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CHEMICAL EFFECTS

Unveiling chemical space, scaffold diversity, critical structural features of pesticides: A comprehensive QSAR, qRASAR, machine learning studies to predict pesticides toxicity

2025-09-19

The increasing use of pesticides in agriculture and urban areas has led to significant contamination of aquatic ecosystems, posing risks to non-target species. Fish, particularly the rainbow trout (Oncorhynchus mykiss), are highly vulnerable due to their gill permeability and ecological importance. As a sensitive and globally distributed species, rainbow trout serves as a key model in ecotoxicological studies and environmental monitoring. Here, a comprehensive cheminformatics workflow was employed to investigate the structural diversity and predictive modeling of a series of pesticides having acute aquatic toxicity to O. mykiss. The chemical space of these pesticides was explored through the Structure-Similarity Activity Trailing (SimilACTrail) map, revealing high structural uniqueness among pesticides, with several clusters exhibiting 80.0 %-90.3 % singleton ratios. A machine learning (ML) classifier model was developed using optimized hyperparameters, achieving robust predictive performance. Additionally, integrating Quantitative Structure-Activity Relationship (QSAR) and quantitative Read-Across Structure-Activity Relationship (q-RASAR) strategies enabled the construction of statistically reliable and mechanistically interpretable models, followed by toxicity data gap filling of 2000+ pesticides from external data sources. This integrated approach provides valuable insights into the structure-activity relationships (SARs) of pesticides and offers a predictive framework for future pesticide prioritization and environmental risk assessment. Developed q-RASAR model also provide an interpretable and reproducible alternative to fish testing, supporting regulatory prioritization efforts under USEPA and ECHA frameworks. At the same time, we recognize the limitations of the present work, including its focus solely on acute rainbow trout toxicity, potential uncertainty for structurally novel pesticides, and exclusion of chronic and mixture toxicity endpoints.

Authors: Supratik Kar, Sk Abdul Amin, Lu Li

Full Source: The Science of the total environment 2025 Sep 19:1001:180489. doi: 10.1016/j.scitotenv.2025.180489.

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Evaluation of the pollution pressures posed by groups of chemicals on British riverine invertebrate populations

2025-09-21

Globally, rivers receive a diverse range of chemicals, including metals, pesticides, persistent organic pollutants, petrochemicals, human and veterinary pharmaceuticals and personal care products. However, the extent to which these different chemical groups affect riverine invertebrate communities is not well defined. Here we set out to evaluate the available evidence for associations between British riverine invertebrate communities and different chemical groups (and individual members of these chemical groups). Our assessment comprised three elements, (i) an evaluation of whether environmental concentrations of these chemicals exceed the lowest effect concentrations (ECs) based on laboratory tests, (ii) an assessment of associations between chemical groups and changes in British riverine invertebrate communities using the existing published literature, and (iii) calculated potential risk of toxicity of the chemical groups to invertebrates based on measured exposures (Environmental Agency monitoring data) and laboratory-based measurements of the lethal concentration required to kill half of the tested population (LC50). Our conclusions indicate that metal and pesticide pollutants (including the veterinary medicine fipronil) are of greatest concern for British riverine invertebrate communities. Petrochemicals were also of potential concern, however, risk calculations indicate this risk is lower than that for metals and pesticides. All other chemical groups assessed appeared to be of relatively low risk to British riverine invertebrates based on the available information. However, the concentrations of some pharmaceuticals and personal care products in British rivers exceeded the lowest ECs for some invertebrate species and require further investigation. Given the widespread concern regarding declines in freshwater invertebrates, studies on chemical impacts on invertebrate populations in British rivers are surprisingly limited and further targeted studies are warranted.

Authors: Imogen P Poyntz-Wright, Xavier A Harrison, Charles R Tyler

Full Source: Biological reviews of the Cambridge Philosophical Society 2025 Sep 21. doi: 10.1111/brv.70075.

Globally, rivers receive a diverse range of chemicals, including metals, pesticides, persistent organic pollutants, petrochemicals, human and veterinary pharmaceuticals and personal care products.

Oxidative potential and cellular toxicity of carbonaceous aerosols undergoing aging in an atmospheric simulation chamber

2025-09-17

This study investigates how chemical composition, atmospheric aging, and environmental conditions affect the oxidative potential (OP) and cellular toxicity of soot particles using an atmospheric simulation chamber (ASC). In the ASC ChAMBRe were simulated real-world summer and winter scenarios, exposing pure soot particles (generated by using the mini-inverted soot generator) and various secondary aerosol precursors (i.e., toluene, 2,5-dimethylfuran and α-pinene) alternatively to light or dark conditions and different oxidants. OP was assessed using multiple assays (namely, 2',7'-dichlorofluorescein - DCFH, Dithiothreitol - DTT and Ascorbic Acid - AA), revealing that soot particles exposed to light, especially in presence of toluene, exhibited higher OP. The presence of toluene also increased cellular reactive oxygen species (ROS) production, leading to elevated cytotoxicity, DNA damage, and release of the proinflammatory cytokine interleukin-8 (IL-8) in BEAS-2B cells. Ammonium sulfate addition reduced OP and do not enhance toxicological responses, suggesting that non-toxic components in aged particulate matter (PM) may mitigate some harmful effects. Toxicological assessment showed increased cytotoxicity, genotoxicity, oxidative stress, and inflammatory responses in soot generated under high irradiance conditions typical of summer and traffic environments, compared to low irradiance winter scenarios. Strong correlations were observed between OP and toxicological endpoints, such as ROS formation, LDH release, micronuclei formation, and IL-8 secretion underscoring the role of chemical composition and environmental aging in determining PM toxicity. The study highlights OP assays as a reliable tool for predicting PM-induced oxidative stress and potential health effects, emphasizing the importance of considering soot chemical composition and aging processes in urban air pollution assessments.

Authors: Virginia Vernocchi, Marco Brunoldi, Silvia Canepari, Emanuela Corsini, Tommaso Isolabella, Lorenzo Massimi, Federico Mazzei, Gloria Melzi, Marco Paglione, Sofia Pantaleoni, Paolo Prati, Marco Rapuano, Matteo Rinaldi, Caterina Tiraboschi, Dario Massabò

Full Source: Toxicology and applied pharmacology 2025 Sep 17:505:117573. doi: 10.1016/j.taap.2025.117573.

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ENVIRONMENTAL RESEARCH

Assessment of potentially toxic elements (PTEs) in surface and groundwater of volcanic and granite regions of Hainan Island, China: Pollution status, sources, and health risk evaluation

2025-09-20

The safety of water resources in regions with naturally high geochemical backgrounds of potentially toxic elements (PTEs) represents a critical environmental issue. This study investigates the concentrations, sources, and health risks of PTEs in surface water and groundwater from volcanic and granite regions of Hainan Island, China. A total of 58 surface water and 26 groundwater samples were collected from the volcanic region, along with 22 surface water samples from the granite region. Ten PTEs (As, Cd, Pb, Se, Hg, B, Cr, I, Mo, and F) were analyzed using a combination of atomic fluorescence spectrometry (AFS), inductively coupled plasma mass spectrometry (ICP-MS), ion-selective electrode method (ISE), and catalytic spectrophotometry (COL). The results showed that surface water generally contained low PTE concentrations, remaining below national regulatory thresholds, whereas groundwater in the volcanic region exhibited significantly elevated levels of As (up to 59 μg/L) and Cr (up to 23.4 μg/L). Pollution index (PI) results indicated that 15.4% of groundwater samples exceeded the acceptable limit for As. Health risk assessments revealed that while non-carcinogenic risks were generally low, arsenic in groundwater posed potential health concerns for children (HQ approaching 1). Carcinogenic risk assessment further identified As and Cr in groundwater as the dominant contributors, with total cancer risk values exceeding the acceptable limit (> 1.0 × 10- 4), reaching 3.67 × 10- 3 for adults and 4.37 × 10- 3 for children. These findings demonstrate the combined influence of geological and anthropogenic factors on groundwater quality in volcanic regions and underscore the urgent need for targeted monitoring and region-specific water safety strategies in Hainan.

Authors: Jianzhou Yang, Yong Li, Shengyue Liang, Min Zhang, Jingjing Gong, Yufang Li, Qiankun Yan, Xiaohui Sun, Zuyang Xu, Xueju Liu, Shuqi Hu, Jianweng Gao, Zhenliang Wang, Liling Tang

Full Source: Environmental geochemistry and health 2025 Sep 20;47(10):447. doi: 10.1007/s10653-025-02757-6.

The safety of water resources in regions with naturally high geochemical backgrounds of potentially toxic elements (PTEs) represents a critical environmental issue.

Degradation of PVDF in photocatalytic membranes in gaseous environments

2025-09-17

Poly(vinylidene fluoride) (PVDF) and poly(vinylidene fluoride-co-hexa-fluoropropylene) (PVDF-HFP) are fluoropolymers used for applications including, but not limited to, immobilization of photocatalytic materials for water and air purification due to its high resistance to ultraviolet (UV) exposure and extreme environmental conditions. The stability of these fluoropolymers in combination with titanium dioxide (TiO2) nanopowder was investigated. Membranes were prepared using the phase inversion method. Fourier transform infrared spectroscopy (FT-IR) and X-ray photoelectron spectroscopy (XPS) analysis after 21 h of intense UV exposure showed a degradation of both PVDF and PVDF-HFP. A decrease in PVDF(-HFP) absorbance relative to TiO2 absorbance in the FT-IR spectra, a decrease of the F (1s) peak and a significant increase of the Ti (2p) peaks in the XPS spectra were observed. It was demonstrated that this degradation results from reaction with TiO2 upon UV exposure. Gas analysis using a quadrupole mass spectrometer (QMS) strongly indicated the gradual formation and subsequent conversion of (highly toxic) carbonic difluoride CF2O, reaching a maximal concentration after 2.5 h and a full removal after 10 h of UV exposure. A strong indication of the production of carbon dioxide (CO2) and tetrafluoromethane (CF4) as end products was obtained.

Authors: Ewoud Cosaert, Hadis Mortazavi Milani, Geraldine J Heynderickx, Dirk Poelman

Full Source: Journal of hazardous materials 2025 Sep 17:498:139576. doi: 10.1016/j.jhazmat.2025.139576.

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PHARMACEUTICAL/TOXICOLOGY

Environmental cadmium exposure promotes lung cancer via DHX34: A molecular toxicology perspective

2025-09-19

Although cadmium (Cd) exposure has been implicated in lung cancer development, systematic investigations into its association with cancer mortality, particularly lung cancer mortality remain limited, and the molecular mechanisms driving Cd-induced tumor progression are not fully understood. In this study, we first conducted a meta-analysis of existing cohort studies to quantitatively assess the association between Cd exposure and cancer- and lung cancer-specific mortality. We then employed an integrative approach combining bioinformatics analyses, LASSO regression, and Mendelian randomization to identify and validate DHX34 as a key gene implicated in Cd-related lung carcinogenesis. These findings were further supported by molecular docking, molecular dynamics simulations, in vitro functional assays, and in vivo tumor models. Our meta-analysis showed that long-term Cd exposure significantly increased cancer mortality risk, especially in males (RR = 1.49, 95 % CI: 1.13-1.96) and in lung cancer (RR = 1.86, 95 % CI: 1.36-2.54). Integration of GSE165549 and TCGA data identified 36 Cd-related genes enriched in tumor associated pathways including cell cycle and DNA replication. LASSO regression and Mendelian randomization suggested a causal role of DHX34 in lung cancer. Molecular docking demonstrated a strong binding affinity between Cd2 + and DHX34 (binding free energy = -5.34

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kcal/mol), and molecular dynamics simulations confirmed the stability of this complex. Functional assays further showed that CdCl2 exposure upregulated DHX34, thereby promoting lung cancer cell proliferation and tumor growth both in vitro and in vivo. Together, these findings provide multi-level evidence that DHX34 mediates Cd-induced lung cancer progression, highlighting the carcinogenic potential of environmental heavy metal exposure and offering new insights into molecular targets for early prevention, risk stratification, and therapeutic intervention.
Authors: Yongbin Lu, Weize Kong, Kaiwen Wang, Zicong Shao, Xu Hui, Xuping Song, Siyu Zhang, Li Ma, Zhiyuan Cheng, Fei Su, Tao Zhang, Kehu Yang
Full Source: Ecotoxicology and environmental safety 2025 Sep 19:304:119087. doi: 10.1016/j.ecoenv.2025.119087.

Dysregulation of Immune Checkpoint LAG3 in Mice Exposed to Silica

2025-09-18
Silica exposure can cause silicosis, and its pathogenesis is not fully understood. This study investigates the role of immune checkpoint lymphocyte activation gene 3 (LAG3) in silicosis. Mice were intratracheally exposed to silica, and tissues were collected and analyzed after 7 and 28 days. Additionally, peripheral blood samples were also collected from silicosis patients. The mRNA and protein expression levels of LAG3 in various tissues were quantified using qRT-PCR and western blot techniques. The localization of LAG3 in the lung, spleen, thymus and hilar lymph nodes was visualized by immunochemistry. Our data showed that silica exposure induced systemic changes in LAG3 expression in an organ-specific manner. In mouse lungs, LAG3 levels were significantly upregulated after silica exposure. In mouse spleen, LAG3 expression changed only during early stage of silica exposure. In mouse thymus, the level of LAG3 decreased during early stage of silica exposure but reversed to increase during late stage. In mouse hilar lymph nodes, expression of LAG3 increased significantly. A marked increase in the concentration of soluble LAG3 was observed in the plasma of mice exposed to silica. Plasma soluble LAG3 levels in silicosis patients were found to be significantly higher than healthy controls. These findings suggest that LAG3 may be involved in the pathogenesis of silicosis and that immune disorders in lung tissue may further affect systemic immune homeostasis.
Authors: Meixiu Duan, Youliang Zhao, Yaqian Qu, Changfu Hao, Wu Yao
Full Source: Toxicology letters 2025 Sep 18:111729. doi: 10.1016/j.toxlet.2025.111729.

Silica exposure can cause silicosis, and its pathogenesis is not fully understood.

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Oral exposure to tire rubber-derived contaminant 6PPD and 6PPD-quinone induces intestinal toxicity in mice

2025-09-19

Oral exposure to tire rubber-derived contaminant 6PPD and 6PPD-quinone induces intestinal toxicity in mice

2025-09-19
N-(1,3-dimethylbutyl)-N′-phenyl-p-phenylenediamine (6PPD) is a commonly used rubber protectant that continuously enters the environment via groundwater. Its oxidation product, N-(1,3-dimethylbutyl)-N′-phenyl-p-phenylenediamine quinone (6PPDQ), has garnered significant concern due to its reported toxicity in animals. This study aims to evaluate the intestinal toxicity and potential metabolic impact of 6PPD and 6PPDQ in mice following oral exposure to various doses. Our results demonstrate that both compounds compromise the intestinal barrier, as evidenced by significant increases in the expression of tight junction proteins (claudin-1 and occludin) and mucin protein (MUC2). These changes suggest an impairment of both the physical and chemical barriers of the intestine. Following exposure, there was a marked increase in pro-inflammatory cytokines (IL-6, IL-22, and NOD-1), indicating an inflammatory response associated with the disruption of lipid metabolism and macrophage polarization. Specifically, the shift from M2 to M1 macrophage polarization correlates with increased expression of M1 markers despite no change in the M1/M2 ratio over prolonged exposure. Furthermore, 6PPD exposure significantly reduced gut microbiota richness and evenness, with more pronounced changes observed in the 6PPDQ-treated group. Correlation analysis suggested that these microbial shifts may influence host carnitine and lipid metabolism pathways. Ultimately, both 6PPD and 6PPDQ exposure led to elevated levels of total cholesterol (TC), triglycerides (TG), and low-density lipoprotein (LDL) in the bloodstream, attributed to decreased TC esterification. These findings highlight the potential long-term health risks associated with environmental exposure to 6PPD and 6PPDQ, particularly concerning gut integrity and metabolic dysregulation. SYNOPSIS: This study investigates the toxicity of 6PPD and its transformation product 6PPDQ, revealing their detrimental effects on intestinal health, disruption of gut microbiota, and

Oral exposure to tire rubber-derived contaminant 6PPD and 6PPD-quinone induces intestinal toxicity in mice

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alterations in lipid metabolism, highlighting significant implications for both environmental and human health.
Authors: Liya Fang, Jinhua Xu, Chanlin Fang, Yuanxiang Jin
Full Source: Toxicology 2025 Sep 19:518:154285. doi: 10.1016/j.tox.2025.154285.

OCCUPATIONAL

Associations of ambient exposure to benzene, toluene, ethylbenzene, and xylene with daily mortality: a multicountry time-series study in 757 global locations

2025-09-16

Background: The presence of benzene, toluene, ethylbenzene, and xylene isomers (BTEX) in the environment is of increasing concern due to their toxicity and ubiquity. Although the adverse health effects of BTEX exposure have been documented, robust epidemiological evidence from large-scale, multicountry studies using advanced exposure assessment methodologies remains scarce. We aimed to assess the association of short-term ambient exposure to individual BTEX components and their mixture with daily total, cardiovascular, and respiratory mortality on a global scale.

Methods: Daily data on mortality, meteorological factors, and air pollution were collected from 757 locations across 46 countries or regions. Data on individual chemicals (ie, benzene, toluene, xylenes [summation of ethylbenzene, m-xylene, p-xylene, and o-xylene]) and the aggregate mixture (ie, BTEX) were estimated using a chemistry-climate model. We examined the short-term associations of each individual chemical as well as the BTEX mixture with daily total, cardiovascular, and respiratory mortality in a multicountry framework. Using a two-stage time-series design, we first applied generalised additive models with a quasi-Poisson distribution to obtain location-specific associations, which were subsequently pooled using random-effects meta-analysis. Two-pollutant models were used to assess the independent effects of BTEX after adjusting for co-pollutants (PM2·5, PM10, nitrogen dioxide, sulphur dioxide, ozone, and carbon monoxide). Additionally, we assessed the overall exposure-response curves with spline terms.

Findings: An IQR increment of BTEX concentration on lag 0-2 days (3-day moving average of the present day and the previous 2 days) was associated with increases of 0·57% (95% CI 0·49-0·65), 0·42% (0·30-0·54), and 0·68% (0·50-0·86) in total, cardiovascular, and respiratory mortality,

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respectively. The corresponding effect estimates for an IQR increment in individual chemicals (benzene, toluene, and xylenes) were 0·38-0·61%, 0·44-0·70%, and 0·41-0·65%, respectively. The associations remained significant after adjusting for co-pollutants, with a general decline in magnitude, except for a slight increase after adjustment for ozone. The shape of the exposure-response curves for all pollutants and causes of death was almost linear, with steeper slopes at low concentrations and no discernible thresholds.

Interpretation: This global study provides novel evidence linking short-term exposure to ambient BTEX, both individually and as a mixture, with increased daily total, cardiovascular, and respiratory mortality. Our findings underscore the need for comprehensive air pollution mitigation policies, including stringent controls on BTEX emissions, to protect public health.

Funding: Noncommunicable Chronic Diseases-National Science and Technology Major Project, National Natural Science Foundation of China, Shanghai Municipal Science and Technology Major Project, Shanghai B&R Joint Laboratory Project, and Shanghai International Science and Technology Partnership Project.

Authors: Lu Zhou, Ying Xiong, Francesco Sera, Ana Maria Vicedo-Cabrera, Rosana Abrutzky, Yuming Guo, Shilu Tong, Micheline de Sousa Zanotti Stagliorio Coelho, Paulo Hilario Nascimento Saldiva, Eric Lavigne, Patricia Matus Correa, Nicolás Valdés Ortega, Samuel Osorio, Dominic Roye, Jan Kyselý, Hans Orru, Marek Maasikmets, Jouni J K Jaakkola, Niilo Ryti, Mathilde Pascal, Veronika Huber, Susanne Breitner-Busch, Alexandra Schneider, Klea Katsouyanni, Evangelia Samoli, Alireza Entezari, Fatemeh Mayvaneh, Patrick Goodman, Ariana Zeka, Raanan Raz, Matteo Scortichini, Massimo Stafoggia, Yasushi Honda, Masahiro Hashizume, Chris Fook Sheng Ng, Barrak Alahmad, Magali Hurtado Diaz, Eunice Elizabeth Félix Arellano, Ala Overcenco, Jochem Klompmaker, Shilpa Rao, Gabriel Carrasco, Xerxes Seposo, Paul Lester Carlos Chua, Susana das Neves Pereira da Silva, Joana Madureira, Iulian-Horia Holobaca, Noah Scovronick, Rebecca M Garland, Ho Kim, Whanhee Lee, Aurelio Tobias, Carmen Íñiguez, Bertil Forsberg, Martina S Ragettli, Yue Leon Guo, Shih-Chun Pan, Shanshan Li, Pierre Masselot, Valentina Colistro, Michelle Bell, Antonella Zanobetti, Joel Schwartz, Tran Ngoc Dang, Do Van Dung, Antonio Gasparrini, Yaoxian Huang, Haidong Kan
Full Source: The Lancet. Planetary health 2025 Sep 16:101306. doi: 10.1016/j.lanplh.2025.101306.