CHEMWATCH

Bulletin Board

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CONTACT US

subscribers@chemwatch.net
tel +61 3 9572 4700
fax +61 3 9572 4777

1227 Glen Huntly Rd
Glen Huntly
Victoria 3163 Australia

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SEP. 10, 2021

CHEMICAL EFFECTS

QSAR modelling of inhalation toxicity of diverse volatile organic molecules using no observed adverse effect concentration (NOAEC) as the endpoint

2021-08-27

Nowadays, air pollution due to urbanization and reduction of forestry is emerging as a serious threat to humans and the environment. According to the World Health Organization, respiratory diseases are the third most mortality factor in the world. Chemical research organizations and industries are producing a large number of new chemical compounds continuously. Although toxicity testing of those chemicals on animals is costly, resource and time consuming, these data cannot be properly extrapolated to humans and other animals, and also these raise ethical issues. In this background, we have developed Quantitative Structure-Activity Relationship (QSAR) models using the No Observed Adverse Effect Concentration (NOAEC) as the endpoint to assess inhalation toxicity of diverse organic chemicals, commonly used and exposed by us in our daily life. No Observed Adverse Effect Concentration (NOAEC) can be used for long term toxicity studies towards the human inhalation risk assessment, as recommended by Organization for Economic Co-operation and Development (OECD) in guidance document 39. A particular QSAR model may not be equally effective for prediction of all query compounds from a given set of compounds; therefore, we have developed multiple models, which are robust, sound and well predictive from the statistical point of view to forecast the NOAEC values for the new untested compounds. Subsequently the validated individual models were employed to generate consensus models, in order to improve the quality of predictions and to reduce prediction errors. We have investigated some crucial structural features from these models which may regulate inhalation toxicity for newly produced molecules. Thus, our developed models may help in toxicity assessment towards reducing the health hazards for new chemicals.

Nowadays, air pollution due to urbanization and reduction of forestry is emerging as a serious threat to humans and the environment.

Authors: Aniket Nath, Priyanka De, Kunal Roy

Full Source: Chemosphere 2021 Aug 27;287(Pt 1):131954. doi: 10.1016/j.chemosphere.2021.131954.

Silica encapsulation of ZnO nanoparticles reduces their toxicity for cumulus cell-oocyte-complex expansion

2021-09-03

Background: Metal oxide nanoparticles (NPs) are increasingly used in many industrial and biomedical applications, hence their impact on occupational and public health has become a concern. In recent years, interest on the effect that exposure to NPs may exert on human reproduction has grown, however data are still scant. In the present work, we investigated whether different metal oxide NPs interfere with mouse cumulus cell-oocyte complex (COC) expansion.

Methods: Mouse COCs from pre-ovulatory follicles were cultured in vitro in the presence of various concentrations of two types of TiO2 NPs (JRC NM-103 and NM-104) and four types of ZnO NPs (JRC NM-110, NM-111, and in-house prepared uncoated and SiO2-coated NPs) and the organization of a muco-elastic extracellular matrix by cumulus cells during the process named cumulus expansion was investigated.

Results: We show that COC expansion was not affected by the presence of both types of TiO2 NPs at all tested doses, while ZnO NM-110 and NM-111 induced strong toxicity and inhibited COCs expansion at relatively low concentration. Medium conditioned by these NPs showed lower toxicity, suggesting that, beside ion release, inhibition of COC expansion also depends on NPs per se. To further elucidate this, we compared COC expansion in the presence of uncoated or SiO2-coated NPs. Differently from the uncoated NPs, SiO2-coated NPs underwent slower dissolution, were not internalized by the cells, and showed an overall lower toxicity. Gene expression analysis demonstrated that ZnO NPs, but not SiO2-coated ZnO NPs, affected the expression of genes fundamental for COC expansion. Dosimetry analysis revealed that the delivered-to-cell mass fractions for both NPs was very low. Conclusions: Altogether, these results suggest that chemical composition, dissolution, and cell internalization are all responsible for the adverse effects of the tested NPs and support the importance of a tailored, safer-by-design production of NPs to reduce toxicity.

Authors: Antonella Camaioni, Micol Massimiani, Valentina Lacconi, Andrea Magrini, Antonietta Salustri, Georgios A Sotiriou, Dilpreet Singh, Dimitrios Bitounis, Beatrice Bocca, Anna Pino, Flavia Barone, Valentina Prota, Ivo Iavicoli, Manuel Scimeca, Elena Bonanno, Flemming R Cassee, Philip Demokritou, Antonio Pietroiusti, Luisa Campagnolo

Full Source: Particle and fibre toxicology 2021 Sep 3;18(1):33. doi: 10.1186/s12989-021-00424-z.

Background: Metal oxide nanoparticles (NPs) are increasingly used in many industrial and biomedical applications, hence their impact on occupational and public health has become a concern.

Predicting molecular mechanisms, pathways, and health outcomes induced by Juul e-cigarette aerosol chemicals using the Comparative Toxicogenomics Database

2021-08-05

There is a critical need to understand the health risks associated with vaping e-cigarettes, which has reached epidemic levels among teens. Juul is currently the most popular type of e-cigarette on the market. Using the Comparative Toxicogenomics Database (CTD; http://ctdbase.org), a public resource that integrates chemical, gene, phenotype and disease data, we aimed to analyze the potential molecular mechanisms of eight chemicals detected in the aerosols generated by heating Juul e-cigarette pods: nicotine, acetaldehyde, formaldehyde, free radicals, crotonaldehyde, acetone, pyruvaldehyde, and particulate matter. Curated content in CTD, including chemical-gene, chemical-phenotype, and chemical-disease interactions, as well as associated phenotypes and pathway enrichment, were analyzed to help identify potential molecular mechanisms and diseases associated with vaping. Nicotine shows the most direct disease associations of these chemicals, followed by particulate matter and formaldehyde. Together, these chemicals show a direct marker or mechanistic relationship with 400 unique diseases in CTD, particularly in the categories of cardiovascular diseases, nervous system diseases, respiratory tract diseases, cancers, and mental disorders. We chose three respiratory tract diseases to investigate further, and found that in addition to cellular processes of apoptosis and cell proliferation, prioritized phenotypes underlying Juul-associated respiratory tract disease outcomes include response to oxidative stress, inflammatory response, and several cell signaling pathways (p38MAPK, NIK/NFkappaB, calcium-mediated).

There is a critical need to understand the health risks associated with vaping e-cigarettes, which has reached epidemic levels among teens.

Authors: Cynthia J Grondin, Allan Peter Davis, Jolene A Wiegers, Thomas C Wiegers, Daniela Sciaky, Robin J Johnson, Carolyn J Mattingly

Full Source: Current research in toxicology 2021 Aug 5;2:272-281. doi: 10.1016/j.crtox.2021.08.001.

Characterization of aerosols produced during shampoo use and harmful chemicals in shampoo aerosols

2021-08-31

To declare a shampoo toxicologically safe, one should evaluate the hazards posed by the inhalation of aerosols produced during its use. Herein, tap water was sprayed into a shampoo-filled plastic container to investigate the formation of shampoo aerosols and the possibility of their inhalation. The aerosols thus obtained had higher mass concentrations (geometric

mean = 5779 µg m-3 (PM10) and 2249 µg m-3 (PM2.5)) than water aerosols (geometric mean = 927 µg m-3 (PM10) and 476 µg m-3 (PM2.5)). In particular, shampoo aerosol particles with an aerodynamic diameter of 2.5 µm, which can penetrate the alveoli when inhaled, had the highest mass concentration (geometric mean = 2000 µg m-3). The volatile organic compounds contained in shampoo aerosols featured alcohol and ether groups attached to dodecane and tetradecane backbones; these compounds were generated by the thermal decomposition of surfactants (i.e., lauryl and laureth sulfates) during instrumental analysis. The acquired data suggest that inhalation exposure and chronic inhalation toxicity evaluations should be performed for various shampoo usage conditions to ensure inhalation safety.

Authors: Kim Yong-Hyun, Kyuhong Lee

Full Source: Environmental research 2021 Aug 31;111957. doi: 10.1016/j.envres.2021.111957.

ENVIRONMENTAL RESEARCH

Potential Impacts of Climate Change on the Toxicity of Pesticides towards Earthworms

2021-08-20

This review examined one of the effects of climate change that has only recently received attention, i.e., climate change impacts on the distribution and toxicity of chemical contaminants in the environment. As ecosystem engineers, earthworms are potentially threatened by the increasing use of pesticides. Increases in temperature, precipitation regime changes, and related extreme climate events can potentially affect pesticide toxicity. This review of original research articles, reviews, and governmental and intergovernmental reports focused on the interactions between toxicants and environmental parameters. The latter included temperature, moisture, acidification, hypoxia, soil carbon cycle, and soil dynamics, as altered by climate change. Dynamic interactions between climate change and contaminants can be particularly problematic for organisms since organisms have an upper and lower physiological range, resulting in impacts on their acclimatization capacity. Climate change variables such as temperature and soil moisture also have an impact on acidification. An increase in temperature will impact precipitation which might impact soil pH. Also, an increase in precipitation can result in flooding which can reduce the population of earthworms by not giving juvenile earthworms enough time to develop into reproductive adults. As an independent stressor, hypoxia can affect soil organisms, alter bioavailability, and

This review examined one of the effects of climate change that has only recently received attention, i.e., climate change impacts on the distribution and toxicity of chemical contaminants in the environment.

increase the toxicity of chemicals in some cases. Climate change variables, especially temperature and soil moisture, significantly affect the bioavailability of pesticides in the soil and the growth and reproduction of earthworm species.
Authors: H Kaka, P A Opute, M S Maboeta
Full Source: Journal of toxicology 2021 Aug 20;2021:8527991. doi: 10.1155/2021/8527991.

Juvenile hormone and transcriptional changes in honey bee worker larvae when exposed to sublethal concentrations of thiamethoxam

2021-09-01
Thiamethoxam, an insecticide with high usage and large amounts of environmental residues, has been reported to affect the pupation and survival of honey bee larvae at sublethal concentrations. The molecular mechanisms are not fully understood. In this study, we measured the response of juvenile hormone (JH) to environmental concentrations of thiamethoxam using liquid chromatography-tandem mass spectrometry (LC-MS/MS), monitored the dynamic changes in the transcription of genes encoding major JH metabolic enzymes (CYP15A1, FAMET, JHAMT and JHE) using RT-qPCR, and analysed the transcriptome changes in worker larvae under thiamethoxam stress using RNA-seq. Thiamethoxam significantly increased the levels of JH3 in honey bee larvae, but no significant changes in the transcript levels of the four major metabolic enzymes were observed. Thiamethoxam exposure resulted in 140 differentially expressed genes (DEGs). P450 CYP6AS5 was upregulated, and some ion-related, odourant-related and gustatory receptors for sugar taste genes were altered significantly. The Kyoto Encyclopedia of Genes and Genomes (KEGG) analysis revealed that amino acid metabolism and protein digestion and absorption were influenced by thiamethoxam. These changes may do harm to honey bee caste differentiation, foraging behaviour related to sensory perception and nutrient levels of bee colonies. These results represent the first assessment of the effects of thiamethoxam on JH in honey bee larvae and provides a new perspective and molecular basis for the study of JH regulation and thiamethoxam toxicity to honey bees.
Authors: Honghong Li, Sheng Liu, Lichao Chen, Jie Luo, Dongqiang Zeng, Xuesheng Li
Full Source: Ecotoxicology and environmental safety 2021 Sep 1;225:112744. doi: 10.1016/j.ecoenv.2021.112744.

Thiamethoxam, an insecticide with high usage and large amounts of environmental residues, has been reported to affect the pupation and survival of honey bee larvae at sublethal concentrations.

OCCUPATIONAL

Impact of Heat on Biological Concentrations of Toluene and Acetone Resulting from Exposure by Inhalation: a pilot study

2021-09-01

Climatic conditions raise new concerns about the potential impact of heat on the absorption and kinetics of certain chemicals. The impact of 3 temperatures (21, 25 and 30 °C WBGT) on the toxicokinetics of toluene and acetone was therefore evaluated in five human subjects during controlled exposures in an inhalation chamber. Biological samples were collected and analyzed by GC-MS/MS. Increases between 4 and 85% were observed for solvents concentrations in blood (30 vs 21 °C) while decreases in urine samples for acetone and o-cresol were measured at the end of the exposure period (4 h). Mean blood concentrations at 4 h are well correlated with temperature. Results suggest an increased absorption and/or a decreased elimination of volatile chemicals in the presence of heat. Higher increases of blood chemical concentrations were observed in heavier individuals. Further studies should include physiologically based toxicokinetic models to help in better understanding the mechanisms involved and their respective contribution.

Authors: Axelle Marchand, Jessie Ménard, Pierre Brochu, Sami Haddad

Full Source: Environmental toxicology and pharmacology 2021 Sep 1;103737. doi: 10.1016/j.etap.2021.103737.

Climatic conditions raise new concerns about the potential impact of heat on the absorption and kinetics of certain chemicals.

Analysis of Early Biomarkers Associated With Noise-Induced Hearing Loss Among Shipyard Workers

2021-09-01

Importance: It is important to determine what frequencies and auditory perceptual measures are the most sensitive early indicators of noise-induced hearing impairment. Objectives: To examine whether hearing loss among shipyard workers increases more rapidly at extended high frequencies than at clinical frequencies and whether subtle auditory processing deficits are present in those with extensive noise exposure but little or no hearing loss.

Design, setting, and participants: This cross-sectional study collected audiometric data (0.25-16 kHz), survey questionnaires, and noise exposure levels from 7890 shipyard workers in a Shanghai shipyard from 2015 to 2019. Worsening hearing loss was evaluated in the group with hearing loss. Speech processing and temporal processing were evaluated in 610

participants with noise exposure and clinically normal hearing to identify early biomarkers of noise-induced hearing impairment. Data analysis was conducted from November to December 2020.
Main outcomes and measures: Linear regression was performed to model the increase in hearing loss as function of cumulative noise exposure and compared with a group who were monitored longitudinally for 4 years. Auditory processing tests included speech-in-noise tests, competing sentence tests, dichotic listening tests, and gap detection threshold tests and were compared with a control group without history of noise exposure.
Results: Of the 5539 participants (median [interquartile range (IQR)] age, 41.0 [34.0-47.0] years; 3861 [86.6%] men) included in the cross-sectional analysis, 4459 (80.5%) were hearing loss positive and 1080 (19.5%) were hearing loss negative. In younger participants (ie, ≤40 years), the maximum rate of increase in hearing loss was 0.40 (95% CI, 0.39-0.42) dB per A-weighted dB-year (dB/dBA-year) at 12.5 kHz, higher than the growth rates of 0.36 (95% CI, 0.35-0.36) dB/dBA-year at 4 kHz, 0.32 (95% CI, 0.31-0.33) dB/dBA-year at 10 kHz, 0.31 (95% CI, 0.30-0.31) dB/dBA-year at 6 kHz, 0.27 (95% CI, 0.26-0.27) dB/dBA-year at 3 kHz, and 0.27 (95% CI, 0.27-0.28) dB/dBA-year at 8 kHz. In the 4-year longitudinal analysis of hearing loss among 403 participants, the mean (SD) annual deterioration in hearing was 2.70 (2.98) dB/y at 12.5 kHz, almost twice as that observed at lower frequencies (eg, at 3kHz: 1.18 [2.15] dB/y). The auditory processing scores of participants with clinically normal hearing and a history of noise exposure were significantly lower than those of control participants (eg, median [IQR] score on speech-in-noise test, noise-exposed group 1 vs control group: 0.63 [0.55-0.66] vs 0.78 [0.76-0.80]; P < .001).
Conclusions and relevance: These findings suggest that the increase in hearing loss among shipyard workers was more rapid at 12.5 kHz than at other frequencies; workers with clinically normal hearing but high cumulative noise exposure are likely to exhibit deficits in speech and temporal processing.

Authors: Zhuang Jiang, Jiping Wang, Yanmei Feng, Daoyuan Sun, Xunmiao Zhang, Haibo Shi, Jian Wang, Richard Salvi, Hui Wang, Shankai Yin
Full Source: JAMA network open 2021 Sep 1;4(9):e2124100. doi: 10.1001/jamanetworkopen.2021.24100.

The role of maternal high fat diet on mouse pup metabolic endpoints following perinatal PFAS and PFAS mixture exposure

2021-08-28

Per- and polyfluoroalkyl substances (PFAS) are a family of chemicals that are ubiquitous in the environment. Some of these chemicals, such as perfluorooctanesulfonic acid (PFOS), perfluorohexanesulfonate (PFHxS) and perfluorooctanoic acid (PFOA), are found in human sera and have been shown to cause liver steatosis and reduce postnatal survival and growth in rodents. The purpose of this work is to evaluate the impact of diet and PFAS exposure to mouse dam (mus musculus) on the risk to pup liver and metabolism endpoints later in life, as well as evaluate PFAS partitioning to pups. Timed-pregnant dams were fed a standard chow diet or 60% kcal high fat diet (HFD). Dams were administered either vehicle, 1 mg/kg PFOA, 1 mg/kg PFOS, 1 mg/kg PFHxS, or a PFAS mixture (1 mg/kg of each PFOA, PFOS, and PFHxS) daily via oral gavage from gestation day 1 until postnatal day (PND) 20. At PND 21, livers of dams and 2 pups of each sex were evaluated for lipid changes while remaining pups were weaned to the same diet as the dam for an additional 10 weeks. Dam and pup serum at PND 21 and PND 90 were also evaluated for PFAS concentration, alanine aminotransferase (ALT), leptin and adiponectin, and glycosylated hemoglobin A1c. Perinatal exposure to a HFD, as expected, increased pup body weight, maternal liver weight, pup liver triglycerides, pup serum ALT, and pup serum leptin. PFOA and the PFAS mixture increased liver weights, and. treatment with all three compounds increased liver triglycerides. The maternal HFD increased dam and pup serum PFAS levels, however, was protective against PFOA-induced increase in serum ALT and observed increases in liver triglycerides. The PFAS mixture had very distinct effects when compared to single compound treatment, suggesting some cumulative effects, particularly when evaluating PFAS transfer from dam to pup. This data highlights the importance of diet and mixtures when evaluating liver effect of PFAS and PFAS partitioning.

Authors: Emily S Marques, Juliana Agudelo, Emily M Kaye, Seyed Mohamad Sadegh Modaresi, Marisa Pfohl, Jitka Be□anová, Wei Wei, Marianne Polunas, Michael Goedken, Angela L Slitt

Full Source: Toxicology 2021 Aug 28;152921. doi: 10.1016/j.tox.2021.152921.

Per- and polyfluoroalkyl substances (PFAS) are a family of chemicals that are ubiquitous in the environment.

PHARAMACEUTICAL/TOXICOLOGY

Human health risk assessment of selected pharmaceuticals in the five major river basins, China

2021-08-18

Pharmaceuticals in aquatic environment have raised wide attention in recent years due to their potential adverse effects and bioaccumulation in biota. China has been a major producer and consumer of pharmaceuticals, however, the potential human health risk of these chemicals is yet to be determined in China. In this study, we evaluated available exposure data for twenty pharmaceuticals in surface waters from Chinese five major river basins (the Yangtze, Haihe, Pearl, Songliao, and Yellow River Basins), and human health risk assessment was performed. Based on the concentration data and risk data, we conducted research on the source, cause, and control measures of the pharmaceuticals. The twenty pharmaceuticals were found to be ubiquitous in China with median concentrations between 0.09 and 304 ng/L. The estimated daily intake of pharmaceuticals from drinking water and eating fish was calculated. The intake via drinking water was significantly lower than that via eating fish. The risk quotients via water intake and fish consumption ranged from 0 to 17.2, with estrogen and sulfapyridine highest among the twenty pharmaceuticals. High risks of exposure were mainly in North China, including the Haihe and Songliao River Basins. This is the first analysis in Chinese major river basins that has filled the gaps in the research on the human health risks of pharmaceuticals. The results of the study provide basic information of pharmaceutical intake from drinking water and eating fish in China and provide insights into the risk management guidance of pharmaceuticals, and will facilitate the optimization of health advisories and policy making.

Authors: Chaomeng Dai, Si Li, Yanping Duan, Kah Hon Leong, Yaojen Tu, Lang Zhou

Full Source: The Science of the total environment 2021 Aug 18;801:149730. doi: 10.1016/j.scitotenv.2021.149730.

Pharmaceuticals in aquatic environment have raised wide attention in recent years due to their potential adverse effects and bioaccumulation in biota.