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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

CHEMICAL EFFECTS

Computational Modeling of Mixture Toxicity

2022-01-01

Environmental pollution has become an inevitable problem and a relevant global issue of the twenty-first century. The fast industrial growth has caused the production and release of various chemical species and multicomponent mixtures to the environment which affect the entire living world adversely. Various industrial regulatory agencies are working in this domain to regulate the production of chemical entities, proper release of chemical wastes, and the risk assessment of the industrial and hazardous chemicals; however, they mostly rely upon the single chemical risk assessment instead of considering the toxicity of multicomponent mixtures. In this era of chemical advances, single chemical exposure is a myth. The entire living world is always being exposed to the environmental chemical mixtures but the scarcity of toxicity data of chemical mixtures is a serious concern. The nature of toxicity of mixtures is entirely different and complex from the individual chemicals because of the interactions (synergism/antagonism) among the mixture components. Various regulatory authorities and the scientific world have come up with a handful of methodologies and guidelines for evaluating the harmful effects of the multicomponent mixtures, though there is no such significant, standard, and reliable approach for the toxicity evaluation of chemical mixtures and their management across diverse fields. Toxicity experimentations on laboratory animals are troublesome, time-consuming, costly, and unethical. Thus, to reduce the animal experimentations, the scientific communities, regulatory agencies, and the industries are now depending upon the already proven computational alternatives. The computational approaches are capable of predicting toxicities, prioritizing chemicals, and their risk assessment. Besides these, the in silico methods are cost-effective, less time-consuming, and easy to understand. It has been found out that most of the in silico toxicity predictions are on single chemicals and till date there are very few computational studies available for chemical mixtures in the scientific literature. Therefore, the current chapter illustrates the importance of determination of toxicity of mixtures, the conventional methods for toxicity evaluation of chemical mixtures, and the role of in silico methods to assess the toxicity, followed by the types of various computational methods used for such purpose. Additionally, few successful applications of computational tools in toxicity prediction of mixtures have been discussed in detail. At the end of this chapter, we have discussed some

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future perspectives toward the role and applications of in silico techniques for toxicity prediction of mixtures.

Authors: Mainak Chatterjee, Kunal Roy
Full Source: Methods in molecular biology (Clifton, N.J.) 2022;2425:561-587. doi: 10.1007/978-1-0716-1960-5_22.

ENVIRONMENTAL RESEARCH

Chimpanzee exposure to pollution revealed by human biomonitoring approaches

2022-02-23

Wildlife is increasingly exposed to environmental pollution, but data illustrating to what extent this exposure can impact health and survival of endangered species is missing. In humans, hair matrix analysis is a reliable tool for assessing cumulative exposure to organic pollutants such as pesticides but has rarely been used in other primates for this purpose. LC/MS-MS and GC/MS-MS multi-residue methods were used to screen the presence of 152 organic pollutants and their metabolites belonging to 21 different chemical families in hair samples from our closest relative, the chimpanzee. Samples were collected from 20 wild chimpanzees in Sebitoli, Kibale National Park, Uganda and 9 captive chimpanzees in the Réserve Africaine de Sigean, France. In total, 90 chemicals were detected, 60 in wild chimpanzees and 79 in captive chimpanzees. The median concentrations of detected chemicals in captive individuals were significantly higher than those in wild chimpanzees. Hair from the captive individuals at RAS was sampled a second time after 6 months in an environment of reduced exposure to these pollutants (diet of organic food, decreased use of plastic food and water containers). The number of chemicals detected in captive chimpanzees reduced from 79 to 63, and their concentrations were also significantly reduced. In the present study we report for the first time the use of hair analysis to detect organic pollutants in primate hair. We conclude that both wild and captive chimpanzees are exposed to a large range of different chemicals through their diet. Our study provides surprising and alarming evidence that besides the direct threats of poaching, deforestation and diseases, wild chimpanzees might be endangered by indirect consequences of anthropic activities. As

Wildlife is increasingly exposed to environmental pollution, but data illustrating to what extent this exposure can impact health and survival of endangered species is missing.

chimpanzees are our closest relatives, our results should be considered as an alert for human health as well.
Authors: Sabrina Krief, Alba Iglesias-González, Brice M R Appenzeller, Lyna Rachid, Marielle Beltrame, Edward Asalu, John-Paul Okimat, Nicole Kane-Maguire, Petra Spirhanzlova
Full Source: Ecotoxicology and environmental safety 2022 Feb 23;233:113341. doi: 10.1016/j.ecoenv.2022.113341.

Quantifying Emission Factors and Setting Conditions of Use According to ECHA Chapter R.14 for a Spray Process Designed for Nanocoatings-A Case Study

2022-02-10
Spray coatings' emissions impact to the environmental and occupational exposure were studied in a pilot-plant. Concentrations were measured inside the spray chamber and at the work room in Near-Field (NF) and Far-Field (FF) and mass flows were analyzed using a mechanistic model. The coating was performed in a ventilated chamber by spraying titanium dioxide doped with nitrogen (TiO2N) and silver capped by hydroxyethylcellulose (Ag-HEC) nanoparticles (NPs). Process emission rates to workplace, air, and outdoor air were characterized according to process parameters, which were used to assess emission factors. Full-scale production exposure potential was estimated under reasonable worst-case (RWC) conditions. The measured TiO2-N and Ag-HEC concentrations were 40.9 TiO2-µg/m3 and 0.4 Ag-µg/m3 at NF (total fraction). Under simulated RWC conditions with precautionary emission rate estimates, the worker's 95th percentile 8-h exposure was ≤171 TiO2 and ≤1.9 Ag-µg/m3 (total fraction). Environmental emissions via local ventilation (LEV) exhaust were ca. 35 and 140 mg-NP/g-NP, for TiO2-N and Ag-HEC, respectively. Under current situation, the exposure was adequately controlled. However, under full scale production with continuous process workers exposure should be evaluated with personal sampling if recommended occupational exposure levels for nanosized TiO2 and Ag are followed for risk management.
Authors: Antti Joonas Koivisto, Benedetta Del Secco, Sara Trabucco, Alessia Nicosia, Fabrizio Ravegnani, Marko Altin, Joan Cabellos, Irini Furxhi, Magda Blosi, Anna Costa, Jesús Lopez de Ipiña, Franco Belosi
Full Source: Nanomaterials (Basel, Switzerland) 2022 Feb 10;12(4):596. doi: 10.3390/nano12040596.

Spray coatings' emissions impact to the environmental and occupational exposure were studied in a pilot-plant.

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PHARMACEUTICAL/TOXICOLOGY

Evaluation of the binding performance of flavonoids to estrogen receptor alpha by Autodock, Autodock Vina and Surflex-Dock

2022-02-17
Molecular docking is a widely used method to predict the binding modes of small-molecule ligands to the target binding site. However, it remains a challenge to identify the correct binding conformation and the corresponding binding affinity for a series of structurally similar ligands, especially those with weak binding. An understanding of the various relative attributes of popular docking programs is required to ensure a successful docking outcome. In this study, we systematically compared the performance of three popular docking programs, Autodock, Autodock Vina, and Surflex-Dock for a series of structurally similar weekly binding flavonoids (22) binding to the estrogen receptor alpha (ERα). For these flavonoids-ERα interactions, Surflex-Dock showed higher accuracy than Autodock and Autodock Vina. The hydrogen bond overweighting by Autodock and Autodock Vina led to incorrect binding results, while Surflex-Dock effectively balanced both hydrogen bond and hydrophobic interactions. Moreover, the selection of initial receptor structure is critical as it influences the docking conformations of flavonoids-ERα complexes. The flexible docking method failed to further improve the docking accuracy of the semi-flexible docking method for such chemicals. In addition, binding interaction analysis revealed that 8 residues, including Ala350, Glu353, Leu387, Arg394, Phe404, Gly521, His524, and Leu525, are the key residues in ERα-flavonoids complexes. This work provides reference for assessing molecular interactions between ERα and flavonoid-like chemicals and provides instructive information for other environmental chemicals.
Authors: Qiao Xue, Xian Liu, Paul Russell, Jin Li, Wenxiao Pan, Jianjie Fu, Aiqian Zhang
Full Source: Ecotoxicology and environmental safety 2022 Feb 17;233:113323. doi: 10.1016/j.ecoenv.2022.113323.

Molecular docking is a widely used method to predict the binding modes of small-molecule ligands to the target binding site.

The Effects of E-Cigarette Aerosol on Oral Cavity Cells and Tissues: A Narrative Review

2022-02-06
A wealth of research has comprehensively documented the harmful effects of traditional cigarette smoking and nicotine on human health.

The lower rate of exposure to harmful chemicals and toxic substances offered by alternative electronic smoking devices (e-cigarettes, vaping, etc.) has made these methods of smoking popular, especially among adolescents and young adults, and they are regarded frequently as safer than regular cigarettes. During vaporization of these so-called e-liquids, toxins, carcinogens and various other chemical substances may be released and inhaled by the user. Data on the potential human health effect attendant on exposure to e-vapor are based mainly on animal and in vitro studies. The oral tissues are the first locus of direct interaction with the components of the inhaled vapor. However, the short-term as well as long-term effects of the exposure are not known. The aim of the review is to briefly present data on the effects of the chemical components and toxins of e-cigarette vapor on oral cavity cells and tissues of oral health.

Authors: Paweł Szumilas, Aleksandra Wilk, Kamila Szumilas, Beata Karakiewicz

Full Source: Toxics 2022 Feb 6;10(2):74. doi: 10.3390/toxics10020074.

Effects of co-exposure to multiple metals on children's behavior problems in China

2022-02-22

Exposure to single metals have been linked to childhood behavior problems, But little is known about the effects of metals mixtures on children. We aimed to evaluate associations of multiple metals exposures in urine with childhood behavior in China. For this population-based study, the children eligible for inclusion provided urine samples and their parents agreed to take in-person interview. A total of 831 children were remained from three cities for the final analysis. Urinary metals concentrations were measured by inductively coupled plasma mass spectrometry (ICP-MS). The childhood behavior scores was calculated by the Conners' Parent Rating Scale (CPRS). Variable selection was achieved by the least absolute shrinkage and selection operator (LASSO) regularization and stepwise regression to for all metals in the study. Linear regression models and Bayesian kernel machine regression (BKMR) were applied to estimate the associations of urinary metals concentrations with children's behavior. In BKMR models, the overall effect of mixture was significantly associated with conduct problems, learning problems and hyperactive index when urinary metals concentrations were all above the 50th percentile compared to all of them at their medians. The models also suggested marginally significant interaction effects of Se and Fe as well as Se and Sb (PSe Fe = 0.063; PSe Sb = 0.061), with a decline in estimate of Se on learning problems when Sb/Fe levels were relatively high. The concentrations of 22 metals in boys were higher than girls. In summary, multiple metals are associated with an increased risk of childhood behavioral problems in China. Potential interaction effects of Se and Fe as well as Se and Sb on childhood behavior should be taken into consideration.

Exposure to single metals have been linked to childhood behavior problems, But little is known about the effects of metals mixtures on children.

Authors: Chengcheng Zhang, Danrong Jing, Xiaoyan Huang, Yi Xiao, Zhihao Shu, Dan Luo, Yanying Duan, Meian He, Shuiyuan Xiao, Xiang Chen, Zhijun Huang, Minxue Shen

Full Source: The Science of the total environment 2022 Feb 22;154062. doi: 10.1016/j.scitotenv.2022.154062.

OCCUPATIONAL

Mask-induced skin changes during COVID pandemic: A cross-sectional web-based survey among physicians in a tertiary care teaching hospital

2022-02-25

Background: The COVID pandemic has affected the human race both physically and mentally. Mask use remains the standard way of preventing the spread of this virus. The continuous mask use has led to the emergence of various dermatoses like acne, pigmentation, and seborrhea in mask contact areas. The present survey has been undertaken to describe the various dermatoses encountered in the medical fraternity especially doctors, who are frequently exposed to prolonged mask use. Aims: To estimate the frequency of various cutaneous manifestations seen among doctors following mask use via web-based online questionnaire survey. Methods: It was a cross-sectional web-based study conducted at a tertiary care teaching institute from June 2021 to August 2021. All the doctors of the hospital completing the questionnaire were included in the study with informed consent. Results: A total of 178 participants completed the survey. The most common complaint was increased sweating (55.6%) followed by acne (34.3%) and oily skin (34.3%). Significant association was found between skin changes and duration (>6 h/day) of mask use, increasing number, and type of mask (N 95) used (p value <0.05). Conclusion: The knowledge of various mask-induced/aggravated dermatoses will help

Background:
The COVID pandemic has affected the human race both physically and mentally.

formulate proper precautionary protocols enhancing efficient mask usage for prolonged periods.
Authors: Gaurav Dash, Nibedita Patro, Binayak Chandra Dwari, Kumar Abhisekh
Full Source: Journal of cosmetic dermatology 2022 Feb 25. doi: 10.1111/jocd.14881.

Occurrence of newly identified plasticizers in handwipes; development and validation of a novel analytical method and assessment of human exposure via dermal absorption

2022-02-19
A novel analytical method for the monitoring of four newly identified plasticizers, namely di-propylene glycol dibenzoate (DiPGDB), tri-n-butyl trimellitate (TBTM), isooctyl 2-phenoxyethyl terephthalate (IOPhET) and bis 3,5,5-trimethylhexyl phosphate (TMHPh), in handwipes based on pulverization was developed and in-house validated. In total, 164 handwipe samples (paired with house dust and human urine) were collected during winter (n = 82) and summer (n = 82) 2019 from adults and toddlers living in Flanders, Belgium. Method LOQs ranged from 1 to 200 ng/g. The ranges of Σplasticizers were 70-5400 ng/g for winter and 70-3720 ng/g for summer. The detection frequencies were 39% for DiPGDB, 27% for TBTM and <5% for IOPhET and TMHPh in winter samples and 33% for DiPGDB, 21% for TBTM and <10% for IOPhET and TMHPh in summer ones. The dominant compound in handwipes was DiPGDB, with mean contributions of 74% and 83% for winter and summer, followed by TBTM (24% and 9.2%), TMHPh (1.8% and 8.1%) and IOPhET (<1% and <1%). Σplasticizers concentrations were positively correlated in summer with the use of sanitizer ($r = 0.375$, $p < 0.05$) and negatively correlated in winter with the use of personal care products ($r = -0.349$, $p < 0.05$). DiPGDB was found positively correlated with the age of the participants ($r = 0.363$, $p < 0.05$) and the time spent indoors ($r = 0.359$, $p < 0.05$), indicating indoor environment as a potential source. Levels of TBTM in handwipes were positively correlated with dust samples collected from the same households ($r = 0.597$, $p < 0.05$), and those detected in toddler handwipes were significantly higher compared to adults ($p < 0.05$). Human daily exposure via dermal absorption was evaluated using the dermal derived no effects level values (DNEL), available in the database of the European Chemicals Agency (ECHA) and estimated using the theoretical bio-accessible fractions per compound. Toddler exposure to TBTM was significantly higher compared to adults (T-test, $p < 0.05$). No risk for

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adverse human health effects was derived from the comparison with DNELs for all compounds.
Authors: Christina Christia, Giulia Poma, Noelia Caballero-Casero, Adrian Covaci
Full Source: Environmental research 2022 Feb 19;210:112983. doi: 10.1016/j.envres.2022.112983.

Silicone Wristbands in Exposure Assessment: Analytical Considerations and Comparison with Other Approaches

2022-02-09
Humans are exposed to numerous potentially harmful chemicals throughout their lifetime. Although many studies have addressed this issue, the data on chronic exposure is still lacking. Hence, there is a growing interest in methods and tools allowing to longitudinally track personal exposure to multiple chemicals via different routes. Since the seminal work, silicone wristbands (WBs) have been increasingly used to facilitate human exposure assessment, as using WBs as a wearable sampler offers new insights into measuring chemical risks involved in many ambient and occupational scenarios. However, the literature lacks a detailed overview regarding methodologies being used; a comprehensive comparison with other approaches of personal exposure assessment is needed as well. Therefore, the aim of this review is fourfold. First, we summarize hitherto conducted research that employed silicone WBs as personal passive samplers. Second, all pre-analytical and analytical steps used to obtain exposure data are discussed. Third, we compare main characteristics of WBs with key features of selected matrices used in exposure assessment, namely urine, blood, hand wipes, active air sampling, and settled dust. Finally, we discuss future needs of research employing silicone WBs. Our work shows a variety of possibilities, advantages, and caveats associated with employment of silicone WBs as personal passive samplers. Although further research is necessary, silicone WBs have already been proven valuable as a tool for longitudinal assessment of personal exposure.
Authors: Małgorzata Wacławik, Wojciech Rodzaj, Bartosz Wielgomas
Full Source: International journal of environmental research and public health 2022 Feb 9;19(4):1935. doi: 10.3390/ijerph19041935.

Humans are exposed to numerous potentially harmful chemicals throughout their lifetime.

Occupational exposure to physicians working with a Zero-Gravity™ protection system in haemodynamic and electrophysiology labs and the assessment of its performance against a standard ceiling suspended shield

2022-02-26

A two centre clinical study was performed to analyse exposure levels of cardiac physicians performing electrophysiology and haemodynamic procedures with the use of state of the art Zero-Gravity™ radiation protective system (ZG). The effectiveness of ZG was compared against the commonly used ceiling suspended lead shield (CSS) in a haemodynamic lab. The operator's exposure was assessed using thermoluminescent dosimeters (TLDs) during both ablation (radiofrequency ablation (RFA) and cryoablation (CRYA)) and angiography and angioplasty procedures (CA/PCI). The dosimeters were placed in multiple body regions: near the left eye, on the left side of the neck, waist and chest, on both hands and ankles during each measurement performed with the use of ZG. In total 29 measurements were performed during 105 procedures. To compare the effectiveness of ZG against CSS an extra 80 measurements were performed with the standard lead apron, thyroid collar and ceiling suspended lead shield during CA/PCI procedures. For ZG, the upper values for the average eye lens and whole body doses per procedure were 4 µSv and 16 µSv for the left eye lens in electrophysiology lab (with additionally used CSS) and haemodynamic lab (without CSS), respectively, and about 10 µSv for the remaining body parts (neck, chest and waist) in both labs. The skin doses to hands and ankles non-protected by the ZG were 5 µSv for the most exposed left finger and left ankle in electrophysiology lab, while in haemodynamic lab 150 µSv and 17 µSv, respectively. The ZG performance was 3 times ($p < 0.05$) and at least 15 times ($p < 0.05$) higher for the eye lenses and thoracic region, respectively, compared to CSS (with dosimeters on the apron/collar). However, when only ZG was used slightly higher normalised doses were observed for the left finger compared to CSS (5.88e - 2 Sv/Gym2 vs. 4.31 e - 2 Sv/Gym2, $p = 0.016$). The study results indicate that ZG performance is superior to CSS. It can be simultaneously used with the ceiling suspended lead shield to ensure the protection to the hands as long as this is not obstructive for the work.

Authors: Joanna Domienik-Andrzejewska, Mateusz Mirowski, Marek Jastrzębski, Tomasz Górnik, Konrad Masiarek, Izabela Warchoł, Włodzimierz Grabowicz

Full Source: Radiation and environmental biophysics 2022 Feb 26;1-8. doi: 10.1007/s00411-022-00968-4.

A two centre clinical study was performed to analyse exposure levels of cardiac physicians performing electrophysiology and haemodynamic procedures with the use of state of the art Zero-Gravity™ radiation protective system (ZG).