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CHEMICAL EFFECTS

A Relevant Screening of Organic Contaminants Present on Freshwater and Pre-Production Microplastics

2020-11-09

Microplastics (MPs) have recently been discovered as considerable pollutants of all environmental matrices. They can contain a blend of chemicals, some of them added during the manufacture of plastic to improve their quality (additives) and others adsorbed from the surrounding environment. In light of this, a detailed study about the identification and quantification of target organic pollutants and qualitative screening of non-target compounds present on MPs was carried out in different types of samples: environmental MPs, collected from an Italian river, and pre-production MPs, taken from the plastic industry. Polychlorobiphenyls (PCBs), organochlorine pesticides (OCPs), and polycyclic aromatic hydrocarbons (PAHs) were chosen as target compounds to be quantified by Gas Chromatography-Mass Spectrometry (GC-MS), while the non-target screening was carried out by High Resolution Gas Chromatography-Mass Spectrometry (HRGC-MS). The target analysis revealed concentrations of 16 priority Polycyclic Aromatic Hydrocarbons by Environmental Protection Agency (EPA-PAHs) in the range of 29.9-269.1 ng/g; the quantification of 31 PCBs showed values from 0.54 to 15.3 ng/g, identifying CB-138, 153, 180, 52, and 101 primarily; and the detected OCPs (p,p'-DDT and its metabolites) ranged between 14.5 and 63.7 ng/g. The non-target screening tentatively identified 246 compounds (e.g., phthalates, antioxidants, UV-stabilizers), including endocrine disruptors, toxic and reprotoxic substances, as well as chemicals subjected to risk assessment and authorisation. The large assortment of plastic chemicals associated with MPs showed their role as a presumable source of pollutants, some of which might have high bioaccumulation potential, persistence, and toxicity.

Authors: Claudia Campanale, Georg Dierkes, Carmine Massarelli, Giuseppe Bagnuolo, Vito Felice Uricchio

Full Source: *Toxics* 2020 Nov 9;8(4):E100. doi: 10.3390/toxics8040100.

In Silico Assessment of Acute Oral Toxicity for Mixtures

2020-11-18

While exposure of humans to environmental hazards often occurs with complex chemical mixtures, the majority of existing toxicity data are for single compounds. The Globally Harmonized System of chemical

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classification (GHS) developed by the Organization for Economic Cooperation and Development uses the additivity formula for acute oral toxicity classification of mixtures, which is based on the acute toxicity estimate of individual ingredients. We evaluated the prediction of GHS category classifications for mixtures using toxicological data collected in the Integrated Chemical Environment (ICE) developed by the National Toxicology Program (United States Department of Health and Human Services). The ICE database contains in vivo acute oral toxicity data for 10,000 chemicals and for 582 mixtures with one or multiple active ingredients. By using the available experimental data for individual ingredients, we were able to calculate a GHS category for only half of the mixtures. To expand a set of components with acute oral toxicity data, we used the Collaborative Acute Toxicity Modeling Suite (CATMoS) implemented in the Open Structure-Activity/Property Relationship App to make predictions for active ingredients without available experimental data. As a result, we were able to make predictions for 503 mixtures/formulations with 72% accuracy for the GHS classification. For 186 mixtures with two or more active ingredients, the accuracy rate was 76%. The structure-based analysis of the misclassified mixtures did not reveal any specific structural features associated with the mispredictions. Our results demonstrate that CATMoS together with an additivity formula can be used to predict the GHS category for chemical mixtures.

Authors: Yaroslav Chushak, Jeffery M Gearhart, Darrin Ott

Full Source: *Chemical research in toxicology* 2020 Nov 18. doi: 10.1021/acs.chemrestox.0c00256.

Plastic debris is ubiquitous in aquatic systems and has been proven vehicles for the transport of various pollutants including trace organic compounds.

ENVIRONMENTAL RESEARCH

Adsorption of ciprofloxacin to functionalized nano-sized polystyrene plastic: Kinetics, thermochemistry and toxicity

2021-01-01

Plastic debris is ubiquitous in aquatic systems and has been proven vehicles for the transport of various pollutants including trace organic compounds. Nanoplastics have large specific surface area and hydrophobic characteristics and therefore are capable of adsorbing other organic or inorganic chemicals from the environment. Antibiotics, as another class of emerging contaminants, have raised significant research concern in recent years as they pose threats to the ecosystems and human health. Nevertheless, little information is available on the adsorption behaviors of antibiotics onto nano-sized plastics. The toxicity of combined nanoplastics and antibiotics is also largely unknown. In this study, the

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physicochemical and thermodynamic interactions between representative nanoplastics, which containing a carboxyl functional group of polystyrene nanoplastics (PS-COOH), and typical antibiotic, i.e., ciprofloxacin (CIP) were investigated in a batch adsorption experiment. The specific thermodynamic correlation function of PS-COOH combined with CIP was obtained through isothermal titration microcalorimetry (ITC) analysis. The adsorption kinetics and isotherm of CIP on PS-COOH closely fit the pseudo-second-order kinetic model ($r_2 = 0.99$) and Freundlich isotherm ($r_2 = 0.99$). The ITC results showed that the adsorption reaction of PS-COOH with CIP was a spontaneous exothermic reaction. The adsorption of antibiotics on nanoplastics may aggravate the negative impacts of these two pollutants on aqueous ecosystems, and we hypothesized that would be reflected in the survival rate of model organism of *Caenorhabditis elegans* when exposed to this combination. This work used a mechanistic approach to unravel the adsorption behavior of antibiotics on nanoplastics and shed light on their potential impact on aquatic ecosystems.

Authors: Mihebai Yilimulati, Longfei Wang, Xiaoli Ma, Chuanwang Yang, Nuzahat Habibul

Full Source: The Science of the total environment 2021 Jan 1;750:142370. doi: 10.1016/j.scitotenv.2020.142370.

Physical activity attenuated the association of air pollutants with telomere length in rural Chinese adults

2020-11-11

Background: Exposure to air pollutants (nitrogen dioxide (NO₂) and particulate matters (PMs)) or physical inactivity is linked to telomere length (TL) shortening. However, there is a lack of research on combined effects of either NO₂ or PMs and physical activity (PA) on TL. This study aimed to explore the joint associations of air pollutants (NO₂ or PMs) and PA with relative TL in rural Chinese adults. Methods: This study

was conducted among 2704 participants aged 18-79 years in rural China. Concentrations of NO₂ and PMs (PM with an aerodynamics diameter $\leq 1.0 \mu\text{m}$ (PM₁), $\leq 2.5 \mu\text{m}$ (PM_{2.5}) or $\leq 10 \mu\text{m}$ (PM₁₀)) were estimated using random forest models incorporated with satellites data, meteorological data, and land use information. Relative TL of each participant was measured by a quantitative real-time polymerase chain reaction. Linear regression models were applied to examine the independent associations between PA, NO₂ or PMs and relative TL. Interaction plots were used to depict the altered associations between NO₂, PM₁, PM_{2.5}, or PM₁₀ and relative TL along with increasing PA levels.

Background: Exposure to air pollutants (nitrogen dioxide (NO₂) and particulate matters (PMs)) or physical inactivity is linked to telomere length (TL) shortening.

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Results: Each 1 $\mu\text{g}/\text{m}^3$ increment in NO₂, PM₁, PM_{2.5}, or PM₁₀ was associated with a 0.038 (95% confidence intervals (CI): -0.044, -0.033), 0.036 (95% CI: -0.041, -0.031), 0.052 (95% CI: -0.059, -0.045), or 0.022 (95% CI: -0.025, -0.019) decrease in relative TL among all participants; similar findings were observed among normal glucose tolerance or impaired fasting glucose (IFG) participants as well as type 2 diabetes mellitus (T2DM) patients. PA at certain levels counteracted the association of air pollutants (NO₂, PM₁, PM_{2.5}, and PM₁₀) with relative TL among IFG participants or T2DM patients. Conclusions: Long-term exposure to NO₂ and PMs was associated with relative TL shortening and these effects may be counteracted by PA at certain levels in IFG participants or T2DM patients.

Authors: Ruiying Li, Shanshan Li, Mingming Pan, Hao Chen, Xiaotian Liu, Gongbo Chen, Ruoling Chen, Zhenxing Mao, Wenqian Huo, Xian Wang, Songcheng Yu, Yanying Duan, Yuming Guo, Jian Hou, Chongjian Wang
Full Source: The Science of the total environment 2020 Nov 11;143491. doi: 10.1016/j.scitotenv.2020.143491.

Long-Term Ambient Air Pollution Exposures and Brain Imaging Markers in Korean Adults: The Environmental Pollution-Induced Neurological Effects (EPINEF) Study

2020-11

Background: Only a limited number of neuroimaging studies have explored the effects of ambient air pollution in adults. The prior studies have investigated only cortical volume, and they have reported mixed findings, particularly for gray matter. Furthermore, the association between nitrogen dioxide (NO₂) and neuroimaging markers has been little studied in adults.

Objectives: We investigated the association between long-term exposure to air pollutants (NO₂, particulate matter (PM) with aerodynamic diameters of $\leq 10 \mu\text{m}$ (PM₁₀) and $\leq 2.5 \mu\text{m}$ (PM_{2.5}), and neuroimaging markers.

Methods: The study included 427 men and 530 women dwelling in four cities in the Republic of Korea. Long-term concentrations of PM₁₀, NO₂, and PM_{2.5} at residential addresses were estimated. Neuroimaging markers (cortical thickness and subcortical volume) were obtained from brain magnetic resonance images. A generalized linear model was used, adjusting for potential confounders. Results: A 10- $\mu\text{g}/\text{m}^3$ increase in PM₁₀ was associated with reduced thicknesses in the frontal [-0.02mm (95% CI: -0.03, -0.01)] and temporal lobes [-0.06mm (95% CI: -0.07, -0.04)]. A 10- $\mu\text{g}/\text{m}^3$ increase in PM_{2.5} was associated with a thinner temporal

Background: Only a limited number of neuroimaging studies have explored the effects of ambient air pollution in adults.

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cortex [-0.18mm (95% CI: -0.27, -0.08)]. A 10-ppb increase in NO₂ was associated with reduced thicknesses in the global [-0.01mm (95% CI: -0.01, 0.00)], frontal [-0.02mm (95% CI: -0.03, -0.01)], parietal [-0.02mm (95% CI: -0.03, -0.01)], temporal [-0.04mm (95% CI: -0.05, -0.03)], and insular lobes [-0.01mm (95% CI: -0.02, 0.00)]. The air pollutants were also associated with increased thicknesses in the occipital and cingulate lobes. Subcortical structures associated with the air pollutants included the thalamus, caudate, pallidum, hippocampus, amygdala, and nucleus accumbens. Discussion: The findings suggest that long-term exposure to high ambient air pollution may lead to cortical thinning and reduced subcortical volume in adults. <https://doi.org/10.1289/EHP7133>.

Authors: Jaelim Cho, Young Noh, Sun Young Kim, Jungwoo Sohn, Juhwan Noh, Woojin Kim, Seong-Kyung Cho, Hwasun Seo, Gayoung Seo, Seung-Koo Lee, Seongho Seo, Sang-Baek Koh, Sung Soo Oh, Hee Jin Kim, Sang Won Seo, Dae-Seock Shin, Nakyoung Kim, Ho Hyun Kim, Jung Il Lee, Changsoo Kim

Full Source: Environmental health perspectives 2020 Nov;128(11):117006. doi: 10.1289/EHP7133.

Diphenylamine Antioxidants in wastewater influent, effluent, biosolids and landfill leachate: Contribution to environmental releases

2020-11-03

Diphenylamine antioxidants (DPAs) are widely used industrial chemicals. Wastewater effluents and biosolids are important pathways for DPAs to enter the environment. Information on the fate of DPAs in wastewater treatment plants (WWTPs) and their environmental releases is limited. In this study, we characterized the occurrence, removal efficiencies, distribution, mass balance, and environmental releases of 17 DPAs in ten Canadian WWTPs and four landfill sites from 2013 to 2015. These WWTPs are different in sizes, and treatment technologies. Median concentrations of ΣDPAs were 78 ng/L in influent, 6.9 ng/L in effluent, 326 ng/L in leachate, and 445 ng/g in biosolids (dry weight), respectively. Diphenylamine (DPA) and ditertoctyl-diphenylamine (DTO-DPA) were the predominant congeners of DPAs in all the matrices. Residues of DPAs were not completely removed during wastewater treatment processes: most DPAs were detected in at least one sample of WWTP effluent with the highest concentration of 117 ng/L (DPA). Overall, high removal efficiencies (median > 90%) of most of the DPAs were observed in the secondary and advanced treatment, as well as in the facultative and aerated lagoons. In contrast, primary treatment exhibited a lower removal efficiency of

Diphenylamine antioxidants (DPAs) are widely used industrial chemicals.

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the DPAs. Mass balance analysis shows that sorption to biosolids is the major removal pathway of DPAs in WWTPs. The results also highlight that environmental releases of DPAs via biosolid applications (70 mg/d/1000 people) can be over several times higher than that via wastewater effluent (2.5-36 mg/d/1000 people).

Authors: Zi-Feng Zhang, Xue Zhang, Xianming Zhang, Ed Sverko, Shirley Anne Smyth, Yi-Fan Li

Full Source: Water research 2020 Nov 3;189:116602. doi: 10.1016/j.watres.2020.116602.

OCCUPATIONAL

Transfer of short-, medium-, and long-chain chlorinated paraffins to eggs of laying hens after dietary exposure

2020-11-04

Chlorinated paraffins (CPs) are a complex family of contaminants. Lack of exposure data and an understanding of the fate of these chemicals in the environment affect our ability to reliably assess the human health risk associated with CP exposure. The present study focused on the evaluation of CP transfer from feed to eggs of laying hens exposed over 91 days. Laying hens were provided feed spiked with five technical mixtures of short-, medium- or long-chain CPs and featuring low or high chlorine contents, at concentrations of 200 ng/g each. Eggs were collected daily. All mixtures except the LCCPs with high chlorine content transferred into the eggs, with accumulation ratios increasing with the chain length and chlorine content. Concentrations at the steady-state varied between 41 and 1397 ng/g lw depending on the mixture. Additionally, the homologue-dependant transfer resulted in a change of pattern compared to that from the spiked feed.

Authors: Marie Mézière, Philippe Marchand, Sébastien Hutinet, Frédéric Larvor, Elisabeth Baéza, Bruno Le Bizec, Gaud Dervilly, Ronan Cariou

Full Source: Food chemistry 2020 Nov 4;128491. doi: 10.1016/j.foodchem.2020.128491.

Chlorinated paraffins (CPs) are a complex family of contaminants.

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Characteristics of Exposure to Chloromethylisothiazolinone (CMIT) and Methylisothiazolinone (MIT) among Humidifier Disinfectant-Associated Lung Injury (HDLI) Patients in South Korea

2020-11-12

This study aimed to quantify both chloromethylisothiazolinone (CMIT) and methylisothiazolinone (MIT) dissolved in different product brands and to characterize the exposure to these chemicals among humidifier disinfectant-associated lung injury (HDLI) patients. Both CMIT and MIT dissolved in different humidifier disinfectant (HD) products were quantified using gas chromatography-mass spectrometry. The inhalation level of CMIT and MIT was estimated based on HD-associated factors as reported by HDLI patients. A total of eleven HD products marketed until the end of 2011 were found to contain CMIT and/or MIT. The level of combined CMIT and/or MIT dissolved in these HD products ranged from 12 to 353 ppm. The level varied among HD products and the year of manufacture. The average inhalation levels were estimated to be 7.5, 4.1, and 3.2 $\mu\text{g}/\text{m}^3$ for the definite, probable, and possible groups, respectively. If probable and possible groups were collapsed together, the inhalation level of the collapsed group was significantly different from that of the definite group ($p < 0.001$). All HDLI patients responded as having used HD not only while sleeping, but also as having a humidifier treated with HD within close proximity every day in insufficiently ventilated spaces. These HD use characteristics of patients may be directly/indirectly linked to the HDLI development.

Authors: Dong-Uk Park, Seon-Kyung Park, Jiwon Kim, Jihoon Park, Seung-Hun Ryu, Ju-Hyun Park, So-Yeon Lee, Han Bin Oh, Sungkyoon Kim, Kyung Ehi Zoh, Soyoung Park, Jung-Hwan Kwon

Full Source: *Molecules* (Basel, Switzerland) 2020 Nov 12;25(22):E5284. doi: 10.3390/molecules25225284.

PHARMACEUTICAL/TOXICOLOGY

Environmental chemicals, breast cancer progression and drug resistance

2020-11-17

Breast cancer (BC) is one of the most common causes of cancer in the world and the second leading cause of cancer deaths among women. Mortality is associated mainly with the development of metastases. Identification of the mechanisms involved in metastasis formation is,

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therefore, a major public health issue. Among the proposed risk factors, chemical environment and pollution are increasingly suggested to have an effect on the signaling pathways involved in metastatic tumor cells emergence and progression. The purpose of this article is to summarize current knowledge about the role of environmental chemicals in breast cancer progression, metastasis formation and resistance to chemotherapy. Through a scoping review, we highlight the effects of a wide variety of environmental toxicants, including persistent organic pollutants and endocrine disruptors, on invasion mechanisms and metastatic processes in BC. We identified the epithelial-to-mesenchymal transition and cancer-stemness (the stem cell-like phenotype in tumors), two mechanisms suspected of playing key roles in the development of metastases and linked to chemoresistance, as potential targets of contaminants. We discuss then the recently described pro-migratory and pro-invasive Ah receptor signaling pathway and conclude that his role in BC progression is still controversial. In conclusion, although several pertinent pathways for the effects of xenobiotics have been identified, the mechanisms of actions for multiple other molecules remain to be established. The integral role of xenobiotics in the exposome in BC needs to be further explored through additional relevant epidemiological studies that can be extended to molecular mechanisms.

Authors: Meriem Koual, Céline Tomkiewicz, German Cano-Sancho, Jean-Philippe Antignac, Anne-Sophie Bats, Xavier Coumoul

Full Source: *Environmental health : a global access science source* 2020 Nov 17;19(1):117. doi: 10.1186/s12940-020-00670-2.

Enhanced activation of peroxydisulfate by strontium modified BiFeO₃ perovskite for ciprofloxacin degradation

2021-01

A series of Sr-doped BiFeO₃ perovskites (Bi_{1-x}Sr_xFeO₃, BSFO) fabricated via sol-gel method was applied as peroxydisulfate (PDS) activator for ciprofloxacin (CIP) degradation. Various technologies were used to characterize the morphology and physicochemical features of prepared BSFO samples and the results indicated that Sr was successfully inserted into the perovskites lattice. The catalytic performance of BiFeO₃ was significantly boosted by strontium doping. Specifically, Bi_{0.9}Sr_{0.1}FeO₃ (0.1BSFO) exhibited the highest catalytic performance for PDS activation to remove CIP, where 95% of CIP (10 mg/L) could be degraded with the addition of 1 g/L 0.1BSFO and 1 mmol/L PDS within 60 min. Moreover, 0.1BSFO displayed high reusability and stability with lower metal leaching. Weak acidic condition was preferred to neutral and alkaline conditions

A series of Sr-doped BiFeO₃ perovskites (Bi_{1-x}Sr_xFeO₃, BSFO) fabricated via sol-gel method was applied as peroxydisulfate (PDS) activator for ciprofloxacin (CIP) degradation.

This study aimed to quantify both chloromethylisothiazolinone (CMIT) and methylisothiazolinone (MIT) dissolved in different product brands and to characterize the exposure to these chemicals among humidifier disinfectant-associated lung injury (HDLI) patients.

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in 0.1BSFO/PDS system. The boosted catalytic performance can be interpreted as the lower oxidation state of Fe and the existence of affluent oxygen vacancies generated by Sr doping, that induced the formation of singlet oxygen (1O_2) which was confirmed as the dominant reactive species by radical scavenging studies and electron spin resonance (ESR) tests. The catalytic oxidation mechanism related to major 1O_2 and minor free radicals was proposed. Current study opens a new avenue to develop effective A-site modified perovskite and expands their application for PDS activation in wastewater remediation.

Authors: Caicai Wang, Shengwang Gao, Jianchao Zhu, Xunfeng Xia, Mingxin Wang, Yanna Xiong

Full Source: Journal of environmental sciences (China) 2021 Jan;99:249-259. doi: 10.1016/j.jes.2020.04.026.