CHEMWATCH
Bulletin Board

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CHEMICAL EFFECTS

Which of the (Mixed) Halogenated n-Alkanes Are Likely To Be Persistent Organic Pollutants?

2021-11-21

Short-chain polychlorinated n-alkanes are ubiquitous industrial chemicals widely recognized as persistent organic pollutants. They represent only a small fraction of the 184,600 elemental compositions (C10-25) and the myriad isomers of all possible (mixed) halogenated n-alkanes (PXAs). This study prioritizes the PXAs on the basis of their potential to persist, bioaccumulate, and undergo long-range transport guided by quantitative structure-property relationships (QSPRs), density functional theory (DFT), chemical fate models, and partitioning space. The QSPR results narrow the list to 966 elemental compositions, of which 352 (23 Br, 83 Cl/F, 119 Br/Cl, and 127 Br/F) are likely constituents of substances used as lubricants, plasticizers, and flame retardants. Complementary DFT calculations suggest that an additional 1367 elemental compositions characterized by a greater number of carbon and fluorine atoms but fewer chlorine and bromine atoms may also pose a risk. The results of this study underline the urgent need to identify and monitor these suspected pollutants, most appropriately using mass spectrometry. We estimate that the resolving power required to distinguish   74% of the prioritized elemental compositions from the most likely interferents, i.e., chlorinated alkanes, is approximately 60,000 (full width at half-maximum). This indicates that accurate identification of the PXAs is achievable using most high-resolution mass spectrometers.

Authors: Xiaolei Li, Tannia Chevez, Amila O De Silva, Derek C G Muir, Sonya Kleywegt, Andre Simpson, Myrna J Simpson, Karl J Jobst
Full Source: Environmental science & technology 2021 Nov 21. doi: 10.1021/acs.est.1c05465.

Updating the European Union's regulation on classification, labelling and packaging of substances and mixtures (CLP): A key opportunity for consumers, workers and stakeholders with interests in the legislation and toxicology of hazardous chemicals

2021-11-17

Recent advancements in toxicology and the European Union's Green Deal, with its Chemicals Strategy for Sustainability, have paved the way for

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major changes in EU legislation on the control of environmental chemicals for a cleaner and safer environment. Another substantial legislative advancement underway is the update of the "Regulation on Classification, Labelling and Packaging of Substances and Mixtures (CLP)," an ambitious piece of EU legislation with exceptional scientific toxicological background in identifying a hazard, aiming at better protecting its citizens and the environment from the risk of chemical substances and products, the occupational settings included. Update of CLP legislation additionally aims at facilitating the free exchange of chemicals in the European Internal Market, provided that proper labelling and packaging processes are implemented. Participation in the ongoing online public consultation on these issues, ending on November 15, 2021, is of key relevance to ensure a transparent and effective definition of such an important piece of legislation, fully compliant with current EU priorities in terms of human and environmental protection and animal welfare.

Authors: Silvio Roberto Vinceti, Anca Oana Docea, Christina Tsitsimpikou, Tommaso Filippini
Full Source: Toxicology reports 2021 Nov 17;8:1865-1868. doi: 10.1016/j.toxrep.2021.11.011.

Persistent organic pollutants (POPs) - QSPR classification models by means of Machine learning strategies

2022-01

Persistent Organic pollutants (POPs) are toxic chemicals with a shallow degradation rate and global negative impact. Their physicochemical is combined with the complex effects of long-term POPs accumulation in the environment and transport function through the food chain. That is why POPs have been linked to adverse effects on human health and animals. They circulate globally via different environmental pathways, and could be detected in regions far from their source of origin. The primary goal of the present study is to carry out classification of various representatives of POPs using different theoretical descriptors (molecular, structural) to develop quantitative structure-properties relationship (QSPR) models for predicting important properties POPs. Multivariate statistical methods such as hierarchical cluster analysis, principal components analysis and self-organizing maps were applied to reach excellent partitioning of 149 representatives of POPs into 4 classes using ten most appropriate descriptors (out of 63) defined by variable reduction procedure. The predictive capabilities of the defined classes could be applied as a pattern recognition for new and unidentified POPs, based only on structural properties that similar molecules may have. The additional self-organizing

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maps technique made it possible to visualize the feature-space and investigate possible patterns and similarities between POPs molecules. It contributes to confirmation of the proper classification into four classes. Based on SOM results, the effect of each variable and pattern formation has been presented.
Authors: Ekaterina Vakarelska, Miroslava Nedyalkova, Mahdi Vasighi, Vasil Simeonov
Full Source: Chemosphere 2022 Jan;287(Pt 2):132189. doi: 10.1016/j.chemosphere.2021.132189.

ENVIRONMENTAL RESEARCH

Toxic chemicals from uncontrolled e-waste recycling: Exposure, body burden, health impact

2021-11-14
Uncontrolled electronic-waste (e-waste) recycling processes have induced serious environmental pollution and human health impacts. This paper reviewed studies on the wide range of toxic chemicals through the use of primitive recycling techniques, their transfer to various ecological compartments, and subsequent health impacts. Results indicated that local food items were heavily polluted by the pollutants emitted, notably heavy metals in vegetables, rice, fish and seafood, and persistent organic pollutants (POPs) in livestock. Dietary exposure is the most important exposure pathway. The associations between exposure to e-waste and high body burdens of these pollutants were evident. It seems apparent that toxic chemicals emitted from e-waste activities are causing a number of major illnesses related to cardiovascular, digestive and respiratory systems, according to the information provided by a local hospital (Taizhou, an e-waste recycling hot spot in China). More epidemiological data should be made available to the general public. It is envisaged that there are potential dangers of toxic chemicals passing on to the next generation via placental transfer and lactation. There is a need to monitor the development and health impacts of infants and children, born and brought up in the e-waste sites.
Authors: Siyi Lin, Muhammad Ubaid Ali, Chunmiao Zheng, Zongwei Cai, Ming Hung Wong
Full Source: Journal of hazardous materials 2021 Nov 14;127792. doi: 10.1016/j.jhazmat.2021.127792.

> Uncontrolled electronic-waste (e-waste) recycling processes have induced serious environmental pollution and human health impacts.

New Models to Predict the Acute and Chronic Toxicities of Representative Species of the Main Trophic Levels of Aquatic Environments

2021-11-19
To assess the impact of chemicals on an aquatic environment, toxicological data for three trophic levels are needed to address the chronic and acute toxicities. The use of non-testing methods, such as predictive computational models, was proposed to avoid or reduce the need for animal models and speed up the process when there are many substances to be tested. We developed predictive models for Raphidocelis subcapitata, Daphnia magna, and fish for acute and chronic toxicities. The random forest machine learning approach gave the best results. The models gave good statistical quality for all endpoints. These models are freely available for use as individual models in the VEGA platform and for prioritization in JANUS software.
Authors: Cosimo Toma, Claudia I Cappelli, Alberto Manganaro, Anna Lombardo, Jürgen Arning, Emilio Benfenati
Full Source: Molecules (Basel, Switzerland) 2021 Nov 19;26(22):6983. doi: 10.3390/molecules26226983.

Environmental Health Risk Evaluation Model for Coastal Chemical Industry

2021-11-10
There are numerous uncertainties associated with environmental health risk assessment (EHRA), and it is unavoidable to apply the best models and information available to save human lives. The EHRA is a method for determining the type and likelihood of adverse health effects on people who are exposed to chemicals in the workplace. To address the environmental health problems caused by harmful gas leakage and water pollution generated by the coastal regional chemical industry, a novel EHRA model for the coastal chemical industry has been developed. The premise of the Gauss plume diffusion model is used to define the model's parameters and the evaluation criterion for harmful gas concentration health risk. The EHRA model is evaluated against the leakage of harmful gases and consists of three steps. The first step is to identify the threat posed by the chemical industry in the coastal region; the second step is to quantify the risk; the third step is to develop a model for assessing water-related environmental health risk. The water-related environmental health assessor analyzes the pollutant variables and parameters of the assessment model to estimate the health risk caused by dangerous

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compounds in the water, using the assessment model of chemical carcinogen health risk and noncarcinogen health risk Type B. The experiments' findings suggest that the model can effectively assess the dangers to human health from hazardous gases and heavy metals in the water bodies of chemical factories in coastal communities.
Authors: Chen Zhao, Yongsheng Zhang, Tong Niu, Melkamu Teshome Ayana
Full Source: Journal of healthcare engineering 2021 Nov 10;2021:6896929. doi: 10.1155/2021/6896929.

Pharmaceuticals in the Environment: Just One Stressor Among Others or Indicators for the Global Human Influence on Ecosystems

2021-11-22
The beneficial use of chemicals in modern human society inevitably leads to their emission into the environment. Pharmaceuticals are crucial for improving and safeguarding public health, whether treating acute infections with historically poor prognoses or increasing the length and quality of our lives by treating chronic conditions such as cardiovascular diseases, cancer, endocrine disorders and improving psychiatric well-being. The use of pharmaceuticals is unlikely to diminish and as such we expect their continuous or even increasing discharge into aquatic and terrestrial environments, predominantly through excretion by patients. This article is protected by copyright. All rights reserved.
Authors: Gerd Maack, Mike Williams, Thomas Backhaus, Laura Carter, Sigrun Kulik, Dean Leverett, Fabiana L Lo Nostro, J Brett Sallach, Jane Staveley, Chris Van den Eede
Full Source: Environmental toxicology and chemistry 2021 Nov 22. doi: 10.1002/etc.5256.

OCCUPATIONAL

Short-Term Acute Exposure to Wildfire Smoke and Lung Function among Royal Canadian Mounted Police (RCMP) Officers

2021-11-10
The increasing incidence of extreme wildfire is becoming a concern for public health. Although long-term exposure to wildfire smoke is associated with respiratory illnesses, reports on the association between short-term occupational exposure to wildfire smoke and lung function

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remain scarce. In this cross-sectional study, we analyzed data from 218 Royal Canadian Mounted Police officers (mean age: 38 ± 9 years) deployed at the Fort McMurray wildfires in 2016. Individual exposure to air pollutants was calculated by integrating the duration of exposure with the air quality parameters obtained from the nearest air quality monitoring station during the phase of deployment. Lung function was measured using spirometry and body plethysmography. Association between exposure and lung function was examined using principal component linear regression analysis, adjusting for potential confounders. In our findings, the participants were predominantly male (71%). Mean forced expiratory volume in 1 s (FEV1), and residual volume (RV) were 76.5 ± 5.9 and 80.1 ± 19.5 (% predicted). A marginal association was observed between air pollution and higher RV [β: 1.55; 95% CI: -0.28 to 3.37 per interquartile change of air pollution index], but not with other lung function indices. The association between air pollution index and RV was significantly higher in participants who were screened within the first three months of deployment (2.80; 0.91 to 4.70) than those screened later (-0.28; -2.58 to 2.03), indicating a stronger effect of air pollution on peripheral airways. Acute short-term exposure to wildfire-associated air pollutants may impose subtle but clinically important deleterious respiratory effects, particularly in the peripheral airways.
Authors: Subhabrata Moitra, Ali Farshchi Tabrizi, Dina Fathy, Samineh Kamravaei, Noushin Miandashti, Linda Henderson, Fadi Khadour, Muhammad T Naseem, Nicola Murgia, Lyle Melenka, Paige Lacy
Full Source: International journal of environmental research and public health 2021 Nov 10;18(22):11787. doi: 10.3390/ijerph182211787.

Body Composition, Anemia, and Kidney Function among Guatemalan Sugarcane Workers

2021-11-02
Rates of anemia among agricultural workers, who are also at risk for kidney injury and chronic kidney disease of unknown cause (CKDu), are unknown. We evaluated body composition through the sum of three skinfolds among 203 male sugarcane cutters and assessed the relationship of variables related to nutrition, anemia (hemoglobin < 13 g/dL), and elevated hemoglobin A1c (HbA1c ≥ 5.7%) with estimated glomerular filtration rate (eGFR) using linear regression. Eleven percent of workers were at the level of essential body fat (2-5%). Anemia was present among 13% of workers, 70% of which were normochromic normocytic, a type of anemia suggesting potential underlying chronic disease. Anemia was more common among those with lower BMI and fat free mass. The

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prevalence of elevated HbA1c was 21%. A moderate negative correlation was found between hemoglobin and HbA1c (Pearson's r = -0.32, p <0.01) which suggests that HbA1c values should be interpreted with caution in populations that have high rates of anemia. Twelve percent of workers had reduced kidney function with an eGFR < 90 mL/min/1.73 m2. On average, the eGFR was 18 mL/min per 1.73 m2 lower [(95% CI:-24, -12), p <0.01)] for those with anemia than those without, and 8 mL/min per 1.73 m2 lower among those with elevated HbA1c [(95% CI: -13, -2), p < 0.01]. Results will inform future studies examining the role of anemia in the evaluation of CKDu and interventions to improve nutrition for workers in low-resource settings.

Authors: Lyndsay Krisher, Jaime Butler-Dawson, Karen Schlosser, Claudia Asensio, Elisa Sinibaldi, Hillary Yoder, Lynn Dexter, Miranda Dally, Daniel Pilloni, Alex Cruz, Diana Jaramillo, Lee S Newman
Full Source: Nutrients 2021 Nov 2;13(11):3928. doi: 10.3390/nu13113928.

PHARAMACEUTICAL/TOXICOLOGY

Association between Maternal Exposure to Chemicals during Pregnancy and the Risk of Foetal Death: The Japan Environment and Children's Study

2021-11-09
Scarce knowledge is available on the relationship between maternal chemical exposure during pregnancy and foetal deaths. We studied the association of spontaneous abortions and stillbirths with occupational or daily maternal exposure to chemicals commonly used by pregnant women. Data from the Japan Environment and Children's Study (JECS), a nationwide prospective birth cohort study, were used. The participants of the study were asked about the frequency of their use of gasoline, pesticides, hair dye, and chlorine bleach during the first and the second to third trimesters of pregnancy. We investigated the relationship between the frequency of the use of chemicals and foetal death. Of the 104,065 foetuses, 923 (0.91%) were spontaneous abortions and 379 (0.37%) were stillbirths. Any type of exposure during the first trimester was not significantly associated with spontaneous abortions. Nevertheless, a more than weekly occupational use of hair dye from the first to the second/third trimester was significantly associated with stillbirth. The results of this study suggest that the frequent use of hair dye during pregnancy can have severe adverse effects on the foetus. These findings can help pregnant

> Scarce knowledge is available on the relationship between maternal chemical exposure during pregnancy and foetal deaths.

women, especially hairdressers, refrain from the continuous use of hair dyes.

Authors: Tadao Ooka, Sayaka Horiuchi, Ryoji Shinohara, Reiji Kojima, Yuka Akiyama, Kunio Miyake, Sanae Otawa, Hiroshi Yokomichi, Zentaro Yamagata, On Behalf Of The Japan Environment And Children's Study Group
Full Source: International journal of environmental research and public health 2021 Nov 9;18(22):11748. doi: 10.3390/ijerph182211748.