CHEMWATCH

# Bulletin Board

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## CHEMICAL EFFECTS

### Contact Allergy to Shellac. Retrospective Cross-Sectional Study With Data From the Spanish Registry of Research in Contact Dermatitis and Cutaneous Allergy (REIDAC)

2023-04-06

Introduction: Shellac is a known allergen present mainly in cosmetics used on the eyelids and lips, although new sources of exposure have recently been described. Our objective was to assess the use of shellac as a contact allergen in Spain and the clinical profile of patients allergic to shellac.

Methods: This retrospective cross-sectional study included patients patch tested for shellac between 2018 and 2021 from the Spanish Registry of Contact Dermatitis and Cutaneous Allergy (REIDAC).

Results: A total of 980 patients were patch tested for shellac (20% in ethanol), and 37 (3.77%, 95% confidence interval [CI], 2.58-3.97%) showed positive results. Most of these patients were tested for shellac due to a suspicion of cosmetic contact dermatitis. Seven patients with present relevance were found, five with relation to cosmetics, and the other two with an occupational background of food handling. The reaction index for shellac was 0.51 and the positivity ratio was 67.56% (95% CI, 52.48-82.65%).

Conclusions: Shellac appears to be a prevalent allergen in patients with suspected contact dermatitis related with cosmetics or foodstuff. However, further studies are needed to validate its use in other patients.

Authors: Pedro Mercader-García, Inmaculada Ruiz-Gonzalez, Ricardo Gonzalez-Perez, Tatiana Sanz-Sanchez, Javier Sanchez-Pérez, Leopoldo Borrego, REIDAC

Full Source: Actas dermo-sifiliograficas 2023 Apr 6;S0001-7310(23)00248-X. doi: 10.1016/j.ad.2023.04.010.

### A dynamic inventory database for assessing age-, gender-, and route-specific chronic internal exposure to chemicals in support of human exposome research

2023-04-05

In this study, we proposed a dynamic inventory database to evaluate chronic internal exposure to chemicals at a population level, which enables users to perform modeling exercises specific to a particular chemical, route of exposure, age group, and gender. The database was built based on the steady-state solution of physiologically based kinetic (PBK) models. The biotransfer factors [BTF, the steady-state ratio between

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the chemical concentration in human tissues and the average daily dose (ADD) of the chemical] of 931 organic chemicals in major organs and tissues were simulated for a total of 14 population age groups for males and females. The results indicated that infants and children had the highest simulated BTFs of chemicals, and middle-aged adults had the lowest simulated BTFs. The route-specific analysis of the simulated BTFs indicated that the biotransformation half-life and octanol-water partition coefficient of chemicals had a profound impact on the BTFs. Organ- and chemical-specific results indicated that the biotransfer potential of chemicals in human bodies was primarily determined by bio-thermodynamic variables (e.g., lipid contents). In conclusion, the proposed inventory database can be conveniently used to access chronic internal exposure doses of chemicals by multiplying the route-specific ADD values for different population groups. In future studies, we recommend incorporating human biotransformation data, partition coefficients of ionizable chemicals, age-specific vulnerable indicators (e.g., the degree of maturation of immune systems), physiological variations within the same age group (e.g., intensity of daily physical activities), growth rates (i.e., the dilution effect on chemical biotransfer), and all possible target organs of carcinogenicity (e.g., bladder) into the proposed dynamic inventory database to help promote human exposome research.

Authors: Zijian Li, Jie Xiong

Full Source: Journal of environmental management 2023 Apr 5;339:117867. doi: 10.1016/j.jenvman.2023.117867.

## ENVIRONMENTAL RESEARCH

### Insight into mixed chlorine/chloramines conversion and associated water quality variability in drinking water distribution systems

2023-04-05

Mixed chlorine/chloramines are common in drinking water distribution systems (DWDSs); however, their transformation and impact on chemical and microbial characteristics are not well understood. We systematically investigated water quality parameters associated with mixed chlorine/chloramine species conversion in 192 samples (including raw, finished, and tap water) collected throughout the year in a city in East China. Various chlorine/chloramine species (free chlorine, monochloramine [NH2Cl], dichloramine [NHCl2], and organic chloramines [OC]) were detected in both chlorinated and chloraminated DWDSs. NHCl2 + OC

Mixed chlorine/chloramines are common in drinking water distribution systems (DWDSs); however, their transformation and impact on chemical and microbial characteristics are not well understood.

increased with transport distance along the pipeline network. The maximum proportion of NHCl2 + OC in over total chlorine in tap water reached 66 % and 38 % from chlorinated and chloraminated DWDSs, respectively. Both free chlorine and NH2Cl showed a rapid decay in the water pipe systems, but NHCl2 and OC were more persistent. Correlations between chlorine/chloramine species and physicochemical parameters were established. Models for predicting the sum of chloroform/TCM, bromodichloromethane/BDCM, chlorodibromomethane/CBDM, and bromoform/TBM (THM4) (R2 = 0.56) and haloacetic acids (HAAs) (R2 = 0.65) exhibited greater accuracy based on machine learning tuned with chlorine/chloramine species, particularly NHCl2 + OC. The predominant bacterial communities in mixed chlorine/chloramine systems were those resistant to chlorine or chloramine such as proteobacteria. NH2Cl was the most significant explanatory factor (28.1 %) for the variation in microbial community assemblage in chloraminated DWDSs. Although residual free chlorine and NHCl2 + OC, accounted for a smaller proportion of chlorine species in chloraminated DWDSs, they played an essential role (12.4 % and 9.1 %, respectively) in the microbial community structure.

Authors: Renjie Pan, Tian-Yang Zhang, Zheng-Xiong Zheng, Jian Ai, Tao Ye, Heng-Xuan Zhao, Chen-Yan Hu, Yu-Lin Tang, Jing-Jing Fan, Bing Geng, Bin Xu

Full Source: The Science of the total environment 2023 Apr 5;163297. doi: 10.1016/j.scitotenv.2023.163297.

## Impacts of hydraulic fracturing wastewater from oil and gas industries on drinking water: Quantification of 69 disinfection by-products and calculated toxicity

2023-04-06

Oil and gas production generates large amounts of brine wastewater called “produced water” with various geogenic and synthetic contaminants. These brines are generally used in hydraulic fracturing operations to stimulate production. They are characterized by elevated halide levels, particularly geogenic bromide and iodide. Such salt concentrations in produced water may be as high as thousands of mg/L of bromide and tens of mg/L of iodide. Large volumes of produced water are stored, transported, reused in production operations, and ultimately disposed of by deep well injection into saline aquifers. Improper disposal may potentially contaminate shallow freshwater aquifers and impact drinking water sources. Because conventional produced water treatment typically does not remove halides, produced water contamination of groundwater aquifers may cause the formation of brominated and

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iodinated disinfection by-products (I-DBPs) at municipal water treatment plants. These compounds are of interest because of their higher toxicity relative to their chlorinated counterparts. This study reports a comprehensive analysis of 69 regulated and priority unregulated DBPs in simulated drinking waters fortified with 1 % (v/v) oil and gas wastewater. Impacted waters produced 1.3×-5× higher levels of total DBPs compared to river water after chlorination and chloramination. Individual DBP levels ranged from (<0.1-122 µg/L). Overall, chlorinated waters formed highest levels, including trihalomethanes that would exceed the U.S. EPA regulatory limit of 80 µg/L. Chloraminated waters had more I-DBP formation and highest levels of haloacetamides (23 µg/L) in impacted water. Calculated cytotoxicity and genotoxicity were higher for impacted waters treated with chlorine and chloramine than corresponding treated river waters. Chloraminated impacted waters had the highest calculated cytotoxicity, likely due to higher levels of more toxic I-DBPs and haloacetamides. These findings demonstrate that oil and gas wastewater if discharged to surface waters could adversely impact downstream drinking water supplies and potentially affect public health.

Authors: Dallas G Abraham, Hannah K Liberatore, Md Tareq Aziz, David B Burnett, Leslie H Cizmas, Susan D Richardson

Full Source: The Science of the total environment 2023 Apr 6;163344. doi: 10.1016/j.scitotenv.2023.163344.

## Molecular insights into the dissolved organic matter of leather wastewater in leather industrial park wastewater treatment plant

2023-04-05

Leather wastewater (LW) effluent is characterized by complex organic matter, high salinity, and poor biodegradability. To meet the discharge standards, LW effluent is often mixed with municipal wastewater (MW) before being treated at a leather industrial park wastewater treatment plant (LIPWWTP). However, whether this method efficiently removes the dissolved organic matter (DOM) from LW effluent (LWDOM) remains debatable. In this study, the transformation of DOM during full-scale treatment was revealed using spectroscopy and Fourier transform ion cyclotron resonance mass spectrometry. LWDOM exhibited higher aromaticity and lower molecular weight than DOM in MW (MWDOM). The DOM properties in mixed wastewater (MixW) were similar to those in LWDOM and MWDOM. The MixW was treated using a flocculation/primary sedimentation tank (FL1/PST), anoxic/oxic (A/O) process, secondary sedimentation tank (SST), flocculation/sedimentation tank, denitrification

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filter (FL2/ST-DNF), and an ozonation contact reactor (O3). The FL1/PST unit preferentially removed the peptide-like compounds. The A/O-SST units had the highest removal efficiencies for dissolved organic carbon (DOC) (61.34 %) and soluble chemical oxygen demand (SCOD) (52.2 %). The FL2/ST-DNF treatment removed the lignin-like compounds. The final treatment showed poor DOM mineralization efficiency. The correlation between water quality indices, spectral indices, and molecular-level parameters indicated that lignin-like compounds were strongly correlated with spectral indices and CHOS compounds considerably contributed to the SCOD and DOC. Although the effluent SCOD met the discharge standard, some refractory DOM from LW remained in the effluent. This study illustrates the composition and transformation of DOM and provides theoretical guidance for improving the current treatment processes.

Authors: Xiao-Xu Gao, Yun-Wen Wang, Ye-Chen An, Rui-Yun Ren, Yao-Hui Lin, Ning Wang, Yi-Fan Wang, Jing-Long Han, Zhi-Neng Hao, Jing-Fu Liu, Ai-Jie Wang, Nan-Qi Ren

Full Source: The Science of the total environment 2023 Apr 5;163174. doi: 10.1016/j.scitotenv.2023.163174.

## PHARMACEUTICAL/TOXICOLOGY

### Connections Between Air Pollution, Climate Change & Cardiovascular Health

2023-04-06

Globally, more people die from cardiovascular disease than any other cause.

Globally, more people die from cardiovascular disease than any other cause. Climate change, through amplified environmental exposures, will promote and contribute to many non-communicable diseases including cardiovascular disease. Air pollution, too, is responsible for millions of deaths from cardiovascular disease each year. While they may appear independent, interchangeable relationships and bi-directional cause-effect arrows between climate change and air pollution can eventually lead to poor cardiovascular health. In this topical review we show that climate change and air pollution worsen each other leading to several ecosystem-mediated impacts. We highlight how increases in hot climates as a result of climate change have increased the risk of major air pollution events such as severe wildfires and dust storms. Additionally, we show how altered atmospheric chemistry and changing patterns of weather conditions can promote the formation and accumulation of air pollutants; a phenomenon known as the climate penalty. We demonstrate these amplified environmental exposures and their associations to adverse cardiovascular health outcomes. The community of health professionals, and cardiologists in particular, cannot afford to overlook the risks that climate change and air pollution bring to the public's health.

Authors: Barrak Alahmad, Haitham Khraisha, Khalid Althalji, William Borchert, Fahd Al-Mulla, Petros Koutrakis

Full Source: The Canadian journal of cardiology 2023 Apr 6;S0828-282X(23)00299-4. doi: 10.1016/j.cjca.2023.03.025.

### Lead exposure disturbs ATP7B-mediated copper export from brain barrier cells by inhibiting XIAP-regulated COMMD1 protein degradation

2023-04-04

The brain barrier is an important structure for metal ion homeostasis.

The brain barrier is an important structure for metal ion homeostasis. According to studies, lead (Pb) exposure disrupts the transportation of copper (Cu) through the brain barrier, which may cause impairment of the nervous system; however, the specific mechanism is unknown. The previous studies suggested the X-linked inhibitor of apoptosis (XIAP) is a sensor for cellular Cu level which mediate the degradation of the MURR1 domain-containing 1 (COMMD1) protein. XIAP/COMMD1 axis was thought to be an important regulator in Cu metabolism maintenance. In this study, the role of XIAP-regulated COMMD1 protein degradation in Pb-induced Cu disorders in brain barrier cells was investigated. Pb exposure significantly increased Cu levels in both cell types, according to atomic absorption technology testing. Western blotting and reverse transcription PCR (RT-PCR) showed that COMMD1 protein levels were significantly increased, whereas XIAP, ATP7A, and ATP7B protein levels were significantly decreased. However, there were no significant effects at the messenger RNA (mRNA) level (XIAP, ATP7A, and ATP7B). Pb-induced Cu accumulation and ATP7B expression were reduced when COMMD1 was knocked down by transient small interfering RNA (siRNA) transfection. In addition, transient plasmid transfection of XIAP before Pb exposure reduced Pb-induced Cu accumulation, increased COMMD1 protein levels, and decreased ATP7B levels. In conclusion, Pb exposure can reduce XIAP protein expression, increase COMMD1 protein levels, and specifically decrease ATP7B protein levels, resulting in Cu accumulation in brain barrier cells.

Authors: Yang Liu, Zai-Hua Zhao, Tao Wang, Jin-Yu Yao, Wen-Qing Wei, Li-Hong Su, Shuang-Shuang Tan, Zi-Xuan Liu, Han Song, Jing-Yuan Chen, Wei Zheng, Wen-Jing Luo, Gang Zheng

Full Source: Ecotoxicology and environmental safety 2023 Apr 4;256:114861. doi: 10.1016/j.ecoenv.2023.114861.



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## Amniogenesis in Human Amniotic Sac Embryoids after Exposures to Organophosphate Flame Retardants

2023-04

Background: Amniogenesis is a key event in biochemical pregnancy, and its failure may result in human embryonic death. However, whether and how environmental chemicals affect amniogenesis remain largely unknown.

Objectives: The objective of the present study was to screen chemicals that may disrupt amniogenesis in an amniotic sac embryoid model and to investigate the potential mechanism of amniogenesis failure, with a focus on organophosphate flame retardants (OPFRs).

Methods: This study developed a high-throughput toxicity screening assay based on transcriptional activity of octamer-binding transcription factor 4 (Oct4). For the two positive OPFR hits with the strongest inhibitory activity, we used time-lapse and phase-contrast imaging to assess their effects on amniogenesis. Associated pathways were explored by RNA-sequencing and western blotting, and potential binding target protein was identified through a competitive binding experiment.

Results: Eight positive hits exhibiting Oct4 expression were identified, with 2-ethylhexyl-diphenyl phosphate (EHDPP) and isodecyl diphenyl phosphate (IDDPP) showing the strongest inhibitory activity. EHDPP and IDDPP were found to disrupt the rosette-like structure of the amniotic sac or inhibit its development. Functional markers of squamous amniotic ectoderm and inner cell mass were also found disrupted in the EHDPP- and IDDPP-exposed embryoids. Mechanistically, embryoids exposed to each chemical exhibited abnormal accumulation of phosphorylated nonmuscle myosin (p-MLC-II) and were able to bind to integrin β1 (ITGβ1).

Conclusion: The amniotic sac embryoid models suggested that OPFRs disrupted amniogenesis likely by inhibiting the ITGβ1 pathway, thus providing direct in vitro evidence associating OPFRs with biochemical miscarriage. https://doi.org/10.1289/EHP11958.

Authors: Chenke Xu, Chenhao Zhang, Yanan Liu, Haojia Ma, Feifan Wu, Yingting Jia, Jianying Hu

Full Source: Environmental health perspectives 2023 Apr;131(4):47007. doi: 10.1289/EHP11958.

Background: Amniogenesis is a key event in biochemical pregnancy, and its failure may result in human embryonic death.



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## OCCUPATIONAL

### Bitumen fumes and PAHs in asphalt road paving: Emission characteristics, determinants of exposure and environmental impact

2023-04-06

Background: Asphalt road paving and its subsequent complex airborne emissions have raised concerns about occupational exposures and environmental impacts. Although several studies described bitumen fumes or Polycyclic Aromatic Hydrocarbons (PAH) emissions at specific worksites, no comprehensive studies have characterised road paving emissions and identified the main determinants of exposure.

Methods: A 10-year study from 2012 to 2022 was performed to examine the pollutants resulting from bitumen fume emissions and covering the main processes used in road paving (asphalt production, mechanical rolled asphalt paving, manual paving, mastic asphalt paving, emulsion paving, and coal-tar asphalt milling). A total of 623 air samples were collected at 63 worksites (on 290 workers, in the environment and near emission sources), and bitumen fumes, PAHs, aldehydes and volatile organic compounds were analysed. Biomonitoring campaigns were performed on 130 workers to assess internal exposure to PAHs.

Results: Fume emissions revealed complex mixtures of C10-C30 compounds, including linear saturated hydrocarbons (C6-C12), alicyclic hydrocarbons and aliphatic ketones. PAHs were dominated by 2-3 aromatic ring compounds (naphthalene, fluorene, and phenanthrene), and C1-C13 aldehydes were identified. Binder proportion, paving temperature, outdoor temperature, workload and job category influenced airborne concentrations. A significant temporal trend was observed over the time period of the study, with decreasing BF and PAH exposures. PAH biomonitoring was consistent with air samples, and urinary metabolites of 2-3 ring PAHs dominated over 4-5 ring PAHs. Occupational exposures were generally far lower than exposure limits, except coal-tar asphalt milling activities. Very low environmental concentrations were measured, which highlights a negligible contribution of paving emissions to global environmental pollution. Conclusion: The present study confirmed the complex nature of bitumen fumes and characterised the main determinants of exposure. The results highlight the need to reduce the paving temperature and binder proportion. Recycled asphalt pavement use was not associated with higher emissions. The impact

Background: Asphalt road paving and its subsequent complex airborne emissions have raised concerns about occupational exposures and environmental impacts.

of paving activities on environmental airborne pollution was deemed negligible.
Authors: Julie Germin-Aizac, Anne Maitre, Franck Balducci, Sarah Montlevier, Marie Marques, Justine Tribouiller, Christine Demeilliers, Renaud Persoons
Full Source: Environmental research 2023 Apr 6;115824. doi: 10.1016/j.envres.2023.115824.

## Review of Antimicrobial Nanocoatings in Medicine and Dentistry: Mechanisms of Action, Biocompatibility Performance, Safety, and Benefits Compared to Antibiotics

2023-04-07
This review discusses topics relevant to the development of antimicrobial nanocoatings and nanoscale surface modifications for medical and dental applications. Nanomaterials have unique properties compared to their micro- and macro-scale counterparts and can be used to reduce or inhibit bacterial growth, surface colonization and biofilm development. Generally, nanocoatings exert their antimicrobial effects through biochemical reactions, production of reactive oxygen species or ionic release, while modified nanotopographies create a physically hostile surface for bacteria, killing cells via biomechanical damage. Nanocoatings may consist of metal nanoparticles including silver, copper, gold, zinc, titanium, and aluminum, while nonmetallic compounds used in nanocoatings may be carbon-based in the form of graphene or carbon nanotubes, or composed of silica or chitosan. Surface nanotopography can be modified by the inclusion of nanoprotrusions or black silicon. Two or more nanomaterials can be combined to form nanocomposites with distinct chemical or physical characteristics, allowing combination of different properties such as antimicrobial activity, biocompatibility, strength, and durability. Despite their wide range of applications in medical engineering, questions have been raised regarding potential toxicity and hazards. Current legal frameworks do not effectively regulate antimicrobial nanocoatings in matters of safety, with open questions remaining about risk analysis and occupational exposure limits not considering coating-based approaches. Bacterial resistance to nanomaterials is also a concern, especially where it may affect wider antimicrobial resistance. Nanocoatings have excellent potential for future use, but safe development of antimicrobials requires careful consideration of the "One Health" agenda, appropriate legislation, and risk assessment.
Authors: James Butler, Richard D Handy, Mathew Upton, Alexandros Besinis
Full Source: ACS nano 2023 Apr 7. doi: 10.1021/acsnano.2c12488.

This review discusses topics relevant to the development of antimicrobial nanocoatings and nanoscale surface modifications for medical and dental applications.