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CHEMICAL EFFECTS

Use of (Q)SAR genotoxicity predictions and fuzzy multicriteria decision-making for priority ranking of ethoxyquin transformation products

2021-10-01

Ethoxyquin (EQ; 6-ethoxy-2,2,4-trimethyl-1,2-dihydroquinoline) has been used as an antioxidant in feed for pets and food-producing animals, including farmed fish such as Atlantic salmon. In Europe, the authorization for use of EQ as a feed additive was suspended, due to knowledge gaps concerning the presence and toxicity of EQ transformation products (TPs). Recent analytical studies focusing on the detection of EQ TPs in farmed Atlantic salmon feed and fillets reported the detection of a total of 27 EQ TPs, comprising both known and previously not described EQ TPs. We devised and applied an *in silico* workflow to rank these EQ TPs according to their genotoxic potential and their occurrence data in Atlantic salmon feed and fillet. Ames genotoxicity predictions were obtained applying a suite of five (quantitative) structure-activity relationship ((Q)SAR) tools, namely VEGA, TEST, LAZAR, Derek Nexus and Sarah Nexus. (Q)SAR Ames genotoxicity predictions were aggregated using fuzzy analytic hierarchy process (fAHP) multicriteria decision-making (MCDM). A priority ranking of EQ TPs was performed based on combining both fAHP ranked (Q)SAR predictions and analytical occurrence data. The applied workflow prioritized four newly identified EQ TPs for further investigation of genotoxicity. The fAHP-based prioritization strategy described here, can easily be applied to other toxicity endpoints and groups of chemicals for priority ranking of compounds of most concern for subsequent experimental and mechanistic toxicology analyses.

Authors: J D Rasinger, F Frenzel, A Braeuning, A Bernhard, R Ørnstrud, S Merel, M H G Berntssen

Full Source: Environment international 2021 Oct 1;158:106875. doi: 10.1016/j.envint.2021.106875.

Ethoxyquin (EQ; 6-ethoxy-2,2,4-trimethyl-1,2-dihydroquinoline) has been used as an antioxidant in feed for pets and food-producing animals, including farmed fish such as Atlantic salmon.

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Spatiotemporal distribution, source apportionment and risk assessment of typical hormones and phenolic endocrine disrupting chemicals in environmental and biological samples from the mariculture areas in the Pearl River Delta, China

2021-10-04

The present work studied the levels, distribution, potential sources, ecological and human health risks of typical hormones and phenolic endocrine disrupting chemicals (EDCs) in the mariculture areas of the Pearl River Delta (PRD), China. The environmental levels of 11 hormones (6 estrogens, 4 progestogens, and 1 androgen) and 2 phenolic EDCs were quantified in various matrices including water, sediment, cultured fish and shellfish. Ultrahigh performance liquid chromatography-triple quadrupole tandem mass spectrometry analyses showed that all the 13 target compounds were detected in biotic samples, whereas 10 were detected in water and sediment, respectively. The total concentrations ranged from 35.06-364.53 ng/L in water and 6.31-29.30 ng/g in sediment, respectively. The average contaminant levels in shellfish (*Ostrea gigas*, *Mytilus edulis* and *Mimachlamys nobilis*) were significantly higher than those in fish (*Culter alburnus*, *Ephippus orbis* and *Ephippus orbis*). Source apportionment revealed that the pollution of hormones and phenolic EDCs in PRD mariculture areas was resulted from the combination of coastal anthropogenic discharges and mariculture activities. The hazard quotient values of the contaminants were all less than 1, implying no immediate human health risk. Overall, the present study is of great significance for scientific mariculture management, land-based pollution control, ecosystem protection, and safeguarding human health.

Authors: Yupeng Chen, Haiwen Xie, Muhammad Junaid, Nan Xu, Youchang Zhu, Huchun Tao, Minghung Wong

Full Source: The Science of the total environment 2021 Oct 4;807(Pt 1):150752. doi: 10.1016/j.scitotenv.2021.150752.

The present work studied the levels, distribution, potential sources, ecological and human health risks of typical hormones and phenolic endocrine disrupting chemicals (EDCs) in the mariculture areas of the Pearl River Delta (PRD), China.

[PI3K/Akt/mTOR signal pathway in endocrine disrupting chemicals-induced apoptosis and autophagy of thyroid follicular cells]

2021-09-20

Endocrine disrupting chemicals (EDCs) are a kind of exogenous chemicals widely existing in the environment, which cause serious harm to the environment and human health. At present, the impact

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of this type of substance on the thyroid has attracted much attention. This review summarized the effects of EDCs on thyroid hormones, and phosphatidylinositol 3-kinase (PI3K) /protein kinase B (Akt) /mammalian target of rapamycin (mTOR) (PI3K/Akt/mTOR) signaling pathway and its role in thyroid diseases, and explore the role of PI3K/Akt/mTOR signaling pathway in EDCs-induced apoptosis and autophagy of thyroid follicular epithelial cells. This paper could provide further understandings for thyroid diseases induced by the autophagy and apoptosis of thyroid follicular epithelial cells.

Authors: M Guo, J Xu

Full Source: Zhonghua lao dong wei sheng zhi ye bing za zhi = Zhonghua laodong weisheng zhiyebing zazhi = Chinese journal of industrial hygiene and occupational diseases 2021 Sep 20;39(9):717-720. doi: 10.3760/cma.j.cn121094-20201025-00510.

ENVIRONMENTAL RESEARCH

Point or non-point source: Toxicity evaluation using m-POCIS and zebrafish embryos in municipal sewage treatment plants and urban waterways

2021-10-06

Municipal sewage treatment plants (STPs) have been regarded as an important source of organic contaminants in aquatic environment. To assess the impact of STPs on occurrence and toxicity of STP-associated contaminants in receiving waterways, a novel passive sampler modified from polar organic chemical integrative sampler (m-POCIS) was deployed at the inlet and outlet of a STP and several upstream and downstream sites along a river receiving STP effluent in Guangzhou, China. Eighty-seven contaminants were analyzed in m-POCIS extracts, along with toxicity evaluation using zebrafish embryos. Polycyclic musks were the predominant contaminants in both STP and urban waterways, and antibiotics and current-use pesticides (e.g., neonicotinoids, fiproles) were also ubiquitous. The m-POCIS extracts from downstream sites caused significant deformity in embryos, yet the toxicity could not be explained by the measured contaminants, implying the presence of nontarget stressors. Sewage treatment process substantially reduced embryo deformity, chemical oxygen demand, and contamination levels of some contaminants; however, concentrations of neonicotinoids and fiproles increased after STP treatment, possibly due to the release of chemicals from perturbed sludge. Source identification showed that most of the

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contaminants found in urban waterways were originated from nonpoint runoff, while cosmetics factories and hospitals were likely point sources for musks and antibiotics, respectively. Although the observed embryo toxicity could not be well explained by target contaminants, the present study showed a promising future of using passive samplers to evaluate chemical occurrence and aquatic toxicity concurrently. Zebrafish embryo toxicity significantly decreased after sewage treatment, but higher toxicity was observed for downstream samples, demonstrating that urban runoff may produce detrimental effects to aquatic life, particularly in rainy season. These results highlight the relevance of monitoring nonpoint source pollution along with boosting municipal sewage treatment infrastructure.

Authors: Peihong Xie, Qiankun Yan, Jingjing Xiong, Huizhen Li, Xue Ma, Jing You

Full Source: Environmental pollution (Barking, Essex : 1987) 2021 Oct 6;292(Pt A):118307. doi: 10.1016/j.envpol.2021.118307.

A comparative study on physicochemical properties, pyrolytic behaviour and kinetic parameters of environmentally harmful aquatic weeds for sustainable shellfish aquaculture

2021-09-24

Aquatic weeds pose hazards to aquatic ecosystems and particularly the aquatic environment in shellfish aquaculture due to its excessive growth covering entire freshwater bodies, leading to environmental pollution particularly eutrophication intensification, water quality depletion and aquatic organism fatality. In this study, pyrolysis of six aquatic weed types (wild and cultured species of *Salvinia* sp., *Lemna* sp. and *Spirodella* sp.) were investigated to evaluate its potential to reduce and convert the weeds into value-added chemicals. The aquatic weeds demonstrated high fixed carbon (8.7-47.3 wt%), volatile matter content (39.0-76.9 wt%), H/C ratio (1.5-2.0) and higher heating value (6.6-18.8 MJ/kg), representing desirable physicochemical properties for conversion into biofuels. Kinetic analysis via Coats-Redfern integral method obtained different orders for chemical reaction mechanisms ($n = 1, 1.5, 2, 3$), activation energy (55.94-209.41 kJ/mol) and pre-exponential factor (4.08×10^4 - $4.20 \times 10^{17} \text{ s}^{-1}$) at different reaction zones (zone 1: 150-268 °C, zone 2: 268-409 °C, zone 3: 409-600 °C). The results provide useful information for design

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and optimization of the pyrolysis reactor and establishment of the process condition to dispose this environmentally harmful species.

Authors: Elfina Azwar, Derek Juinn Chieh Chan, Nor Azman Kasan, Hajar Rastegari, Yafeng Yang, Christian Sonne, Meisam Tabatabaei, Mortaza Aghbashlo, Su Shiung Lam

Full Source: Journal of hazardous materials 2021 Sep 24;424(Pt A):127329. doi: 10.1016/j.jhazmat.2021.127329.

Formal waste treatment facilities as a source of halogenated flame retardants and organophosphate esters to the environment: A critical review with particular focus on outdoor air and soil

2021-10-05

Extensive use of halogenated flame retardants (HFRs) and organophosphate esters (OPEs) has generated great concern about their adverse effects on environmental and ecological safety and human health. As well as emissions during use of products containing such chemicals, there are mounting concerns over emissions when such products reach the waste stream. Here, we review the available data on contamination with HFRs and OPEs arising from formal waste treatment facilities (including but not limited to e-waste recycling, landfill, and incinerators). Evidence of the transfer of HFRs and OPEs from products to the environment shows that it occurs via mechanisms such as: volatilisation, abrasion, and leaching. Higher contaminant vapour pressure, increased temperature, and elevated concentrations of HFRs and OPEs in products contribute greatly to their emissions to air, with highest emission rates usually observed in the early stages of test chamber experiments. Abrasion of particles and fibres from products is ubiquitous and likely to contribute to elevated FR concentrations in soil. Leaching to aqueous media of brominated FRs (BFRs) is likely to be a second-order process, with elevated dissolved humic matter and temperature of leaching fluids likely to facilitate such emissions. However, leaching characteristics of OPEs are less well-understood and require further investigation. Data on the occurrence of HFRs and OPEs in outdoor air and soil in the vicinity of formal e-waste treatment facilities suggests such facilities exert a considerable impact. Waste dumpsites and landfills constitute a potential source of HFRs and OPEs to soil, and improper management of waste disposal might also contribute to HFR contamination in ambient air. Current evidence suggests minimal impact of waste incineration plants

Extensive use of halogenated flame retardants (HFRs) and organophosphate esters (OPEs) has generated great concern about their adverse effects on environmental and ecological safety and human health.

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on BFR contamination in outdoor air and soil, but further investigation is required to confirm this.

Authors: Yulong Ma, William A Stubbings, Mohamed Abou-Elwafa Abdallah, Reginald Cline-Cole, Stuart Harrad

Full Source: The Science of the total environment 2021 Oct 5;807(Pt 1):150747. doi: 10.1016/j.scitotenv.2021.150747.

Aging of tire and road wear particles in terrestrial and freshwater environments - A review on processes, testing, analysis and impact

2021-10-05

The environmental fate of tire and road wear particles (TRWPs) receives increasing attention due to the per capita emission volumes of 0.2-5.5 kg/(cap year) and recent reports on the environmental hazard of TRWP constituents. It is expected that aging impacts TRWPs fate in the environment but detailed knowledge is quite limited, yet. Making use of information on tire aging, the available knowledge on environmental aging processes such as thermooxidation, photooxidation, ozonolysis, shear stress, biodegradation and leaching is reviewed here. Experimental techniques to simulate aging are addressed as are analytical techniques to determine aging induced changes of TRWPs, covering physical and chemical properties. The suitability of various tire wear test materials is discussed. Findings and methods from tire aging can be partially applied to study aging of TRWPs in the environment. There is a complex interplay between aging processes in the environment that needs to be considered in future aging studies. In addition to existing basic qualitative understanding of the aging processes, quantitative understanding of TRWP aging is largely lacking. Aging in the environment needs to consider the TRWPs as well as chemicals released. Next steps for filling the gaps in knowledge on aging of TRWPs in the environment are elaborated.

Authors: Stephan Wagner, Philipp Klöckner, Thorsten Reemtsma

Full Source: Chemosphere 2021 Oct 5;132467. doi: 10.1016/j.chemosphere.2021.132467.

The environmental fate of tire and road wear particles (TRWPs) receives increasing attention due to the per capita emission volumes of 0.2-5.5 kg/(cap year) and recent reports on the environmental hazard of TRWP constituents.

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OCCUPATIONAL

Effects of exposure to fine particulate matter on the decline of lung function in rural areas in northwestern China

2021-10-08

Our aim was to clarify the main factors associated with lung function and to analyze the correlation between fine particulate matter (PM_{2.5}) and lung function in a rural Chinese population. We analyzed data of 5195 participants in the China Northwest Natural Population Cohort: Ningxia Project who were ≥ 30 years old. They were recruited from 2018 to 2019, underwent spirometry during the physical examination, and completed a self-report questionnaire. A satellite-based spatiotemporal model was used to estimate the 2-year average PM_{2.5} exposure based on participants' home addresses. A generalized linear mixed model was used to test the relationship between PM_{2.5} concentration and lung function. Sex, age, exposure to cooking oil fumes, and occupational exposure were negatively correlated (P < 0.05) with forced vital capacity (FVC) and forced expiratory volume in 1 s (FEV₁). Educational status, economic level, tea consumption, and alcohol consumption were positively correlated (P < 0.05) with FVC and FEV₁. The adjusted results of each model revealed that FVC and FEV₁ decreased with increased exposure to PM_{2.5}. There was a strong negative correlation between a PM_{2.5} concentration of 35.66 µg/m³ and FVC, FEV₁, and FEV₁/FVC, with unadjusted hazard ratios of - 0.06 [95% confidence interval, - 0.10 to - 0.01], - 0.13 [- 0.17 to - 0.10], and - 22.10 [- 24.62 to - 19.26], respectively. In conclusion, long-term exposure to high concentrations of ambient PM_{2.5} is related to reduce lung function among people in rural areas in northwestern China.

Authors: Di Tian, Xiyuan Chen, Pengyi Hou, Yi Zhao, Yu Zhao, Yajuan Zhang, Jiangping Li, Yuhong Zhang, Faxuan Wang

Full Source: Environmental science and pollution research international 2021 Oct 8. doi: 10.1007/s11356-021-16865-0.

Occupational risk of COVID-19 in the first versus second epidemic wave in Norway, 2020

2021-10

BackgroundThe occupational risk of COVID-19 may be different in the first versus second epidemic wave. AimTo study whether employees in occupations that typically entail close contact with others were at higher risk of SARS-CoV-2 infection and COVID-19-related hospitalisation during

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the first and second epidemic wave before and after 18 July 2020, in Norway. MethodsWe included individuals in occupations working with patients, children, students, or customers using Standard Classification of Occupations (ISCO-08) codes. We compared residents (3,559,694 on 1 January 2020) in such occupations aged 20-70 years (mean: 44.1; standard deviation: 14.3 years; 51% men) to age-matched individuals in other professions using logistic regression adjusted for age, sex, birth country and marital status. ResultsNurses, physicians, dentists and physiotherapists had 2-3.5 times the odds of COVID-19 during the first wave when compared with others of working age. In the second wave, bartenders, waiters, food counter attendants, transport conductors, travel stewards, childcare workers, preschool and primary school teachers had ca 1.25-2 times the odds of infection. Bus, tram and taxi drivers had an increased odds of infection in both waves (odds ratio: 1.2-2.1). Occupation was of limited relevance for the odds of severe infection, here studied as hospitalisation with the disease. ConclusionOur findings from the entire Norwegian population may be of relevance to national and regional authorities in handling the epidemic. Also, we provide a knowledge foundation for more targeted future studies of lockdowns and disease control measures.

Authors: Karin Magnusson, Karin Nygård, Fredrik Methi, Line Vold, Kjetil Telle

Full Source: Euro surveillance : bulletin Européen sur les maladies transmissibles = European communicable disease bulletin 2021 Oct;26(40). doi: 10.2807/1560-7917.ES.2021.26.40.2001875.

PHARMACEUTICAL/TOXICOLOGY

Associations between both legacy and alternative per- and polyfluoroalkyl substances and glucose-homeostasis: The Isomers of C8 health project in China

2021-10-05

Background: Epidemiological studies on the associations of legacy per- and polyfluoroalkyl substances (PFASs) and glucose homeostasis remain discordant. Understanding of PFAS alternatives is limited, and few studies have reported joint associations of PFASs and PFAS alternatives. Objectives: To investigate associations of novel PFAS alternatives (chlorinated perfluoroalkyl ether sulfonic acids, Cl-PFESAs and perfluorobutanoic acid, PFBA) and two legacy PFASs (Perfluorooctanoic acid, PFOA and perfluorooctane sulfonate, PFOS) with glucose-homeostasis

Background: Epidemiological studies on the associations of legacy per- and polyfluoroalkyl substances (PFASs) and glucose homeostasis remain discordant.

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markers and explore joint associations of 13 legacy and alternative PFASs with the selected outcomes.

Methods: We used cross-sectional data of 1,038 adults from the Isomers of C8 Health Project in China. Associations of PFASs and PFAS alternatives with glucose-homeostasis were explored in single-pollutant models using generalized linear models with natural cubic splines for PFASs. Bayesian Kernel Machine Regression (BKMR) models were applied to assess joint associations of exposures and outcomes. Sex-specific analyses were also conducted to evaluate effect modification.

Results: After adjusting for confounders, both legacy (PFOA, PFOS) and alternative (CI-PFESAs and PFBA) PFASs were positively associated with glucose-homeostasis markers in single-pollutant models. For example, in the total study population, estimated changes with 95% confidence intervals (CI) of fasting glucose at the 95th percentile of 6:2CI-PFESA and PFOS against the thresholds were 0.90 (95% CI: 0.59, 1.21) and 0.44 (95% CI: 0.26, 0.62). Positive joint associations were found in BKMR models with 6:2CI-PFESA contributing most. Sex-specific associations existed in both single- and multi-pollutant models.

Conclusions: Legacy and alternative PFASs were positively associated with glucose-homeostasis markers. 6:2CI-PFESA was the primary contributor. Sex-specific associations were also identified. These results indicate that joint associations and effect modification should be considered in risk assessment. However, further studies are recommended to strengthen our findings and to elucidate the mechanisms of action of legacy and alternative PFASs.

Authors: Yun-Ting Zhang, Mohammed Zeeshan, Fan Su, Zheng-Min Qian, Sarah Dee Geiger, Stephen Edward McMillin, Zhi-Bin Wang, Peng-Xin Dong, Yan-Qiu Ou, Shi-Min Xiong, Xu-Bo Shen, Pei-En Zhou, Bo-Yi Yang, Chu Chu, Qing-Qing Li, Xiao-Wen Zeng, Wen-Ru Feng, Yuan-Zhong Zhou, Guang-Hui Dong

Full Source: Environment international 2021 Oct 5;158:106913. doi: 10.1016/j.envint.2021.106913.