemicals (PM chemicals) were searched for in surface waters by hydrophilic interaction liquid chromatography (HILIC) and supercritical fluid chromatography (SFC), both coupled to high resolution mass spectrometry (HRMS). A suspect screening was performed using a newly compiled list of 1310 potential PM chemicals to the data of 11

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surface water samples from two river systems. In total, 64 compounds were identified by this approach. The overlap between HILIC- and SFC-HRMS was limited (31 compounds), confirming the complementarity of the two methods used. The identified PM candidates are characterized by a high polarity (median logD -0.4 at pH 7.5), a low molecular weight (median 187 g/mol), are mostly ionic (54 compounds) and contain a large number of heteroatoms (one per four carbons on average). Among the most frequently detected novel or yet scarcely investigated water contaminants were cyanoguanidine (11/11 samples), adamantan-1-amine (10/11), trifluoromethanesulfonate (9/11), 2-acrylamido-2-methylpropanesulfonate (10/11), and the inorganic anions hexafluorophosphate (11/11) and tetrafluoroborate (10/11). 31% of the identified suspects are mainly used in ionic liquids, a chemically diverse group of industrial chemicals with numerous applications that is so far rarely studied for their occurrence in the environment. Prioritization of the findings of PM candidates is hampered by the apparent lack of toxicity data. Hence, precautionary principles and minimization approaches should be applied for the risk assessment and risk management of these substances. The large share of novel water contaminants among these findings of the suspect screening indicates that the universe of PM chemicals present in the environment has so far only scarcely been explored. Dedicated analytical methods and screening lists appear essential to close the analytical gap for PM compounds.

Authors: Isabelle Neuwald, Matthias Muschket, Daniel Zahn, Urs Berger, Bettina Seiwert, Till Meier, Jochen Kuckelkorn, Claudia Strobel, Thomas P Knepper, Thorsten Reemtsma

Full Source: Water research 2021 Sep 10;204:117645. doi: 10.1016/j.watres.2021.117645.

Organic carbon and acidic ions in PM 2.5 contributed to particle bioreactivity in Chinese megacities during haze episodes

2021-09-22

Fine particulate matter (PM_{2.5}) has been linked to cardiopulmonary disease and systemic effects in humans. However, few studies have investigated the particle bioreactivity in Chinese megacities during haze episodes. The objective of this study was to determine the contributions of chemical components in PM_{2.5} to particle bioreactivity in Chinese megacities during haze episodes. PM_{2.5} samples were collected in 14 megacities across China from 23 December 2013 to 16 January 2014. Average PM_{2.5} concentrations ranged 88.92~199.67 µg/m³. Organic

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carbon (OC), elemental carbon (EC), anions, and cations per unit of PM_{2.5} were linked to cellular bioreactivity (i.e., reactive oxygen species (ROS) as assessed by dichlorodihydrofluorescein diacetate (DCFH) and inflammation as assessed by interleukin (IL)-6 in A549 cells). The contributions of chemicals in PM_{2.5} to ROS and inflammation were examined by the Pearson correlation coefficient and random forests. These results indicated that OC, Ca²⁺, SO₄²⁻, Cl⁻, F⁻, K⁺, and NO₃⁻ contributed to ROS production, whereas OC, Cl⁻, EC, K⁺, F⁻, Na⁺, and Ca²⁺ contributed to inflammation. In conclusion, PM_{2.5}-contained OC and acidic ions are important in regulation of oxidative stress and inflammation during haze episodes. Our findings suggest that severe haze PM_{2.5} events cause deterioration in air quality and may adversely affect human health.

Authors: Kin-Fai Ho, Ya-Chun Lee, Xinyi Niu, Hongmei Xu, Renjian Zhang, Jun-Ji Cao, Cheng-Yu Tsai, Ta-Chih Hsiao, Hsiao-Chi Chuang
Full Source: Environmental science and pollution research international 2021 Sep 22. doi: 10.1007/s11356-021-16552-0.

ENVIRONMENTAL RESEARCH

An integrated approach for chemical water quality assessment of an urban river stretch through Effect-Based Methods and emerging pollutants analysis with a focus on genotoxicity

2021-09-17

The impact of emerging chemical pollutants, on both status and functionality of aquatic ecosystems is worldwide recognized as a relevant issue of concern that should be assessed and managed by researchers, policymakers, and all relevant stakeholders. In Europe, the Reach Regulation has registered more than 100.000 chemical substances daily released in the environment. Furthermore, the effects related to the mixture of substances present in aquatic ecosystems may not be predictable on the basis of chemical analyses alone. This evidence, coupled with the dramatic effects of climate changes on water resources through water scarcity and flooding, makes urgent the application of innovative, fast and reliable monitoring methods. In this context, Effect-Based Methods (EBMs) have been applied in the urban stretch of the Tiber River (Central Italy) with the aim of understanding if detrimental pressures affect aquatic environmental health. In particular, different eco-genotoxicological assays have been used in order to detect genotoxic activity of chemicals present in the river, concurrently characterized by chemical analysis.

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Teratogenicity and embryo-toxicity have been studied in order to cover additional endpoints. The EBMs have highlighted the presence of diffuse chemical pollution and ecotoxicological effects in the three sampling stations, genotoxicological effects have been also detected through the use of different tests and organisms. The chemical analyses confirmed that in the aquatic ecosystems there is a diffuse presence, even at low concentrations, of emerging contaminants such as pharmaceuticals, not routinely monitored pesticides, personal care products, PFAS. The results of this study can help to identify an appropriate battery of EBMs for future studies and the application of more appropriate measures in order to monitor, mitigate or eliminate chemical contamination and remediate its adverse/detrimental effects on the ecosystem health.

Authors: Mario Carere, Antonio Antoccia, Annamaria Buschini, Giada Frenzilli, Francesca Marcon, Cristina Andreoli, Gessica Gorbì, Antonio Suppa, Serena Montalbano, Valentina Prota, Francesca De Battistis, Patrizia Guidi, Margherita Bernardeschi, Mara Palumbo, Vittoria Scarcelli, Marco Colasanti, Veronica D'Ezio, Tiziana Persichini, Massimiliano Scalici, Antonella Sgura, Federica Spani, Ion Udroi, Martina Valenzuela, Ines Lacchetti, Kevin di Domenico, Walter Cristiano, Valentina Marra, Anna Maria Ingelido, Nicola Iacovella, Elena De Felip, Riccardo Massei, Laura Mancini

Full Source: Journal of environmental management 2021 Sep 17;300:113549. doi: 10.1016/j.jenvman.2021.113549.

Organic Markers of Tire and Road Wear Particles in Sediments and Soils: Transformation Products of Major Antiozonants as Promising Candidates

2021-09-07

Tire and road wear particles (TRWPs) are one of the main sources of particulate traffic emissions, but measured data on TRWP contents in the environment are scarce. This study aims at identifying organic compounds suitable as quantitative markers for TRWPs by a tiered multistep selection process involving nontarget screening and subsequent identification by liquid-chromatography high-resolution mass spectrometry. Starting from several thousands of signals recorded in the extract of tire particles, the rigorous selection process considered source specificity, tendency of leaching, analytical sensitivity and precision, and stability during aging. It led to three transformation products of N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine (6-PPD) as the most suitable marker candidates: N-formyl-6-PPD, hydroxylated N-1,3-dimethylbutyl-N-phenyl quinone diimine, and 6-PPD-quinone. A linear response in standard addition experiments

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with tire particles and the correlation with TRWP contents in a diverse set of environmental samples imply that these compounds are promising candidates as markers for the quantification of TRWPs. Organic markers for TRWP contents in the environment would allow TRWP quantification with the traditional tandem MS (LC-MS/MS) equipment of an organic trace analytical laboratory and, thus, allow easy generation of data on TRWP occurrence in sediments and soils and other environmental matrices.

Authors: Philipp Klöckner, Bettina Seiwert, Stephan Wagner, Thorsten Reemtsma

Full Source: Environmental science & technology 2021 Sep 7;55(17):11723-11732. doi: 10.1021/acs.est.1c02723.

Social status modulates the behavioral and physiological consequences of a chemical pollutant in animal groups

2021-09-22

The social environment (i.e., the suite of social interactions that occur among individuals, which can result in variation in social ranks) is a commonly overlooked aspect of biology when scientists evaluate the effects of chemical contaminants. The social environment, however, represents the arena in which individual-level performance shapes group- or population-level outcomes, and may therefore mediate many of the ultimate consequences of chemicals for wildlife. Here, we evaluated the role that the social environment plays in determining the consequences of pollutant exposure. We exposed groups of juvenile brown trout (*Salmo trutta*) to an emerging pharmaceutical pollutant that is commonly detected in freshwaters (the benzodiazepine, oxazepam), and allowed them to form dominance hierarchies. Exposure affected dominant and subordinate fish differently, causing fish to become less aggressive at high doses and subordinate fish to become more competitively successful at low doses. These perturbations had further consequences for growth, fin damage, and survival. Exposure also modulated physiological stress in the hierarchy, and social status itself affected how much oxazepam was absorbed in tissues - potentially creating a dynamic feedback loop that further influences the asymmetric effects of exposure on differing social statuses. Many effects followed a "U-shaped" dose-response, highlighting the importance of non-linear, low dose effects. Altogether, we show that social structure in animal groups can interact with and modulate the effects of an environmental contaminant. We underscore the need to account for an organism's natural ecological context, including their social environment,

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in future experiments and environmental risk assessments to predict the effects of chemical contaminants on wildlife.

Authors: Erin S McCallum, Cody J Dey, Daniel Cervený, Aneesh P H Bose, Tomas Brodin

Full Source: Ecological applications : a publication of the Ecological Society of America 2021 Sep 22;e02454. doi: 10.1002/eap.2454.

[Environmental endocrine disruptors and fertility]

2021-09-21

Endocrine disruptor chemicals (EDCs) are ubiquitous contaminants in the environment, wildlife, and humans. During the last 20 years, several epidemiological, clinical and experimental studies have demonstrated the role of EDCs on the reduction of male and female fertility. The concept of foetal origins of adult disease is particularly topical in the field of reproduction. Moreover, exposure to EDCs during pregnancy has been shown to influence epigenetic programming of endocrine signalling and other important physiological pathways, and provided the basis for multi- and transgenerational transmission of adult diseases. However, the large panel of EDCs simultaneously present in the air, soil and water makes the quantification of human exposition still a challenge. Gas chromatography coupled with mass spectrometry, the measurement of total plasmatic hormonal bioactivity on stably transfected cell lines as well as the EDC analysis in hair samples are useful methods of evaluation. More recently, microRNAs analysis offers a new perspective in the comprehension of mechanisms behind the modulation of cellular response to foetal or post-natal exposure to EDCs. They will help researchers and clinicians in identifying EDCs exposition markers and new therapeutic approaches in the future.

Authors: Laura Gaspari, Françoise Paris, Marie-Odile Soyer-Gobillard, Nicolas Kalfa, Charles Sultan, Samir Hamamah

Full Source: Gynecologie, obstetrique, fertilité & senologie 2021 Sep 21;S2468-7189(21)00219-1. doi: 10.1016/j.gofs.2021.09.009.

Endocrine disruptor chemicals (EDCs) are ubiquitous contaminants in the environment, wildlife, and humans.

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OCCUPATIONAL

Under-reporting of non-fatal occupational injuries among precarious and non-precarious workers in Sweden

2021-09-20

Background: Under-reporting of occupational injuries (OIs) among precariously employed workers in Sweden challenges effective surveillance of OIs and targeted preventive measures.

Objective: To estimate the magnitude of under-reporting of OIs among precarious and non-precarious workers in Sweden in 2013.

Methods: Capture-recapture methods were applied using the national OIs register and records from a labour market insurance company. Employed workers 18-65 resident in Sweden in 2013 were included in the study (n=82 949 OIs). Precarious employment was operationalised using the national labour market register, while injury severity was constructed from the National Patient Register. Under-reporting estimates were computed stratifying by OIs severity and by sociodemographic characteristics, occupations and precarious employment.

Results: Under-reporting of OIs followed a dose-response pattern according to the levels of precariousness (the higher the precarious level, the higher the under-reporting) being for the precarious group (22.6%, 95% CI 21.3% to 23.8%), followed by the borderline precarious (17.6%, 95% CI 17.1% to 18.2%) and lastly the non-precarious (15.0%, 95% CI 14.7% to 15.3%). Under-reporting of OIs, decreased as the injury severity increased and was higher with highest level of precariousness in all groups of severity. We also observed higher under-reporting estimates among all occupations in the precarious and borderline precarious groups as compared with the non-precarious ones.

Conclusions: This is the first register-based study to empirically demonstrate in Sweden that under-reporting of OIs is 50% higher among precariously employed workers. OIs under-reporting may represent unrecognised injuries that especially burden precariously employed workers as financial, health and social consequences shift from the employer to the employee.

Authors: Bertina Kreshpaj, Theo Bodin, David H Wegman, Nuria Matilla-Santander, Bo Burstrom, Katarina Kjellberg, Letitia Davis, Tomas Hemmingsson, Johanna Jonsson, Carin Håkansta, Cecilia Orellana
Full Source: Occupational and environmental medicine 2021 Sep 20;oemed-2021-107856. doi: 10.1136/oemed-2021-107856.

Background: Under-reporting of occupational injuries (OIs) among precariously employed workers in Sweden challenges effective surveillance of OIs and targeted preventive measures.

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Examining the cost-effectiveness of personal protective equipment for formal healthcare workers in Kenya during the COVID-19 pandemic

2021-09-20

Background: Healthcare workers are at a higher risk of COVID-19 infection during care encounters compared to the general population. Personal Protective Equipment (PPE) have been shown to protect COVID-19 among healthcare workers, however, Kenya has faced PPE shortages that can adequately protect all healthcare workers. We, therefore, examined the health and economic consequences of investing in PPE for healthcare workers in Kenya.

Methods: We conducted a cost-effectiveness and return on investment (ROI) analysis using a decision-analytic model following the Consolidated Health Economic Evaluation Reporting Standards (CHEERS) guidelines. We examined two outcomes: 1) the incremental cost per healthcare worker death averted, and 2) the incremental cost per healthcare worker COVID-19 case averted. We performed a multivariate sensitivity analysis using 10,000 Monte Carlo simulations.

Results: Kenya would need to invest \$3.12 million (95% CI: 2.65-3.59) to adequately protect healthcare workers against COVID-19. This investment would avert 416 (IQR: 330-517) and 30,041 (IQR: 7243 - 102,480) healthcare worker deaths and COVID-19 cases respectively. Additionally, such an investment would result in a healthcare system ROI of \$170.64 million (IQR: 138-209) - equivalent to an 11.04 times return.

Conclusion: Despite other nationwide COVID-19 prevention measures such as social distancing, over 70% of healthcare workers will still be infected if the availability of PPE remains scarce. As part of the COVID-19 response strategy, the government should consider adequate investment in PPE for all healthcare workers in the country as it provides a large return on investment and it is value for money.

Authors: Jacob Kazungu, Kenneth Munge, Kalin Werner, Nicholas Risko, Andres I Vecino-Ortiz, Vincent Were

Full Source: BMC health services research 2021 Sep 20;21(1):992. doi: 10.1186/s12913-021-07015-w.

Background: Healthcare workers are at a higher risk of COVID-19 infection during care encounters compared to the general population.

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PHARMACEUTICAL/TOXICOLOGY

The Protective Effect of Natural Compounds on Doxorubicin-Induced Cardiotoxicity via Nicotinamide Adenine Dinucleotide Phosphate Oxidase Inhibition

2021-09-25

Objectives: Doxorubicin (DOX) is widely prescribed for the treatment of several human cancers. Unfortunately, cumulative doses of DOX are the main cause of myocardial dysfunction. Although preclinical and pharmaceutical studies were performed to investigate the potential of natural compounds in minimizing DOX toxicity, a comprehensive review of them is not available. This review can help the researchers for an effective search strategy. **Key findings:** Oxidative stress and p53 play an important role in DOX-associated cardiotoxicity. DOX activates nicotinamide adenine dinucleotide phosphate NADPH oxidase (NOX) in the heart, resulting in excessive reactive oxygen species that can induce cardiomyocyte apoptosis through phosphorylation of p53, DNA damage and/or mitogen-activated protein kinases-mediated cardiomyocyte apoptosis. Although a few chemical drugs with high efficacy are administered along with DOX to prevent or more likely to reduce cardiovascular toxicity, their use is often limited by additional side effects. Recently, attention has been drawn to natural compounds that prevent DOX cardiotoxicity. This review focuses on some of the natural bioactive compounds with potential therapeutic efficacy against DOX-induced cardiotoxicity (DIC).

Summary: Some natural compounds, especially flavonols, flavonoids and proanthocyanidins, have the most protective effects against DIC by forming stable radicals and preventing the assembly of the NOX subunits.

Authors: Mozhdeh Yousefian, Hossein Hosseinzadeh, A Wallace Hayes, Farzin Hadizadeh, Gholamreza Karimi

Full Source: The Journal of pharmacy and pharmacology 2021 Sep 25;rgab109. doi: 10.1093/jpp/rgab109.

Objectives: Doxorubicin (DOX) is widely prescribed for the treatment of several human cancers.