IECTO 2024 Conference

The 1st International Electronic Conference on Toxics

20–22 March 2024 | Online

Program and Abstract Book

Organizers

MDPI Academic Open Access Publishing since 1996

toxics

Media Partners

biology

pharmaceuticals

antioxidants

water

pollutants

CONFERENCE locate.com

CONFERENCE2GO

学术会议云 ALLCONFS.ORG

VEGAHUB

The 1st International Electronic Conference on Toxics

20–22 March 2024 | Online

MDPI

Basel • Beijing • Wuhan • Barcelona • Belgrade • Novi Sad • Cluj • Manchester

Organizing Committees

Conference Chair

Dr. Demetrio Raldúa

Session Chairs

Prof. Dr. Qixing Zhou
Prof. Dr. Yankai Xia
Prof. Dr. Virgínia Cruz Fernandes
Dr. Natalia Garcia-Reyero
Prof. Dr. Youssef Sari

Scientific Committees

Prof. Dr. Xiaojun Luo
Prof. Dr. Sijie Lin
Dr. Louis A. Tremblay
Prof. Dr. João Fernando Pereira Gomes
Dr. Wanli Ma
Dr. Jose V. Tarazona
Prof. Dr. Qing Huang
Dr. Daniel Drage
Prof. Dr. Fayuan Wang
Dr. Catarina Cruzeiro
Dr. Gunnar Toft
Dr. Eduardo V. Soares
Dr. Minjian Chen
Dr. Jamie Dewitt
Prof. Dr. Emilio Benfenati
Dr. Joel Ferreira De Brito
Dr. Noel Aquilina
Prof. Dr. Qi Wang
Prof. Dr. Karina Boltes
Dr. Nikiforos Alygizakis

Organised by

MDPI
Academic Open Access Publishing
since 1996

Conference Secretariat

Email: iecto2024@mdpi.com

Welcome from the Chair

Dear Colleagues,

On behalf of the MDPI journal *Toxics* (ISSN: 2305-6304; Impact Factor: 4.6) and its Scientific Committee, I am pleased to invite you to participate in the **1st International Electronic Conference on Toxics**. This meeting will be held **online** from **20–22 March 2024**.

The aim of this platform is to bring together students, researchers, and scientists from around the world to present their work and exchange ideas on the exposure, effects, and risks of chemicals and materials on humans and the natural environment, as well as on the development of new approaches to assess and/or manage the toxicological and ecotoxicological risks of chemicals and materials. The topics are organized into six sessions, corresponding to the following journal Sections:

This year's conference is dedicated to following sessions:

1. Environmental Contaminants and Health.
2. Drugs Toxicity and Safety.
3. Toxicological Mechanisms of Toxicants.
4. Identification and Quantification of Toxicants.
5. Novel Methods in Toxicology Research.
6. Toxicity Reduction and Environmental Remediation.

Submitted abstracts will be reviewed by the conference committee and, if accepted, authors can choose to submit proceedings papers or posters, potentially alongside a PowerPoint and/or video presentation of their work. All accepted abstracts will be published as one dedicated volume in the Proceedings journal (ISSN: 2504-3900).

The 1st International Electronic Conference on Toxics offers you the opportunity to participate in this international, scholarly conference without having the concern or expenditure of travel fees. We would like to invite you to "attend" this conference by presenting your latest work. Abstracts (in English) should be submitted online before **20 November 2023**.

Conference Chair
Dr. Demetrio Raldúa
Department Environmental Chemistry, IDAEA-CSIC,
Barcelona, Spain

Table of Content

toxics

an Open Access Journal by MDPI

Toxics (ISSN 2305-6304) is an international, peer-reviewed, open access journal which provides an advanced forum for studies related to all aspects of toxic chemicals and materials. It publishes reviews, regular research papers, and short communications. Our aim is to encourage scientists to publish their experimental and theoretical results in detail. There is, therefore, no restriction on the maximum length of the papers, although authors should write their papers in a clear and concise way. The full experimental details must be provided so that the results can be reproduced. Electronic files or software regarding the full details of calculations and experimental procedure can be deposited as supplementary material, if it is not possible to publish them along with the text.

Journal Webpage: https://www.mdpi.com/journal/toxics.

Session Chairs

Prof. Dr. Qixing Zhou
College of Environmental Science and Engineering, Nankai University, Tianjin, China

Dr. Natalia Garcia-Reyero
Environmental Laboratory, US Army Engineer Research & Development Center, Vicksburg, USA

Prof. Dr.Yankai Xia
School of Public Health, Nanjing Medical University, Nanjing, China

Prof. Dr. Youssef Sari
Department of Pharmacology and Experimental Therapeutics, College of Pharmacy and Pharmaceutical Sciences, The University of Toledo, Toledo, USA

Prof. Dr. Virgínia Cruz Fernandes
Instituto Superior de Engenharia, Politécnico do Porto, Porto, Portugal

Scientific Committees

Prof. Dr. Xiaojun Luo
Guangzhou Institute of Geochemistry, Chinese Academy of Sciences, Guangzhou, China

Dr. Gunnar Toft
Department of Public Health, Aarhus University, Denmark

Prof. Dr. Sijie Lin
College of Environmental Science and Engineering, Tongji University, Shanghai, China

Dr. Eduardo V. Soares
ISEP-School of Engineering, Polytechnic Institute of Porto, Porto, Portugal, Centre of Biological Engineering, University of Minho, Braga, Portugal

Dr. Louis A. Tremblay
Cawthron Institute, Nelson, New Zealand, School of Biological Sciences, University of Auckland, Auckland, New Zealand

Dr. Minjian Chen
School of Public Health, Nanjing Medical University, Nanjing, China

Prof. Dr. João Fernando Pereira Gomes
Department of Chemical Engineering (ADEQ), Instituto Superior de Engenharia de Lisboa (ISEL), Lisbon, Portugal

Dr. Jamie Dewitt
Department of Pharmacology and Toxicology, Brody School of Medicine, East Carolina University, Greenville, USA

Dr. Wanli Ma
Harbin Institute of Technology, Harbin, China

Prof. Dr. Emilio Benfenati
Istituto di Ricerche Farmacologiche Mario Negri, Milan, Italy

Dr. Jose V. Tarazona
National Centre for Environmental Health, Instituto de Salud Carlos III, Madrid, Spain

Dr. Joel Ferreira De Brito
IMT Nord Europe, Douai, France

Prof. Dr. Qing Huang
School of Ecology and Environment, Hainan University, Haikou, China

Dr. Noel Aquilina
Department of Chemistry, Faculty of Science, University of Malta, Msida, Malta

Dr. Daniel Drage
School of Geography, Earth & Environmental Sciences, University of Birmingham, Birmingham, UK

Prof. Dr. Qi Wang
Department of Toxicology, Peking University, Beijing, China

Prof. Dr. Fayuan Wang
College of Environment and Safety Engineering, Qingdao University of Science & Technology, Qingdao, China

Prof. Dr. Karina Boltes
Department of Analytical Chemistry, Physical Chemistry and Chemical Engineering, University of Alcala, Alcalá de Henares, Spain

Dr. Catarina Cruzeiro
Helmholtz Munich - German Research Center for Environmental Health, Neuherberg, Germany

Dr. Nikiforos Alygizakis
Department of Chemistry, Laboratory of Analytical Chemistry, National and Kapodistrian University of Athens, Athens, Greece

Speakers

Keynote Speakers

Prof. Dr. Roy M. Harrison
Division of Environmental Health & Risk Management, School of Geography, Earth & Environmental Sciences, University of Birmingham, Birmingham, UK

Prof. Dr. Hartmut Jaeschke
Department of Pharmacology, Toxicology & Therapeutics, University of Kansas Medical Center, Kansas City, USA

Dr. Gunnar Toft
Department of Public Health, Aarhus University, Denmark

Prof. Dr. Emilio Benfenati
Istituto di Ricerche Farmacologiche Mario Negri, Milan, Italy

Invited Speakers

Dr. Di Wu
School of Public Health, Nanjing Medical University, Nanjing, China

Dr. Diogo Pestana
CINTESIS@RISE, Nova Medical School, Universidade Nova de Lisboa, Lisboa, Portugal

Prof. Dr. Jing Liu
College of Environmental and Resource Sciences, Zhejiang University, China

Dr. Yuxia Liu
Department of chemical engineering and environment, China University of Petroleum, Beijing, China

Dr. Maite De Maria
Cherokee Nation System Solutions, contractor to the U.S. Geological Survey- Wetland and Aquatic Research Center, Gainesville, FL, USA

Dr. Kelly Carstens
US EPA, Office of Research and Development

Program at a Glance

The 1st International Electronic Conference on Toxics
20–22 Mar 2024, Online

	20 March 2024 (Wednesday)	**21 March 2024 (Thursday)**	**22 March 2024 (Friday)**
Morning	Opening Ceremony Session C. Toxicological Mechanisms of Toxicants	Session D. Identification and Quantification of Toxicants Session F. Toxicity Reduction and Environmental Remediation	Session A. Environmental Contaminants and Health
	Break	Break	Break
Afternoon	Session B. Drugs Toxicity and Safety Session E. Novel Methods in Toxicology Research	Poster Session	Session A. Environmental Contaminants and Health

IECTO 2024 Program

20 March 2024 (Wednesday) Opening Ceremony
Session C. Toxicological Mechanisms of Toxicants

CET (Central European Time)	CST Asia (China Standard Time)	Speaker	Title
9:30–9:35	16:30–16:35	Welcome from the conference chair—Dr. Demetrio Raldúa	
9:35–10:05	16:35–17:05	Keynote Speaker **Prof. Dr. Roy M. Harrison**	Air pollution and health, past present and future
10:05–10:35	17:05–17:35	Keynote Speaker **Prof. Dr. Emilio Benfenati**	Read-across: Today and tomorrow
10:35–10:45	17:35–17:45	Break	
10:45–11:05	17:45–18:05	Invited Speaker **Prof. Dr. Jing Liu**	Effects of pyrethroid insecticides on glucose homeostasis and gestational diabetes mellitus
11:05–11:20	18:05–18:20	Selected Speaker **Margarida Ribeiro Vilaça**	Unravelling the effects of benzo[k]fluoranthene and temperature on the expression of detoxification genes in the rainbow trout liver RTL-W1 cell line
11:20–11:35	18:20–18:35	Selected Speaker **Fang Chu**	Unveiling the LncRNA–miRNA–mRNA regulatory network in arsenic-induced nerve injury in rats using high-throughput sequencing

Session B. Drugs Toxicity and Safety
Session E. Novel Methods in Toxicology Research

CET (Central European Time)	CST Asia (China Standard Time)	Speaker	Title
14:00–14:10	21:00–21:10	**Welcome from the session chair—Prof. Dr. Youssef Sari**	
14:10–14:40	21:10–21:40	Keynote Speaker **Prof. Dr. Hartmut Jaeschke**	Acetaminophen hepatotoxicity: Novel mechanisms and therapeutic approaches
14:40–14:55	21:40–21:55	Selected Speaker **Archange Michel Emmanuel MBOUNGOU MALONGA**	Neurotoxicity of valproic acid in wistar rats: Effects on memory
14:55–15:10	21:55–22:10	Selected Speaker **Karolina Nowak**	Self-poisonings by use of 'suicide kits' and a 'home-made' multi-xenobiotics mixes: Are they a growing problem in forensic toxicology?
15:10–15:20	22:10–22:20	**Welcome from the session chair—Dr. Natalia Garcia-Reyero**	
15:20–15:40	22:20–22:40	Invited Speaker **Maite De Maria**	Impacts of glyphosate on in-vitro T-lymphocytes in florida manatees
15:40–16:00	22:40–23:00	Invited Speaker **Kelly Carsten**	New approach methods for developmental neurotoxicity: A per- and polyfluoroalkyl substances (PFAS) case study
16:00–16:15	23:00–23:15	Selected Speaker **Jingjie Zhang**	Evaluation of the genotoxic potential of a flavored oral nicotine pouch product using integrated approaches
16:15–16:30	23:15–23:30	Selected Speaker **Martina Palomino-Schätzlein**	ProtoPRED: An innovative platform for the prediction of toxicological properties of small molecules and nanomaterials

21 March 2024 (Thursday)
Session D. Identification and Quantification of Toxicants
Session F. Toxicity Reduction and Environmental Remediation

CET (Central European Time)	CST Asia (China Standard Time)	Speaker	Title
9:30–9:40	16:30–16:40	Welcome from the session chair—Prof. Dr. Virgínia Cruz Fernandes	
9:40–10:00	16:40–17:00	Invited Speaker **Dr. Diogo Pestana**	Nutrition, environment & endocrine disruptors—A translational approach
10:00–10:15	17:00–17:15	Selected Speaker **Tieqing You**	Target analysis and suspect screening of per- and polyfluoroalkyl substances in tap water samples throughout Chinese cities
10:15–10:30	17:15–17:30	Selected Speaker **Kaja Tusiewicz**	A historical drug or a current problem? Determination of methaqualone and its analogs in biological material via UHPLC-QqQ-MS/MS
10:30–10:40	17:30–17:40	Welcome from the session chair—Prof. Dr. Qixing Zhou	
10:40–11:00	17:40–18:00	Invited Speaker **Dr. Yuxia Liu**	Impacts of microplastics on performance and assembly of anaerobic ammonium oxidizing (anammox) bacteria
11:00–11:15	18:00–18:15	Selected Speaker **Louis Tremblay**	Up-the-pipe solutions: A best-practice framework to engage communities in reducing chemical contamination in waste
11:15–11:30	18:15–18:30	Selected Speaker **SBIAA Salah Eddine**	Green and high-performance magnetic catalysts for the toxicity-catalytic reduction of nitroarene
11:30–11:45	18:30–18:45	Selected Speaker **Juan Adrian Ramos Guivar**	Ecotoxicological behavior of functionalized magnetic nanohybrids in water flea *Daphnia magna* and their recovered physicochemical properties

Poster Session

CET (Central European Time - UTC+1)	CST Asia (China Standard Time - UTC+8)	Speaker	Title
14:00–15:30	21:00–22:30	Poster Session	The Poster Sessions will take place in Zoom break-out rooms. The list of names and titles of the posters will be found here.

22 March 2024 (Friday)
Session A. Environmental Contaminants and Health

CET (Central European Time)	CST Asia (China Standard Time)	Speaker	Title
9:30–9:40	16:30–16:40	Welcome from the session chair—Prof. Dr. Yankai Xia	
9:40–10:00	16:40–17:00	Invited Speaker **Dr. Di Wu**	The detection of microplastics in biological samples and their potential health effects
10:00–10:15	17:00–17:15	Selected Speaker **Minjian Chen**	A metabolomic study on spermatogenesis failure induced by heavy metal exposome
10:15–10:30	17:15–17:30	Selected Speaker **Francis Manyori Bigambo**	Impact of temperature and relative humidity variability on children's allergic diseases and critical time window identification
10:30–10:45	17:30–17:45	Selected Speaker **Antonio Peña-Fernández**	Environmental exposure of children to silver in Alcalá de Henares (Spain): Risk assessment due to its presence in topsoils
10:45–11:00	17:45–18:00	Selected Speaker **Sandra Lavandeira**	The impact of occupational exposure on workers' respiratory microbiota
11:00–11:15	18:00–18:15	Selected Speaker **Mingzhi Zhang**	Neonatal cytokines: Mediators and indicators of $PM_{2.5}$ exposure during early pregnancy and childhood eczema
11:15–11:30	18:15–18:30	Selected Speaker **Teetawat Santijitpakde**	Oxidative potential as a health risk estimation of ambient $PM_{2.5}$ in Chiang Mai City, Northern Thailand: A study in 2021
11:30–11:45	18:30–18:45	Selected Speaker **Stefania Gheorghe**	Ecotoxicological effects of polystyrene particles on *Cyprinus carpio:* A laboratory assessment

CET (Central European Time)	CST Asia (China Standard Time)	Speaker	Title
14:00–14:10	21:00–21:10	Welcome from the committee—Dr. Jose V. Tarazona	
14:10–14:40	21:10–21:40	Keynote Speaker **Dr. Gunnar Toft**	Prenatal exposure to endocrine disrupting compounds and offspring reproductive function
14:40–14:55	21:40–21:55	Selected Speaker **Shaohan Zhang**	Human exposure characteristics of liquid crystal monomers (LCMs) and their mechanisms to cross the skin barrier
14:55–15:10	21:55–22:10	Selected Speaker **Bhavana Sivakumar**	PM2.5-induced declined cardiac tolerance to ischemia-reperfusion injury can be ameliorated by hydrogen sulfide
15:10–15:25	22:10–22:25	Selected Speaker **Chayan Munshi**	Arsenic-induced neurotoxicity: A study on the brain–behaviour circuit
15:25–15:40	22:25–22:40	Selected Speaker **Monica Torres-Ruiz**	Effects of acute nanoplastic exposure on thyroid hormone axis and behavior in zebrafish larvae
15:40–15:55	22:40–22:55	Selected Speaker **Pedro Espitia-Pérez**	Genetic damage and multi-elemental exposure in populations in proximity to artisanal and small-scale gold mining areas in North Colombia
15:55–16:10	22:55–23:10	Selected Speaker **Irini Tsiodra**	Spatiotemporal gradients of PAHs in Greek urban environments and subsequent health impacts

Poster List

Poster Session	
Name	**Title**
Nezha MEJJAD	Assessment of potential ecological risk of Cr, Cd, Pb and As, in coastal sediments.
Shankar M Bakkannavar	Fatal Dermal Absorption of Organophosphate Insecticide
Rosária Seabra	Exploring marine-derived fungal preussin toxicity on MDA-MB-231 cells cultured in 2D and 3D
Ishika Pal	Geospatial deposition of toxic heavy metals and metalloid between pond and associated agricultural ecosystem in a non-industrialized rural area in West Bengal, India
Jorge M. S. Faria	Environmental and human health benefits of bionematicidal volatiles in comparison to commercial synthetic nematicides
Rita Couto	Is tamoxifen cytotoxicity against breast cancer cells influenced by xenoestrogens?
Ahmad Mahdavi	Global measures to stop the exportation of Highly Hazardous Pesticides from the EU to Developing Countries
Kevin Castillo-Mendieta	In Silico Discovery of Hemolytic Peptides Through a Novel Approach Based on Network Science and Similarity Searching Methods
Varvara Maksimova	Thiram Effects on HeLa TI Cells
María Carpena	Assessment of the Chemical Hazards in Herbs consumed in Europe: Toxins, Heavy Metals, and Pesticide Residues
Jing Hu	The role of the HIF-1α-BNIP3 pathway in acrylonitrile-induced hippocampal neuronal cell toxicity
Prem Chand	Characterization of rainbow trout hepatic 3D spheroids for next-generation ecotoxicity testing
Natasha Chitakwa	Charge and Size Effects of Microplastics on Human Endometrium Cancer Cell Proliferation
Carlos Seiti Hurtado Shiraishi	Exploring Schiff bases as promising alternatives to traditional drugs in the in silico treatment of leishmaniasis
Mamatha Bhanu L S	Potential risk of cyclopiazonic acid toxicity in Kodo millet (*Paspalum scrobiculatum* L.) poisoning
Tao Zehua	Exploring the Role and Regulation of HIF-1 in Manganese Toxicity Using Caenorhabditiselegans as a Model
Chenxv Hu	Effects of subchronic methylmercury exposure on response to acute hypoxia in mice: role of HIF-1α
Mazhar Sultan	Association of Individual and Combined Exposure to Bisphenol and Serum Thyroid Hormones Level in Adults and Pregnant Woman: A Systematic Review and Meta-Analysis
ABHISHEK KUMAR	Plant-Based Approaches for Wastewater Management: A Comprehensive Review of Phytoremediation Techniques
Mª Ángeles Peña Fernández	Biomonitoring chromium contamination in urban and rural topsoils from Leicestershire, England
Obinna Kenneth Didigwu	Drug-likeness, Pharmacokinetics, and Toxicity Prediction of Phytotoxic Terpenoids
Yinyin Zhang	Impact of Sodium Ion Stress on the Mechanism of Lead Ion Migration in Electrochemical Treatment of Lead-Contaminated Soil
Manuela Dias Machado	Unravelling the formation of a palmelloid-like phenotype in the green microalga Raphidocelis subcapitata when exposed to pollutants
Samira El Aouidi	Distribution Coefficient (Kd) of Stable Cesium in Agricultural Soil in the Rabat Region, Morocco
Lorena González-Gómez	Occurrence of tropane alkaloids in teas. Effect of tea-making on atropine and scopolamine
Osama Ali Abulseoud	Thyrotropin Suppression during Intoxication Mediates a Positive Effect of Alcohol on Kidney Function in Males
Antonio Peña-Fernández	Exposure to platinum group elements in young university students from Leicester, England
Ivan Dolanc	The Antibacterial Efficacy and Drug Safety Profile of Trans-cinnamaldehyde against Acinetobacter baumannii: Bioinformatics and Cheminformatics Approach

Poster Session	
Name	**Title**
José Cabêda	Reuse of wastewater: concerns about the effects of mixtures of chemical substances on human health
Francisco Ríos	Toxicity mechanisms of mixtures of anionic and non-ionic surfactants
Núria Ferrer-Cortés	Development of an ICP-MS/MS-based methodology for the analysis of (ultra) trace elements in follicular fluid samples of patients undergoing IVF treatment
Andreia Garces	Acorn poisoning as a potential threat to animals
Emma Rowan	New Approach Methodologies: Physiological Responses Of Daphnids To Pharmaceutical Mixtures
Lin Yanli	Methylmercury-induced ferroptosis may be attenuated by vitamin K in PC12 cells
Ana Fernandez Agudo	Adding Realism to the Assessment of Occupational Exposure to Pesticides Using Probabilistic Modelling. A Case Study on Aggregate Exposure to Pyrethroids.
Ana Margarida Esteves	Determination and Risk Assessment of PAHs and PCBs in Seawater and Blue Mussels from Vila-do-Conde, Portugal
Despina Paraskevopoulou	Fine aerosol toxicity in urban environments of Eastern Mediterranean
Marta Oliveira	Impact of polycyclic aromatic hydrocarbons on the environment and human health: evidence retrieved from biomonitoring studies
Mat Tamizi Zainuddin	Nanomaterial Exposure Assessment of Carbonaceous Compounds from Carbon Fiber Processing Laboratory
Clara Naccari	Toxic and Essential Metals in Stenella Coeruleoalba: Assessment of Marine Environmental Pollution and Dolphin Health Status
Cristina Tapia-Navarro	Impact of Microfibers on the Marine Microalgae *Phaeodactylum tricornutum*

About Us

Launched in 2009 by MDPI, Sciforum is an event management platform that supports open science by offering the opportunity to participate in, as well as to organize, academic events. Having hosted hundreds of events (be it in-person events, virtual events, or webinars), Sciforum helps organizers reduce their administrative efforts by providing a comprehensive set of tools to successfully manage academic events.

Sciforum Will Help You To

- Easily build your own event's website
- Define your own submission settings
- Manage submissions and its peer-review
- Handle registrations and invoicing
- Easily contact your event attendees and authors
- And much more...

Are you also looking for publication opportunities?
Do you need assistance managing some organizational aspects?
Let us know what else you need!

Where to Find Us

linkedin.com/showcase/sciforum
facebook.com/mdpisciforum
twitter.com/sciforum
info@sciforum.net

sciforum.net

Our Customers

Abstracts

Session A. Environmental Contaminants and Health

sciforum-085626: A Metabolomic Study on Spermatogenesis Failure Induced by Heavy Metal Exposome

Yingtong Jiang, Miaomiao Tang, Yusheng Guan and Minjian Chen

[1] State Key Laboratory of Reproductive Medicine and Offspring Health, Center for Global Health, School of Public Health, Nanjing Medical University, Nanjing 211166, China
[2] Key Laboratory of Modern Toxicology of Ministry of Education, Nanjing Medical University, Nanjing 211166, China

Introduction

Increasing heavy metal pollution may impact spermatogenesis. However, previous research has been limited to a few known toxic metals.

Methods

A total of 962 patients with spermatogenesis failure and healthy controls were recruited for the study. ICP-MS was utilized to detect heavy metal exposome in urine, while UPLC-Q Exactive was employed to analyze metabolome of both urine and seminal plasma. Based on the human study, we established in vivo and in vitro exposure models as well as key metabolic reversal models to observe reproductive indicators and analyze downstream molecules.

Results

Among the 52 heavy metals detected, molybdenum was the most significant element related to spermatogenesis failure with the highest content. The metabolome associational study demonstrated the significant association between molybdenum exposure, adenosine metabolism, and spermatogenic disorders. Mice aged 8 and 56 weeks were exposed to molybdenum with increasing detected molybdenum in urine and testis. Pathological examination showed that molybdenum specifically impaired testis tissue. The number of sperm and the proportion of progressive sperm were decreased, while the sperm deformity rate was increased after molybdenum exposure. There was an exacerbation of apoptosis in both spermatocytes and Sertoli cells in the testicles of mice. The gene expression of Nt5e, Adora1, Bax, Caspase-9, Caspase-3, and oxidative glutathione in the testes were increased. The above effects were partially restored by the reversal of adenosine metabolism. Molybdenum exposure also promoted cell apoptosis and lead to an increase in apoptotic gene expression in GC-2 cells, and the effects were restored in the adenosine metabolism reversal group.

Conclusions

This study provided a global understanding of spermatogenesis failure caused by heavy metal exposome, and further clarified a novel toxic pathway as Molybdenum-Nt5e enzyme-Adenosine-Adenosine A1 receptor-Mitochondrial dependent apoptosis-Spermatogenesis failure, providing new information for male reproductive toxicity caused by heavy metal exposure.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-082924: Acorn Poisoning as a Potential Threat to Animals

Andreia Garces [1], Filipe Silva [2] and Isabel Pires [2]

[1] Universidade de Trás os Montes e Alto Douro
[2] CECAV, University of Trás-os-Montes and Alto Douro, Vila Real, Portugal

The acorn is the nut of oak trees (genera Quercus and Lithocarpus) that can be found in the Northern Hemisphere. They are a valuable source of food for many animals (birds, rats, squirrels, pigs), but can pose health risks when consumed in large quantities. This nut contains gallotannin. When ingested, gallotannin is broken down into gallic acid and tannic acid. Tannic acid is toxic and can cause ulcers in the mouth, esophagus, and intestines, and damage the liver and kidneys. Animals that consume acorns as part of their diets (wild boars, deer, bears, birds, and squirrels) have some defense mechanisms against this toxin, such as waiting to consume them until enough groundwater has percolated through the acorns to leach the tannins or buffering the acorns with other foods. Some animals metabolize tannins better than others. Acorns can be particularly toxic to cattle, horses, and dogs, and fatal to all species when consumed in large quantities due to kidney failure. Animals with acorn poisoning may begin showing symptoms within hours or even several days after eating acorns. Symptoms include vomiting, diarrhea, cramping, abdominal tenderness, depression, rapid weight loss, loss of appetite, tiredness, and dehydration. There is no specific treatment for acorn poisoning, with prevention being key. Limiting access to fields with many oak trees to domestic animals during the fall is one measure. Diagnosis is based on clinical findings, necropsy, history, and histopathologic examination of the kidneys. Due to climate change, the weather has become increasingly dry throughout the year and forest fires are common, meaning that during autumn, often the only food available in some regions is acorns, leading to a silent killing of animals due to lack of resources. It is important that farmers and veterinarians are aware so that they can offer faster and more effective treatment.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085701: Adding Realism to the Assessment of Occupational Exposure to Pesticides Using Probabilistic Modelling. A Case Study on Aggregate Exposure to Pyrethroids

Ana Fernandez Agudo [1], Agathi Charistou [2], Niki Arapaki [2], Kyriaki Machera [2], Mercedes Alba Gonzalez [3], Maria del Carmen Gonzalez Caballero [3] and Jose V. Tarazona Lafarga [3]

[1] National Environmental Health Centre. Instituto de Salud Carlos III
[2] Benaki Phytopathological Institute
[2] National Environmental Health Centre

Pyrethroid usage has risen due to restrictions on other insecticides, prompting interest in biomonitoring data as exposure indicators. Occupational exposure, particularly in Plant Protection Product (PPP) applications, is a focus. Regulatory agencies, like the European Food Safety Authority (EFSA), use tools such as OPEX to assess non-dietary exposure, employing worst-case scenarios for increased protection.

This research explores OPEX's suitability for realistic exposure estimations via probabilistic modeling and Monte Carlo simulations. This study uses data from the EU PARC project estimating aggregated pyrethroid exposure. This study uses workflows for operators and workers, integrating tasks and applying Monte Carlo simulations for exposure estimation variability. Probability distributions replace default values, addressing real-world uncertainties.

The intention is to present a conceptual model for three occupational exposure scenarios, highlighting variability in task roles and exposure routes. Monte Carlo simulations offer full probability distributions, aiding sensitivity and uncertainty analyses. This study plans to compare aggregated exposure, including dietary exposure, with some preliminary results. The ongoing project aims to refine default values via a probabilistic assessment strategy.

To conclude, there is a need for aggregate exposure models considering shared neurotoxicity among pyrethroids. The proposed approach, based on the regulatory OPEX tool, facilitates comparisons between regulatory and aggregate assessments. Pyrethroids are chosen due to their proximity to concerning dietary exposure levels. This study's innovative approach aims to refine occupational exposure assessments, identify aggregate exposure risks, and enhance pesticide risk evaluation in occupational settings, contributing valuable insights for future studies.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-086006: Arsenic-Induced Neurotoxicity: A Study on the Brain–Behaviour Circuit

Chayan Munshi

Ethophilia (An Autonomous Research Group), Santiniketan 731235, India

Introduction

Arsenic is a highly toxic metalloid and an environmental contaminant which predominantly affects the aquatic ecosystem. This pollutant is a well-known neurotoxicant and effectively alters neuronal activity by affecting the neurotransmission process. Abnormal neuronal activities manifest as modifications of behavioural biomarkers, which makes them a convenient method of assessing modulations in the neural system of an organism. The aim of this research study is to establish the hypothesis that an environmental toxicant like arsenic can cause repetitive behavioural patterns, which is an index of neurological abnormality.

Methods

Aquatic invertebrates are a reliable model to study ecotoxicity. As a common freshwater prawn species, *Macrobrachium lamarrei* was considered as a model organism to evaluate the critical role of low (non-lethal) concentrations of arsenic trioxide (As_2O_3) as a neurotoxicant in aquatic organisms. Both behavioural and respective gene expression (acetyl cholinesterase, neurexin–neuroligins) data were analysed to corroborate arsenic-induced neurotoxicity.

Results

The effect of arsenic trioxide on *Macrobrachium lamarrei* was robustly manifested in the form of a significant increase in grooming behaviour activity. Grooming is an established marker of neurological stress in several animals. In addition, repetitive behaviour is a marker of Autism Spectrum Disorder (ASD). Here, grooming repetitions were substantiated with neurexin–neuroligin up- and downregulation patterns.

Conclusions

Present-day research on the brain–behaviour circuit is applied for the analysis of psychopathological status in animals and humans. It is also efficiently used in neuropharmaceutical or neurotoxicological examinations of certain neuromodulators and neurotoxic agents (like arsenic) in the ecosystem which can induce transformed neuronal actions and consequently cause behavioural plasticity.

© 2024 by the author. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-086689: Assessment of Potential Ecological Risk of Cr, Cd, Pb and As, in Coastal Sediments

Nezha MEJJAD, Samira El Aouidi and Abdelmourhit Laissaoui

National Centre for Nuclear Energy, Science and Technology (CNESTEN) Morocco

Coastal sediments are a powerful tool for analyzing pollution levels and reconstructing history. The Oualidia lagoon plays an essential role as it provides several ecosystem services, including aquaculture, fisheries, and coastal tourism, among others. Therefore, the conservation and protection of this natural system requires continuous monitoring of its environmental quality. In this sense, the present study evaluates the potential ecological risk of Cr, Cd, Pb and As in coastal sediment cores collected from the Oualidia lagoon. These sediment cores were also dated using lead-210 in order to study the temporal variations of the studied metals. The ecological risk values of the metals show that among the four metals, cadmium indicates a very high ecological risk in the first 25 cm and 15 cm of sediment cores CO-1 and CO-2, respectively. The high potential ecological risk of the sediments recorded in the surface layers suggests that the development of human activities in the last two decades has contributed to the increase of heavy metal concentrations. Activities such as agriculture can be potential sources of Cd. Excessive use of fertilizers and pesticides may contribute to the increase of this heavy metal in the lagoon. This finding highlights the need for careful monitoring and remediation of Cd levels in this aquatic system, as it presents a high ecological risk value among the selected heavy metals.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085628: Association of Individual and Combined Exposure to Bisphenol and Serum Thyroid Hormones Level in Adults and Pregnant Woman: A Systematic Review and Meta-Analysis

Mazhar Sultan [1,2], Guan Quanquan [3,4] and Yankai Xia [3,4]

[1] State Key Laboratory of Reproductive Medicine, Center for Global Health, School of Public Health, Nanjing Medical University, Nanjing 211166, China
[2] Key Laboratory of Modern Toxicology of Ministry of Education, School of Public Health, Nanjing Medical University, Nanjing 211166, China
[3] State Key Laboratory of Reproductive Medicine, Center for Global Health, School of Public Health, Nanjing Medical University, Nanjing 211166, China
[4] Key Laboratory of Modern Toxicology, Ministry of Education, School of Public Health, Nanjing Medical University, Nanjing 211166, China

Background

Environmental factors influence thyroid malfunction. Bisphenols are a class of endocrine-disrupting substances widely detected in global populations. As awareness of its toxicity increased, BPA was substituted with presumably less toxic alternatives, such as bisphenols S, F, and AF. The present meta-analysis examines the association of individual and combined exposure to bisphenol and serum thyroid hormone levels in adults and pregnant women.

Material and Methods

A comprehensive search was conducted on PubMed, Web of Science, Embase, and Cochrane Library databases, resulting in the retrieval of a total of 4160 articles, utilizing both prospective and cross-sectional research designs. In total, aggregate hazards for the reliability of the included studies were also evaluated using a random effect model. The heterogeneity test was performed using the I2.

Results

14 studies were deemed eligible for our analysis. Overall, fixed model summary estimates indicated the negative association between BPA and TSH in adults with regression coefficient $\beta = 0.02$ and [95% CI: -0.04; -0.0]. Meanwhile, marginally significant results also found an association between BPA and TT4 in adults. The overall summary showed that there is no association between bisphenols and thyroid hormones in the 1st and 2nd trimesters of pregnant women. Subgroup analysis in females revealed a positive association between BPA and TSH and a negative relationship with BPA and TSH with the effect size $\beta = 0.01$ [95% CI: 0.00; 0.01] and $\beta = -0.09$ [95% CI: -0.17; -0.01], respectively.

Conclusions

There were notable gender-based disparities in the impact of BP on the levels of thyroid hormones. Bisphenols have the potential to exert a substantial influence on the concentrations of thyroid hormones in males, females, adults, and pregnant women. Data was not enough to analyze BPF and BPB exposure to thyroid hormones, so conducting a comprehensive study on the association of combined exposure to bisphenols and thyroid hormones in adults and pregnant women is suggested.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085605: Biomonitoring Chromium Contamination in Urban and Rural Topsoils from Leicestershire, England

Gurminderjeet S. Jagdev [1], Maria del Carmen Lobo-Bedmar [2], Mª Ángeles Peña Fernández [3], Mark D. Evans [4] and Antonio Peña-Fernández [5]

[1] PhD Research
[2] Research in IMIDRA (Madrid Institute for Rural, Agricultural and Food Research)
[3] University of Alcalá
[4] Professor in Leicester School of Allied Health Sciences, De Montfort University, Leicester
[5] Professor in Department of Surgery, Medical and Social Sciences, Faculty of Medicine and Health Sciences, University of Alcalá

A monitoring study was performed to characterise the risks to chromium (Cr) in Leicestershire, England. 106 wild growing mushrooms were collected from Leicester city and Bradgate Park (a close rural park). Cr was monitored by ICP-MS in cleaned/dried/homogenised mushrooms appropriately mineralised [LoD = 1.012 μg/g dry weight (dw)]. Cr was also monitored in 850 topsoils collected across Leicestershire processed as composite samples by ICP-MS after acid/microwave digestion (LoD = 3.683 μg/g). Cr was detected in 92.2% of the topsoil samples, meanwhile was found in 47.1% of the mushroom samples [median and range, in μg/g dw; 0.863 (1.012–19.466)], showing significant distribution across the four ordinal directions in which Leicestershire was divided [SE (1.908) >NW (1.738) >NE (0.987) >SW (LoD); Peto-Prentice test, $\chi^2(2) = 12.4$, p-value = 0.002]. These results might suggest some level of pollution by Cr in Leicestershire, as they were higher than the proposed reference interval for wild mushrooms that grow in unpolluted areas (0.5–5 μg/g dw). A similar distribution of Cr was found in the topsoils monitored, i.e. the highest concentration in those collected in the southeast and the lowest in the southwest quadrant (123.137 vs. 20.947 μg/g). Moreover, significantly higher levels were found in topsoils collected in the urban area (median and range, in μg/g; Peto-Prentice test, $\chi^2(1) = 1.1$, p-value = 9×10^{-4}): 82.542 (3.683–196.795) vs. 32.806 (3.683–265.069), which might be attributed to different anthropic sources such as vehicles. All bioconcentration factor values were lower than one, suggesting a low bioaccumulation of Cr in the wild mushrooms species collected in Leicestershire. Toxic risks derived from oral, inhalation and dermal exposure to Cr from topsoils in the urban four ordinal directions (NW = 1.95×10^{-1}, NE = 1.40×10^{-1}, SW = 2.53×10^{-1}, SE = 4.30×10^{-2}), were lower than the unit, suggesting a minimal risk for Leicester's population. However, speciation analysis would be needed to rule out carcinogenic risks to hexavalent Cr.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085693: Charge and Size Effects of Microplastics on Human Endometrium Cancer Cell Proliferation

Natasha Chitakwa

Nanjing Medical University

Phthalates and other endocrine-disrupting chemicals (EDCs) used as additives in microplastic (MP) production have been linked to endometrial cancer, one of the most common types of cancer in women. However, the effects of the physical properties of MPs, such as surface charge and size, on endometrial cancer are unclear. Our study aimed to explore the effects of MPs of varying size and surface charge on endometrial cancer using an endometrium epithelial-like cancer cell line, RL95-2. The experiments were divided into aged (Polystyrene, PS 20 nm and 2 μm) and charged (PS 2+ and 2−) MP groups. After incubating the cells in DMEM/F12 medium for 24, 48, and 72 h, the results suggested that smaller-sized MPs and charged MPs increased the proliferation of endometrial cancer cells in a time- and dose-dependent manner, with proliferation rates reducing after longer periods of exposure and at higher exposure concentrations, as assessed via CCK-8. We also observed larger increases in proliferation rates in the cells exposed to charged MPs as opposed to aged MPs. These findings suggest that MPs, a novel, ubiquitous pollutant, may promote the growth of endometrial cancer cells. We are currently conducting further experiments using other methods, such as flow cytometry and Western blot, to explore whether MP exposure will increase the proliferation of endometrial cancer cells. This could provide a basis for research aimed at understanding how to prevent and minimize the aggravation of endometrial cancer in patients.

© 2024 by the author. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084281: Cytotoxicity of Glyphosate Studied in Selected Human Cell Lines

Agata Jabłońska-Trypuć [1], Gabriela Sokołowska [2], Monika Naumowicz [3], Urszula Wydro [2] and Elżbieta Wołejko [2]

[1] Bialystok University of Technology
[2] Department of Chemistry, Biology and Biotechnology, Faculty of Civil Engineering and Environmental Sciences, Bialystok University of Technology, Wiejska 45E Street, 15-351 Białystok, Poland
[3] Department of Physical Chemistry, Faculty of Chemistry, University of Bialystok, Ciolkowskiego 1K Street, 15-245 Bialystok, Poland

Introduction

Glyphosate is a phosphonate herbicide, which has been used for 35 years and it is still the most widely used herbicide in the world. The development of modern methods of in vitro toxicological analysis and the obvious increase in exposure to glyphosate have made it an increasingly studied xenobiotic. The widespread use of pesticides, especially glyphosate, causes it to be largely released into the environment, where it poses a threat to entire ecosystems.

Methods

In our research, we focused on the best research model from the point of view of toxicology, which are human cell lines, which were used in order to test the cytotoxicity of glyphosate. The tested concentrations of this compound reflected the level of human exposure to this active substance and ranged from 0.01 mM to 10 mM. The analyzes were conducted on human cell lines: MCF-7, T98G and DLD-1. In order to estimate cytotoxicity of herbicide MTT assay was used.

Results

A significant increase in cancer cell viability was observed under the influence of studied concentrations of glyphosate. The effect was significant especially under the influence of lower studied concentrations.

Conclusions

The obtained results indicate the carcinogenic and tumor cell-stimulating effects of glyphosate. This indicates the need for prudent use and monitoring of glyphosate in the environment due to its potentially hazardous effects on human health.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-086249: Determination and Risk Assessment of PAHs and PCBs in Seawater and Blue Mussels from Vila-do-Conde, Portugal

Ana Margarida Esteves, Rodrigo Alves, Eduardo Rocha and Maria João Rocha

[1] Laboratory of Histology and Embryology, Department of Microscopy, ICBAS—School of Medicine and Biomedical Sciences, University of Porto, R. Jorge Viterbo Ferreira 228, 4050-313 Porto, Portugal
[2] Team of Animal Morphology and Toxicology, CIIMAR/CIMAR—Interdisciplinary Centre of Marine and Environmental Research, University of Porto, Terminal de Cruzeiros do Porto de Leixões, Av. General Norton de Matos s/n, 4450-208 Matosinhos, Portugal

Polycyclic Aromatic Hydrocarbons (PAHs) and Polychlorinated Biphenyls (PCBs) are persistent organic pollutants that significantly threaten aquatic life. PAHs are formed through incomplete combustion and are found in sources such as oil spills, vehicle emissions, and industrial discharges. PCBs are synthetic chemicals used in electrical equipment and industrial applications before being banned due to their harmful effects. Both groups exhibit hydrophobic properties, leading to their accumulation in sediments and fatty tissues of aquatic organisms. The toxicity of these compounds varies depending on their chemical structure and concentration, with some being carcinogenic, mutagenic, and endocrine-disruptors. This study evaluated fluctuation patterns of 16 priority PAHs and 7 indicator PCBs in seawater and wild mussel samples collected from four sampling sites along the Atlantic Iberian Northwest Coastline (Vila-do-Conde, Portugal). Extraction methods included solid-phase extraction (SPE) for water samples and the QuEChERS method for mussel samples, followed by gas chromatography-mass spectrometry (GC-MS) analysis. Toxicity equivalents (TEQs) and risk quotient (RQ) were calculated to measure environmental risks. Exposure daily intake (EDI), target hazard quotient (THQ) and carcinogenic risk (CR) were calculated to measure potential human health risks. Seawater samples revealed the presence of PAHs and PCBs, indicating moderate contamination in the region. The results suggest that (i) PAHs have petrogenic and pyrogenic origins and pose a low ecological risk with potential carcinogenicity and that (ii) PCBs have minimal toxic potential and sources remain uncertain. Wild mussels showed widespread contamination due to low metabolizing and high accumulation capacities. From our analysis, PAHs posed a moderate environmental risk, exceeding legal levels, but revealed considerable potential carcinogenicity, mainly due to high ingestion rates. The study calls for further monitoring and controlling POPs to protect local communities and ecosystems, as these contaminants are often found in complex mixtures, posing greater risks than the current study's findings.

Funding: ATLANTIDA-NORTE-01-0145-FEDER-000040; FCT-UIDB/UIDB/04423/2020.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085208: Distribution Coefficient (Kd) of Stable Cesium in Agricultural Soil in the Rabat Region, Morocco

Samira El Aouidi [1], Abdelmourhit Laissaoui [1], Moncef Benmansour [1], Zineb El Mouridi [2] and Redouane Saadi [1]

[1] Centre National de l'Energie, des Sciences et des Techniques Nucléaires—Rabat, Morocco
[2] National Institute of Agricultural Research (INRA), BP 6356, CRRA Rabat, Av. Al Irfane, 10100 Rabat, Morocco

The presence of radioactive cesium (Cs) in soil poses a significant risk to both human health and the environment. Plant uptake is an important pathway for the migration of Cs to the human food chain. Therefore, determining the concentrations of 133Cs in soil solutions is crucial for monitoring and predicting the uptake of radiocesium by soils and plants. The mobility and availability of Cs in soil can be measured by using distribution coefficient (Kd) values. In this study, soil was taken from the Rabat region and characterized in terms of granulometric distribution, organic matter, carbonate content, pH, and electrical conductivity. Batch experiments were carried out for the determination of the distribution coefficient (Kd) of cesium in aqueous suspensions. Six experiments were carried out by suspending about 2.5 g of soil particles in 50 mL of 1M CaCl2 solution and spiking it with different amounts of stable Cs, from 22 to 476 μg/L. The suspensions were kept under shaking for almost five days and then centrifuged to separate the particles from the liquid. Cesium concentration was measured in the aqueous phase using ICP-MS. Distribution coefficients were determined as the ratio of the amount of Cs adsorbed on solids to that contained initially in the aqueous phase. The preliminary findings indicated that Kd values increased almost asymptotically as Cs concentration increased. This work is part of an international coordinated research project led by the International Atomic Energy Agency.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085319: Ecotoxicological Effects of Polystyrene Particles on *Cyprinus carpio*: A Laboratory Assessment

Stefania Gheorghe, Stoica Catalina and Harabagiu Maria Anca

National Research and Development Institute for Industrial Ecology—ECOIND

Global consumption has led to an increased and persistent plastic pollution in the aquatic environments. Due to their small size, plastic particles are omnipresent, affecting aquatic biota. Polystyrene is a synthetic polymer and one of the most widely used plastics. Its accumulation in the environment endangers the health of aquatic organisms. This study aims to investigate the acute (7 days) and chronic (75 days) toxicity of spherical polystyrene particles (20, 200, 430 µm) on *Cyprinus carpio* fish using OECD methodology. No mortality or behavioural changes were recorded after acute or chronic tests conducted on 1, 10, 100 mg/L polystyrene particles. Polystyrene showed bioavailability mainly through ingestion with food, causing weight loss in fish. Fish lots exposed to the polystyrene mix (particle sizes of 20, 200, 430 µm and 1.2 mg PS/L total concentration) showed changes in physiological indices but without major significance compared to control lots. After 75 days of chronic exposure of fish to a mix of polystyrene particles, organs were collected for sub-lethal effect investigation. Polystyrene was found to cause oxidative stress in fish organs. A very significant increase in the activity of the enzymes catalase and glutathione reductase, correlated with lipid peroxidation in gills, were observed. In the liver, catalase and glutathione S transferase activity increased, but there were no lipid peroxidation effects. Also, alanine transferase and aspartate transferase activity showed significant changes. Regarding the vitellogenesis initiated in the liver, vitellogenin activity increased by 40%. EROD activity saw a 20% increasecompared to control fish, indicating stress enzyme expression. Instead, acetylcholinesterase showed significant inhibition (>80%) in the brain and muscle. The protein profile showed new stress protein expression compared to the control in the gills and liver. Based on the results of our study, the introduction of new regulations monitoring the accumulation of microplastics in surface water is an urgent matter.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085685: Effects of Acute Nanoplastic Exposure on Thyroid Hormone Axis and Behavior in Zebrafish Larvae

Monica Torres-Ruiz [1], Patricia Iglesias-Hernandez [1,2], Maria Muñoz Palencia [1], Ana Cañas Portilla [1] and Antonio De la Vieja [2]

[1] Environmental Toxicology Unit, Centro Nacional de Sanidad Ambiental (CNSA), Instituto de Salud Carlos III (ISCIII), Ctra. Majadahonda-Pozuelo Km. 2,2., Majadahonda, 28220 Madrid, Spain
[2] Endocrine Tumor Unit, Unidad Funcional de Investigación en Enfermedades Crónicas (UFIEC), Instituto de Salud Carlos III (ISCIII), Ctra. Majadahonda-Pozuelo Km. 2,2., Majadahonda, 28220 Madrid, Spain

Introduction

Plastic production has increased exponentially in recent decades. Macroplastics in the environment are degraded through mechanical, physical, and biological processes, ultimately producing nanoplastics (NPs). NPs have been found in air, water, and soil, and there is a growing concern regarding their effects on the environment and on human health. NPs can accumulate in tissues, affecting them and causing disruptions in metabolism, development, and fertility, although their mechanisms of action are still largely unknown. The zebrafish embryo (ZFE) poses an ideal model to investigate this due to it is high homology with humans. The present work's main objective was to determine the impact of acute exposure to polystyrene (PS) NPs on the thyroid endocrine system in ZF larvae that had largely completed development.

Methods

Larvae were exposed to a concentration gradient of PSNP (0–10 mg/L) at 120 hours post fertilization for 1h. After exposure, alterations in gene transcriptions of thyroid-related genes were examined via qPCR. In addition, behavioral assays were conducted to evaluate activity patterns in reaction to visual and auditory stimuli, and confocal microscopy was performed to assess NP incorporation using fluorescently labeled NPs. Results: NPs were able to enter ZF larvae within 1h of exposure. They altered the expression of different thyroid-related genes in a concentration-dependent or biphasic manner. In addition, acute NP exposure affected larvae locomotion, with both hypo- and hyperactivity observed depending on the type of stimuli and NP concentration. Conclusion: These findings underscore the urgent need for additional studies on the possible impacts of NPs on human health and offer more proof of NPs' possible mode of action as thyroid disruptors.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085651: Effects of Subchronic Methylmercury Exposure on Response to Acute Hypoxia in Mice: Role of HIF-1α

Chenxv Hu

Jiangsu University

Introduction

Methylmercury (MeHg) is a neurotoxic environmental pollutant. A hypoxic response is an adaptive response of organisms to cope with hypoxia, and HIF-1α is a key nuclear transcription factor in response to hypoxia. Acute MeHg exposure can decrease HIF-1α protein in vitro and in vivo, but the impact of subchronic MeHg exposure on hypoxic response has not yet been elucidated.

Methods

Healthy ICR mice were intraperitoneally infected with 0.25, 0.5, and 1.0 mg/kg of methylmercury, treated with hypoxia in a 250 mL of hypoxia bottle for 15 min, and then recorded the time of death and collected blood, heart tissue, and brain tissue for detection via Western blotting. Analyzing the contents of lactic acid (LA), pyruvate kinase (PK), malondialdehyde (MDA), glutathione (GSH), and HIF-1α.

Results

According to the mouse survival curve, after methylmercury exposure, the hypoxic survival time of mice in the medium- and high-dose groups was significantly shorter than that of the normal saline group. The survival rates of mice in the medium- and high-dose groups were 33.3% and 16.7%, respectively, which were significantly lower than those in the normal saline group. The detection results of lactic acid and pyruvate kinase showed that the effect of subchronic MeHg exposure on the hypoxic adaptation ability of mice was promoted by low doses and inhibited by medium and high doses. Malondialdehyde content increased and glutathione content decreased with MeHg treatment in a dose-dependent manner; the expression of hypoxia-inducible factor-1α protein decreased after hypoxia treatment, but its expression showed an increasing trend with MeHg treatment and vascular endothelial growth. The expression of factor proteins showed an overall upward trend.

Conclusions

Subchronic exposure to methylmercury can aggravate the oxidative damage caused by hypoxia and inhibit the hypoxic response in mice by affecting the expression of HIF-1α. However, cute hypoxia will overexpress HIF-1α protein in the brain tissue of mice with subchronic methylmercury poisoning.

© 2024 by the author. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084527: Effects of Wildfire Smoke on the Reproductive Potential of Male Rats

Vera Vokina, Larisa Sosedova, Elizaveta Andreeva, Mikhail Novikov and Evgeniy Titov

Federal State Budgetary Scientific Institution «East-Siberian Institute of Medical and Ecological Research»

Introduction

The negative impact of wildfire smoke on human health is a unique interdisciplinary problem for the modern scientific community. Despite the fact that wildfires have recently become global, many aspects of the toxic effects of smoke and its components on human health remain unknown. Epidemiological data today convincingly prove the negative impact of smoke from wildfires on human health. At the same time, the multi-component composition of smoke and the presence of potential repro- and genotoxicants determines the need for a comprehensive study of the toxic effects of smoke on the reproductive system, including remote effects manifested in the offspring.

Methods

Adult Wistar male rats were exposed to wildfire smoke inhalation for 1 day, 1 week and 4 weeks (4 h/day, 5 days/week). A histological examination of the gonads and the survival and postnatal development of offspring was carried out.

Results

Smoke exposure for 1 day and 7 days did not reveal a pronounced effect on spermatogenesis parameters. However, increasing the duration of exposure to 4 weeks led to a decrease in the spermatogenesis index and Leydig cells. With exposure to smoke for 4 weeks, the incidence of stillbirth was more pronounced and amounted to 29.4%, while the rate of death of rat pups in the first week of life was 3.6%.

Conclusions

The results obtained can be considered as a fundamental basis for the development of preventive health-saving measures for both the general population and forest firefighters. In addition, the identified dependencies will make it possible to contribute to the assessment of environmental damage from natural fires when assessing the potential ability of small mammals to reproduce.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084493: Environmental Exposure of Children to Silver in Alcalá de Henares (Spain): Risk Assessment Due to Its Presence in Topsoils

Antonio Peña-Fernández [1,2], Manuel Higueras [3], María de los Ángeles Peña [4] and Maria de Carmen Lobo-Bedmar [5]

[1] Department of Surgery, Medical and Social Sciences, Faculty of Medicine and Health Sciences, University of Alcalá, Ctra. Madrid-Barcelona, Km. 33.600, 28871 Alcalá de Henares, Madrid, Spain
[2] Leicester School of Allied Health Sciences, De Montfort University, Leicester, LE1 9BH, UK
[3] Scientific Computation & Technological Innovation Center (SCoTIC), Universidad de La Rioja, Logroño, Spain
[4] Departamento de Ciencias Biomédicas, Universidad de Alcalá, Crta. Madrid-Barcelona Km, 33.6, 28871 Alcalá de Henares, Madrid, Spain
[5] Departamento de Investigación Agroambiental. IMIDRA. Finca el Encín, Crta. Madrid-Barcelona Km, 38.2, 28800 Alcalá de Henares, Madrid, Spain

Silver (Ag) is extensively used in a broad spectrum of personal care products and industrial products. Ag was analysed in scalp hair from 120 children (6 to 9 years old; 70 females) born/residing in Alcalá de Henares (Spain), and in randomly collected topsoils from different urban parks (n = 97) across Alcalá. Ag was detected in all samples (LoDs in hair and topsoils in µg/g: 0.0036, 0.049), except in three hair samples. Levels of Ag were significantly higher in females (median and range, in µg/g): 0.1199 (0.0168-0.4906) vs. 0.08916 (0.0139–0.3841), and slightly lower compared to those reported in hair from children (6–10 years-old) living in Madrid [0.1107 (0.0139–0.4906) vs. 0.251 (0.132–491); all in µg/g]. These authors also reported the deposition of Ag in hair was higher in females. The Spanish capital, Madrid, is more polluted than Alcalá, which could explain our results. Thus, the levels of Ag in Alcalá's topsoils [0.0680 (0.0492–4.0493)] were lower than those reported in other urban areas such as in Athens, Greece [0.260 (0.017–7.430); all in mg/kg]. Although the examination of the pollution index values (2.46; 0.65–53.55; data provided as mean and range) suggest some anthropogenic origin for the Ag found in the topsoils, the distribution of this contaminant was minimal and was only detected in 62 of the topsoil samples collected. Hazard quotients (HQs) for Ag were determined for ingestion and dermal contact; all values were lower than the safety thresholds for HQs (unity), suggesting a minimal risk for the population. Our results suggest that the monitored child population from Alcalá has a minimal exposure to Ag, as the geometric mean was lower than that reported in children living in Iglesias (0.095 vs. 0.13, 0–3 years-old) and much lower than that reported in children living in the polymetallic mining area in the Bolivian Altiplano (0.33, average 7.9 years-old ; all in µg/g).

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084492: Exposure to Platinum Group Elements in Young University Students from Leicester, England

Antonio Peña-Fernánde [1,2], Manuel Higueras [3], Maria del Carmen Lobo-Bedmar [4], Edna Segura [3] and María de los Ángeles Peña [5]

1 Department of Surgery, Medical and Social Sciences, Faculty of Medicine and Health Sciences, University of Alcalá, Ctra. Madrid-Barcelona, Km. 33.600, 28871 Alcalá de Henares, Madrid, Spain
2 Leicester School of Allied Health Sciences, De Montfort University, Leicester, LE1 9BH, UK
3 Scientific Computation & Technological Innovation Center (SCoTIC), Universidad de La Rioja, Logroño, Spain
4 Departamento de Investigación Agroambiental. IMIDRA. Finca el Encín, Crta. Madrid-Barcelona Km, 38.2, 28800 Alcalá de Henares, Madrid, Spain
5 Departamento de Ciencias Biomédicas, Universidad de Alcalá, Crta. Madrid-Barcelona Km, 33.6, 28871 Alcalá de Henares, Madrid, Spain

We assessed dietary exposure to platinum group elements (PGEs; platinum (Pt), palladium (Pd) and rhodium (Rh)) in young adults (18–23 yrs–old) at De Montfort University (DMU, England). In total, 111 (20.45 ± 1.16 yrs-old; 78 female) DMU students completed a validated Food Frequency Questionnaire. PGEs were analysed viaICP-MS in scalp hair provided by 73 of these participants (58 females), as human hair has been described as a reliable tool to monitor environmental exposure to Pd and Pt. Data were processed with the statistical package 'NADA' in R due to a high presence of censored results (data presented as censored percentages and LoDs in µg/g for Pd, Pt and Rh, respectively: 100%, 0.0057; 75.34%, 0.00046; 82.19%, 0.0014). Pt was detected in hair from sixteen female (median and IQR, in µg/g: 0.00014 (0.000036, 0.000551)) and two male participants (P95 = 0.00205, in µg/g); Rh was detected in seven female (P95 = 0.0038, in µg/g) and six male participants (median and IQR, in µg/g: 0.00097 (0.00028, 0.00335)). Only Rh showed sex-dependency (p-value = 0.00392), possibly due to the high presence of censored values in female/male participants. The concentrations of Pt were similar to those reported in adolescents' hair from Palermo, where higher levels in females were also reported. Pt was positively correlated with fatty fish intake (r = 0.292; p-value 0.05) and Rh with the intake of dairy products and fish (r = 0.293, 0.286; p-value 0.05) and very positively with the intake of eggs, meat and crisps and snacks (r = 0.311, 0.315, 0.335; p-value 0.01). The differences in the intake of these foods might explain the sex differences found for Rh in hair. Thus, the intake of eggs (17.625 vs. 16.998 g/day) and meat (271.55 vs. 193.06 g/day) was higher in male counterparts. The differences found for Pt may similarly be explained by the fact that female participants ate more fatty fish (13.41 vs. 10.05 g/day). Our results suggest that DMU students would have experienced a minimal exposure to PGEs.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084545: Fine Aerosol Toxicity in Urban Environments of the Eastern Mediterranean

Despina Paraskevopoulou [1,2], Kalliopi Tavernaraki [1], Irene Maria Vrettou [2], Maria Tsagkaraki [1], Aikaterini Bougiatioti [2] and Nikolaos Mihalopoulos [1,2]

[1] ECPL, Department of Chemistry, University of Crete, P.O. Box 2208, 71003 Heraklion, Greece
[2] IESRD, National Observatory of Athens, I. Metaxa and Vas. Pavlou, 15236, P. Penteli, Athens, Greece

In October 2022, the European Commission published a proposal for a revision of the Ambient Air Quality Directive, introducing stricter thresholds for pollution, more closely aligned with new limits set by the WHO, and strengthening rules for air quality monitoring to support preventive action and targeted measures. One of the latter is the monitoring of the Reactive Oxygen Species (ROS) contained in ambient aerosol. Although a direct mechanism linking PM exposure to health outcomes has not yet been well established, it is believed that ROS (redox-active components, like metals and several organic species), present in polluted air or generated from photochemical reactions, can induce oxidative stress in the human organism. During an intensive measurement campaign, daytime and nighttime $PM_{2.5}$ samples were collected at the urban environment of Ioannina, a rural mountainous moderately inhabited city (0.15M inhabitants), impacted by intense residential wood burning (RWB) for heating purposes especially during winter nighttime, that in combination with its topography, results in a magnified accumulation of atmospheric pollutants. The oxidative potential of the collected samples was determined using a semi-automated system, applying the dithiothreitol (DTT) assay. It is worth noting that nighttime DTT values were three times higher than the daytime ones, highlighting the critical role of RWB in population exposure. Furthermore, the measured OP levels were compared with carcinogenic markers such as polycyclic aromatic hydrocarbons (PAHs) and their oxygenated derivatives (OPAHs). All the aforementioned levels were also compared to the respective values from Athens, the capital of Greece with almost 4 million inhabitants, and from Heraklion, an urban center in Crete, with 0.2M inhabitants. The results elucidate the importance of regional aerosol transportation during the warmest period of the year, and the dominant impact of local sources in wintertime.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084537: Genetic Damage and Multi-Elemental Exposure in Populations in Proximity to Artisanal and Small-Scale Gold Mining Areas in North Colombia

Pedro Espitia-Pérez [1], Lyda Espitia-Pérez [1], Claudia Galeano- Páez [1], Karina Pastor-Sierra [1], Ana Marcela Peñata-Taborda [1], Tatiana Dillenburg Saint´Pierre [2], Solange Cristina García [3] and Hugo Brango [4]

[1] Facultad de Ciencias de la Salud, Grupo de Investigación Biomédica y Biología Molecular, Universidad del Sinú, Calle 38 Carrera 1W, Barrio Juan XXIII, Montería, Córdoba, Colombia
[2] Departamento de Química, Pontifícia Universidade Católica do Rio de Janeiro (PUC-Rio), Rio de Janeiro, Rio de Janeiro, Brasil
[3] Laboratorio de Toxicologia (LATOX), Universidade Federal do Rio Grande do Sul, Avenida Ipiranga, 2752, Porto Alegre, Rio Grande do Sul, Brasil
[4] Departamento de Matemáticas y Estadística, Universidad del Norte, Barranquilla, Colombia

Colombia has seen a significant increase in total gold production. The bulk of auriferous material extraction and processing is conducted through artisanal and small-scale gold mining (ASGM), predominantly focusing on exploiting alluvial deposits. In the northern region of Colombia, a highly active zone for gold production, the intense ASGM activities have result in substantial release of pollutants into the environment, adding to the already present Hg contamination. These pollutants, notably As, Co, Pb, Mn, and Zn, are recognized carcinogens, posing potential combined health risks to the local populations through unknown additive or synergistic effects. This study aimed to assess cytogenetic damage in isolated human peripheral lymphocytes using the cytokinesis-block micronucleus cytome assay (CBMN-Cyt) and its association with multi-elemental exposure measured via Inductively Coupled Plasma Atomic Emission Spectrometry (ICP-AES) analysis of hair samples. The study encompassed 112 healthy subjects, comprising 39 individuals from an unexposed area (Cotorra municipality) and 73 residents from the 'La Mojana' region, known for a high Hg contamination and intense gold mining activities. The findings revealed a significant increase in micronuclei (MNBN), nucleoplasmic bridges (NPB), and frequencies of necrotic and apoptotic cells in binucleated cells among individuals living in proximity to ASGM areas. Hair samples indicated elevated levels of toxic elements such as Pb, Hg, As, Cd, and Ba in exposed residents, while essential elements like Mg, Mn, V, and Sr showed a similar pattern. Positive associations were observed between Hg exposure and MNBN, whereas increased Mn and Pb levels correlated with NPB. Considering MNBN frequency as a predictive biomarker of cancer risk, our results underscore the potential risks posed by this economic activity and multi-elemental exposure to environmentally exposed communities. This emphasizes the critical need for further research in this specific area to inform governmental decision-making.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084429: Human Exposure Characteristics of Liquid Crystal Monomers (LCMs) and Their Mechanisms to Cross the Skin Barrier

Shaohan Zhang, Zhipeng Cheng and Hongwen Sun

Nankai University

Introduction

Liquid crystal monomers (LCMs) are persistent, bio-accumulative, and toxic substances widely used in liquid crystal displays of smart devices. However, little has been known about the human exposure and health risks of LCMs. Here, the human exposure characteristics of LCMs and their mechanisms to cross the skin barrier were explored.

Methods

A suite of 60 LCMs were selected as target compounds. A total of 149 dust samples and 43 paired hand–forehead wipe samples of workers were collected from October to November 2020 in an e-waste recycling industrial park in central China. Forty-eight indoor and ninety-seven outdoor dust samples were collected across mainland China from March to August 2017. The estimated daily intake (EDI) based on the above samples was evaluated to assess the workers' and residents' exposure risks of LCMs. Three-dimensional human skin equivalents were used to quantitatively assess the percutaneous penetration of LCMs. Transporters in the skin were explored via molecular docking analysis.

Results

LCMs were widely detected not only in e-waste areas but also in residents both indoors and outdoors. The median EDI of the total LCMs (ΣLCMs) via dust ingestion and dermal contact of workers were 48.3 and 16.5 ng/kg body weight/day, respectively, indicating a high occupational exposure risk of LCMs. The median EDI of ΣLCMs via dust ingestion, dermal contact, and inhalation of residents were 1.50×10^{-2}, 2.90×10^{-2}, and 8.57×10^{-6} ng/kg body weight/day, suggesting exposure risks of LCMs to residents. LCMs with higher log Kow and molecular weight had more difficulty in crossing the skin barrier. Additionally, ABCG2 (an efflux transporter) may be responsible for the percutaneous penetration of LCMs.

Conclusions

There were exposure risks of LCMs to both workers and residents. Passive diffusion and active transport may be involved in the percutaneous penetration of LCMs.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085607: Human Health Risks to Copper from Urban and Rural Topsoils from East Midlands, England

Gurminderjeet S. Jagdev [1], Carmen Lobo-Bedmar [2], Mª Ángeles Peña Fernández [3], Mark D. Evans [4] and Antonio Peña-Fernández [5]

[1] PhD Research
[2] Research in IMIDRA (Madrid Institute for Rural, Agricultural and Food Research)
[3] University of Alcalá
[4] Professor in Leicester School of Allied Health Sciences, De Montfort University, Leicester
[5] Professor in Department of Surgery, Medical and Social Sciences, Faculty of Medicine and Health Sciences, University of Alcalá

Introduction

The purpose was to determine the distribution of copper (Cu) in topsoils from urban public parks across Leicester and its rural surroundings (Leicestershire, England).

Methods

A total of 850 topsoil samples were collected (2017-18). 26 composite samples were appropriately prepared after mixing samples collected per location (18 urban, 8 rural), which were further processed in duplicate. Cu was measured twice in each of the 52 composite samples by ICP-MS after acid/microwave digestion with nitric acid (69%)/chlorhydric acid (37%).

Results

Cu was found in all composites examined (LoD = 1.335 mg/kg). Significantly higher levels were found in the urban areas [43.784 (27.200, 56.190) vs. 32.678 (20.280, 35.710); data presented as median and IQR, in mg/kg; Peto-Prentice test, $\chi^2(1) = 7.4$, p-value = 0.007)], which might be logical as this metal is associated with traffic density. This would be supported by the enrichment factors calculated for rural topsoils (EF = 0.101), which suggests minimal anthropogenic influence. Moreover, significant differences (p-value = 3E-05) were found between the four ordinal directions dividing the Leicestershire region monitored to study the distribution of Cu, showing the following distribution SW (51.345) > NW (43.827) > SE (37.262) > NE (20.052; all medians in mg/kg), suggesting a wide distribution in Leicestershire. Toxic risks derived from oral, inhalation and dermal exposure to Cu from topsoils in the urban four ordinal directions and in all rural topsoils monitored were 1, suggesting minimal non-carcinogenic risks from the exposure to Cu present in topsoils.

Conclusions

Thus, the presence and distribution of Cu in Leicestershire's topsoils would not represent a significant risk for the population. In general, the range of Cu found (9.580–101.229 mg/kg) would suggest that the monitored topsoils were not polluted, if we consider the threshold proposed by the Finnish and Swedish legislations to denote unpolluted soils (100 mg/kg). However, a continuous monitoring would be recommended to protect the public.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084291: Impact of Microfibers on the Marine Microalgae *Phaeodactylum tricornutum*

Francisco Ríos, Cristina Tapia-Navarro, Josefa Nuñez-Olea, Juan Francisco Martínez-Gallegos and Mercedes Fernández-Serrano

University of Granada

Introduction

During each wash of textile materials, millions of natural and plastic microfibers (MFs) are discharged into wastewater due to the wear and friction generated on fabrics during the washing process. MFs reach wastewater treatment plants (WWTPs) or are directly released into aquatic bodies (rivers, lakes, lagoons, or oceans). Up to 20% of these MFs cannot be captured in WWTPs and are likely released directly into aquatic environments.

Several studies have discussed the environmental and health impacts caused by MFs, which are toxic to some aquatic organisms and persist in the environment. In this work, we study the effects of synthetic and natural MFs on the marine microalgae Phaeodactylum tricornutum.

Methods

In this study, we used two types of microfibers, namely MF A, composed of 100% polyester, and MF B, composed of 100% cotton. Microfibers were obtained via micro-cutting of standard fabrics supplied by the Center For Test Materials B.V.

A toxicity test was carried out on the marine microalgae following the ISO 10253:2006 Guideline. The specific growth rates and the percentages of growth inhibition were calculated at 24, 48, and 72 hours.

Results

The results reveal that the specific growth rate of Phaeodactylum tricornutum decreased due to the presence of MFs.This effect was more pronounced in the case of natural MFs (B) when compared with a control without MFs. The percentage of growth inhibition was 12.8% for polyester MFs (A), whereas in the case of cotton MFs (B), it reached 37.1% after 72 hours

Conclusions

Microfibers, both synthetic and natural, have a negative effect on the normal growth of the marine microalgae Phaeodactylum tricornutum.

The negative effects of cotton MFs on microalgae are more pronounced compared with those caused by polyester MFs, probably due to the higher adsorption of nutrients onto natural MFs.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084507: Impact of Polycyclic Aromatic Hydrocarbons on the Environment and Human Health: Evidence Retrieved from Biomonitoring Studies

Joana Teixeira [1], Cristina Delerue-Matos [2], Simone Morais [2], Marta Oliveira [3]

[1] REQUIMTE/LAQV-Instituto Superior de Engenharia, Instituto Politécnico do Porto; REQUIMTE/UCIBIO, Unidade Biociências Moleculares Aplicadas, Departamento de Ciências Biológicas, Faculdade de Farmácia da Universidade do Porto
[2] REQUIMTE/LAQV-Instituto Superior de Engenharia, Instituto Politécnico do Porto
[3] REQUIMTE-LAQV-Instituto Superior de Engenharia do Porto

The presence of polycyclic aromatic hydrocarbons (PAHs) in different environmental matrices has significant repercussions on ecosystems and human health. There is a need to reunite and revise the available literature to improve the evaluation of the impact of PAHs on the environment and human health. This work compiles, for the first time, the concentrations of PAHs in the air, aquatic ecosystems, and soils, with a global overview of the results from environmental and human biomonitoring studies. The higher incidence of anthropogenic occupancy is directly associated with the presence of PAHs in the environmental matrices (1344.4–12300 ng/m^3 versus 0.03–0.60 ng/m^3 in the air in industrial/urban and rural areas, respectively; 2.00–1.66 × 10^7 ng/L and 7.00 × 10^{-4}–1.00× 109 ng/g in the water systems and aquatic sediments from coastal areas, respectively; 0.14–1.77 × 10^6 ng/g and 1.59–5.87 × 10^3 ng/g in urban and rural soils, respectively). Benzo(a)pyrene, a carcinogenic PAH, was found in all the environmental matrices. The potential of some sentinel species (e.g., mosses, lichens, tree leaves, bivalves, and cephalopods) used as biomonitors in environmental biomonitoring studies is described. Despite the growing concern about the negative impacts of PAH exposure, more biomonitoring studies are crucial to characterize the impact of PAHs on the environment and human health and estimate the associated risks for wildlife and humans. Mitigation and preventive measures for PAH exposure can be beneficial to protect human health due to the improvement in the human–animal–environment interface.

Funding: This work was funded by project PCIF/SSO/0090/2019 by the Fundação para a Ciência e a Tecnologia, Ministério da Ciência, Tecnologia e Ensino Superior (FCT-MCTES) through national funds.

Acknowledgements: This work received support from UIDB/50006/2020, UIDP/50006/2020, LA/P/0008/2020, 2022.05381.PTDC, and PCIF/SSO/0017/2018 by FCT-MCTES. M. Oliveira thanks to the scientific contract CEEC—Individual 2017 Program Contract CEECIND/03666/2017.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085624: Impact of Temperature and Relative Humidity Variability on Children'S Allergic Diseases and Critical Time Window Identification

Shumin Yu [1], Francis Manyori Bigambo [2], Zhiyu Zhou [3], Sabitina Mrisho Mzava [4], Haiyue Qin [5], Ling Gao [6] and Xu Wang [7]

[1] Department of Toxicology, School of Public Health, Nanjing Medical University
[2] Department of Endocrinology, Children's Hospital of Nanjing Medical University
[3] Department of Orthopedics, Children's Hospital of Nanjing Medical University
[4] Muhimbili National Hospital
[5] Nanjing Foreign Language School
[6] Department of Clinical Laboratory, Children's Hospital of Nanjing Medical University
[7] Nanjing Medical University

Background

Several studies have shown associations between respiratory allergies in children and climate variables such as temperature and relative humidity. However, the effects of average temperature and relative humidity on different types of children's allergic diseases have not been comprehensively evaluated so far. This study aims to assess the impact of temperature and relative humidity variability on children's allergic diseases and to identify the critical time window.

Methods

We collected outpatient data on allergen testing in children between July 2020 and January 2022 from the Affiliated Children's Hospital of Nanjing Medical University. Logistic regression was used to evaluate the effect of temperature and relative humidity on allergic diseases. Subgroup analysis by gender was conducted in different types of allergic diseases, among which propensity score matching was performed for digestive allergies, and age-specific analysis was performed to identify the critical time window.

Results

We found that total allergies and skin allergies were negatively associated with temperature and positively associated with relative humidity. While digestive allergies were positively associated with temperature and negatively associated with relative humidity. Children under 5 years were more susceptible to the effect of temperature and relative humidity. However, we did not find any association between temperature and relative humidity with respiratory allergies.

Conclusions

Our study provides evidence that temperature and relative humidity variability may have a greater risk for the occurrence of allergic diseases in children, especially skin allergies and digestive allergies. Children under 5 years were more susceptible to the effect of temperature and relative humidity.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085819: Is Tamoxifen Cytotoxicity against Breast Cancer Cells Influenced by Xenoestrogens?

Rita Couto [1] Beatriz Cunha [2], Eduardo Rocha [1] and Fernada Malhão [2]

[1] Laboratory of Histology and Embryology, Department of Microscopy, ICBAS – School of Medicine and Biomedical Sciences, University of Porto (U.Porto), Rua Jorge Viterbo Ferreira 228, 4050-313 Porto, Portugal. Team of Animal Morphology and Toxicology, CIIM
[2] Laboratory of Histology and Embryology, Department of Microscopy, ICBAS – School of Medicine and Biomedical Sciences, University of Porto (U.Porto), Rua Jorge Viterbo Ferreira 228, 4050-313 Porto, Portugal. Team of Animal Morphology and Toxicology, CIIMAR

Tamoxifen (TAM) is a chemical widely used in hormone therapy to treat hormone receptor-positive breast cancer (BC). Humans are regularly exposed to xenoestrogens, i.e., chemicals like bisphenol A (BPA) and endosulfan (END), which mimic the natural endogenous estrogens in many pathways and may potentiate (at least in theory) BC risk. BPA is one of the most produced chemicals worldwide used in polycarbonate plastic in food and drink packaging. END is an organochlorine pesticide that, although considered probable and carcinogenic to humans, is still illegally used in some countries. Both xenoestrogens share similar routes of exposure to humans through ingestion, and we wonder if such exposure may model the TAM impacts against BC cells. Therefore, in this study, we aimed to investigate the in vitro cytotoxicity effects of TAM, BPA, and END in single exposures, followed by the effects of co-exposures (TAM+BPA and TAM+END) on the MCF7 cell line (representative of hormone-positive BC). We intended to study the impact of TAM's therapy outcome in ER-positive BC cells when simultaneously exposed to the referred xenoestrogens. The cytotoxic effects were assessed by MTT and SRB assays, and cells' morphology rates were monitored and photographed during the experiments. Overall, TAM, BPA, and END showed a reduction in cell viability relative to the control. The combinations of TAM with BPA and END showed a statistically significant decrease in cell viability compared to the control and the compounds alone. The results support the notion that BPA and END can be cytotoxic to MCF7 alone but also interfere with the TAM effects. The current data call for further research in order to investigate the modulation of these ubiquitous and xenoestrogenic pollutants over established endocrine therapies for BC.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084689: Morphological Changes of Ovaries under the Influence of Lead Acetate and Theit Relations with Biochemical Changes in the Experiment

Yroslav Bilyk

Horbachevsky Ternopil Medical National University

Lead as an environmental pollutant and toxic agent remains to be in the center of attention of specialist from different areas of medicine and biology.

The aim of work was to study the effect of different doses of lead acetate (LA) on biochemical parameters and morphological picture of the ovaries in the experiment.

The study was carried out on 40 nonlinear female rats divided into 4 experimental groups: I—control, II group—rats that during 30 days drink LA solution in the dose of 0.05 mg/kg of body weight, III and IV group—dose of 10 mg/kg and 60 mg/kg, respectively. The blood of animals and ovaries were taken for histological and biochemical examination.

It was determined, that LA caused activation of peroxidation of lipids and proteins in the rats, which is directly dependent on the dose of lead. In response to the activation of free radical oxidation there were changes in the antioxidant system, which depend on the dose of LA: at a dose of 0.05 mg/kg superoxide dismutase and catalase activity were increase, at a dose of 60 mg/kg superoxide dismutase and catalase activity significantly decreased.

Morphological examination showed that structural components of ovary cortex and medulla were changed: moderately increased blood supply of the cortex and medulla was found in the ovaries of animals given low doses of LA. Analysis of the state of follicles in the cortex of the ovaries showed that in group IV animals, there was a slight increase in the number of primordial follicles in non-ovulating ovaries, increase in tunica albuginea thickness, slight decrease in atretic follicles, the number of follicles in the cortex at all stages of their growth and development were decreased.

Conclusions

Small doses of lead did not cause the development of endogenous intoxication, in contrast to high doses, which increased the formation of toxic compounds.

© 2024 by the author. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085767: Microplastic Presence in Commercial Sea Salt: Sampling and Quantification Challenges

Cristina Di Fior [1], Maria Pia Sammartino [2], Cristina Giannattasio [3], Pasquale Avino [1] and Giovanni Visco [2]

[1] Department of Agricultural, Environmental and Food Science, University of Molise, via De Sanctis, I-86100 Campobasso, Italy
[2] Department of Chemistry, University of Rome "La Sapienza", p.le Aldo Moro 5, I-00185 Rome, Italy
[3] Department of Chemistry, University of Rome "La Sapienza", p.le Aldo Moro 5, I-00185 Rome, Italy

Introduction

The presence of microplastics in sea salt has become an issue of a public concern due to the potential negative effects that microplastics could have on human health. Salt, in fact, could be seen as a carrier of microplastics into organisms. However, the quantification of microplastics in sea salt is still hampered by methodological limitations. In Italy, there are three important salterns characterised by global relevance, given the significant export of Italian salt to foreign countries.

Methods

In this work, sea salts collected from Italian salterns were investigated in terms of microplastics contamination. From a methodological point of view, the salt samples were solubilised in MilliQ water and filtered to extract the microplastics. The microplastics were visually quantify using a stereomicroscope. Hence, the microparticles present were classified by their morphological characteristic details, like shape, size and colour. Afterwards, the microparticles isolated were chemically identified using ATR-FTIR and Raman spectroscopy to assess the polymer type.

Results

The results showed an average of 1653 ± 29 microplastics/kg of sea salt. Regarding the shape, 80.6% of the microplastics had a fiber shape, 18.9% had a fragmented shape, and 2.7% were spheres. The sizes of the microplastics ranged between 0 and 500 µm, reflecting the presence of a potentially relevant fraction from a human health perspective. ATR-FTIR and Raman spectroscopy confirmed the plastic nature of the microparticles. Particularly, polypropylene, polyamide, and polyethylene were the most abundant polymer types in the samples.

Conclusions

This work confirmed the presence of microplastics in the sea salt samples, with a fraction of "small" microplastics, which could represent a threat to humans. Further investigations are required to assess the contamination levels of microplastics in the food chain in depth, as well as their impact on humans.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-083806: Multielemental Profile of Peritoneal Fluid in Gynaecology Patients Presenting with Uterine Myomas

Andrea López-Botella [1,2], María José Gómez-Torres [1], José -Luis Todolí-Torró [2], Raquel Sánchez-Romero [2], Irene Velasco [1,3] and Maribel Acién [3,4]

[1] Biotechnology Department, Faculty of Sciences, University of Alicante
[2] Department of Analytical Chemistry, Nutrition and Food Sciences, University of Alicante
[3] Service of Obstetrics and Gynecology, Unit of Human Reproduction, FISABIO
[4] Gynecology Division, Faculty of Medicine, Miguel Hernández University

Introduction

Uterine myomas are benign tumours that usually grow in the uterus. They are considered an estrogen-dependent disease which has been associated with an increased expression of estrogen receptor-α. Exposure to endocrine disruptor compounds (EDCs) acting as exogenous estrogens, such as cadmium, may be associated with the development of the disease. The aim of this study was to describe the multielemental profile of peritoneal fluid (PF), including potentially toxic elements (PTEs) and EDCs such as Pb and Cd in women presenting with uterine leiomyomas compared to control patients.

Methods

Ten PF samples were collected from female patients from the gynaecology division of San Juan de Alicante University Hospital, Spain, during laparoscopic surgery for ovarian cysts. PF samples were collected via aspiration into a sterile syringe, filtered through a 20 µm filter, and transferred to a glass centrifuge tube. The supernatants were stored in the dark at -20 °C until analysis. The diagnosis of uterine leiomyomas was confirmed via ultrasonography prior to surgery. Thus, the patients were divided into two groups: leiomyoma (n: 5) and control group (n: 5). An Agilent 8900 ICP-MS/MS (Agilent Technologies. Santa Clara, CA, USA) was used to analyse the samples. The clinical history of the patients was investigated to obtain clinical data, and information regarding lifestyle and exposition to PTEs was collected using a questionnaire (RedCap).

Results

Concerning the elemental profile of PF, some PTEs (Ba, Ni, and V) were found in higher concentrations in the leiomyoma group. However, EDCs such as Cd and Pb were not quantified in the leiomyoma group.

Conclusions

The preliminary results of our study show that some PTEs, but not EDCs, were found in higher concentrations in the PF of women presenting with uterine leiomyomas. This report reveals that some PTEs could be involved in the development of the disease, although additional research is needed to confirm these differences.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085297: Nanomaterial Exposure Assessment of Carbonaceous Compounds from Carbon Fiber Processing Laboratory

Mat Tamizi Zainuddin, Sudirman Sahid, Mohamad Azmirrudin Ahmad and Nurazilah Mohd Zainon

Industrial Centre of Innovation in Biomedical, SIRIM Berhad, Kulim HiTech Park, MALAYSIA

Expanding applications on nanomaterial-based products of carbon fiber from research to industry should be considered on the concern aspects of potential toxicity especially in occupational safety related to the nano-particulate emission. In order to evaluate this matter as well as their interaction towards biological for hazardous evaluation, it is important to comprehend and precisely determine their physicochemical properties. In spite of that, inconclusive data on physicochemical properties still being a stumbling point for an authoritative framework on nanomaterials to synchronize the relevance of certain physicochemical endpoints toward toxicological effects. The question arise on which physicochemical endpoints or technological solutions are currently available to support the requested characterization of nanomaterial-based products. Established standard test method that could be satisfactory to evaluate physicochemical endpoints has been strategized to pinpoint such decision framework for nanomaterials assessment. This work encompasses chemical and physical methods from multiple points of analytical techniques for determination of physicochemical parameters on nanoparticulate emission within carbon fiber processing laboratory. Microscopic analysis through SEM and TEM revealed the presence of carbon nanofiber with diameter ranging from 80 to 250 nm with several aggregation and agglomeration states whereas data from EDS stated the presence of carbon, oxygen and silicon elements within the collected nano-emission particles. Data from these physicochemical analysis and concentration of exposure have been synchronized toward formation of control banding within nanomaterial risk assessment in order to address exposure prevention and risk management in a consistent manner to be useful and interpretable for future users of nanomaterial risk assessment for such carbon fiber processing. These data have been synchronized in developing the control banding within nanomaterial risk assessment toward formation of exposure prevention and risk management in a consistent manner to be practical and interpretable for future activities in the carbon fiber processing laboratory.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084410: Nanoplastics as a Vehicle for Environmental Pollutants: A Hazard for Human Health

Carina Ladeira [1], José Cabêda [2]

[1] H&TRC—Health & Technology Research Center, Escola Superior de Tecnologia da Saúde de Lisboa (ESTeSL), Instituto Politécnico de Lisboa, Avenida D. João II, lote 4.69.01, Parque das Nações, 1990-096 Lisboa, Portugal; NOVA National School of Public Health
[2] Guarda Nacional Republicana, Destacamento Territorial de Vila Franca de Xira, Núcleo de Proteção Ambiental

Plastic waste degrades into small particles, which depending on their size can be classified as microplastics (0.001–5 mm) or nanoplastics (up to a maximum of 0.001 mm), and which can be transported by air, water and food. In humans, contamination by these particles occurs through the airways, through contact with personal products, and through the consumption of food and water. This causes direct or indirect damage to the body's homeostasis. Studies carried out in the area of nanoplastics verify that due to their size, these particles have a capacity for internalization, causing damage to membranes and organelles, inflammation, cytotoxicity, and cell death, among others.

In addition to these effects per se, nanoplastics are the polymers with the greatest impact on the environment, as they can absorb and, in this way, act as vectors of highly toxic compounds, such as aromatic hydrocarbons, heavy metals, persistent organic pollutants (POPs), and endocrine disrupting chemicals (Bisphenol A, Phthalates), among others. In the specific case of POPs, they are directly linked to hormonal, immunological, neurological, and reproductive dysfunctions. They remain in the environment for a long time and, once ingested, they have the ability to attach themselves to the body fat, blood, and body fluids of animals and humans. Packaged products also contain Bisphenol A in their composition, a known endocrine disruptor, exposure to which is associated with various diseases such as diabetes, polycystic ovary syndrome, infertility, and uterine fibroids, among others.

In summary, given the ubiquity of plastics in the environment, their potential for transporting other toxic substances, as well as their versatility of absorption through different routes of exposure, they meet the conditions to be considered a hazard for human health.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085590: Neonatal Cytokines: Mediator and Indicator of $PM_{2.5}$ Exposure during Early Pregnancy and Childhood Eczema

Mingzhi Zhang [1], Xu Wang [2] and Yankai Xia [1]

[1] Nanjing Medical University
[2] Children's Hospital of Nanjing Medical University

Background

Previous studies have shown that neonatal cytokines could have harmful effects on allergic diseases in childhood. However, the impact of maternal exposure to $PM_{2.5}$ and its components on the development of fetal immune systems and allergic diseases in childhood remains unclear.

Methods

A total of 482 mother-infant pairs were included. Maternal exposure to $PM_{2.5}$ and its six main components was assessed, and 27 kinds of cytokines were detected using heel-prick blood specimens from newborns. General linear regression and weighted quantile sum regression analyses were used to investigate the association between maternal exposure and neonatal cytokines. The K-means algorithm was used for cluster analysis to categorize the infants into different groups based on their cytokines. Principle component analysis was then used to validate it. Finally, general linear regression models and LASSO regression were employed to identify the associations between neonatal cytokines and eczema in childhood.

Results

Negative associations were observed between maternal exposure to $PM_{2.5}$ and components with neonatal IL7 ($\beta = -0.05$, 95%CI: (-0.07, -0.03), p 0.001), IL12 ($\beta = -0.04$, 95%CI: (-0.06, -0.01), $p = 0.05$) and IL13 ($\beta = -0.04$, 95%CI: (-0.06, -0.02), $p = 0.02$) while positive associations with neonatal Eotaxin ($\beta = 0.17$, 95%CI: (0.09, 0.25), p 0.001), PDGFbb ($\beta = 0.05$, 95%CI: (0.07, 0.23), $p = 0.01$), MIP1b ($\beta = 0.10$, 95%CI: (0.05, 0.15), p 0.001), RANTES ($\beta = 0.32$, 95%CI: (0.22, 0.41), p 0.001). Meanwhile, WQS indexes were statistically associated with all seven neonatal cytokines in both robust and fully adjusted models (p0.001). In addition, children with higher IL7 (OR = 10.57, 95%CI: (1.60,73.82) , $p = 0.02$) and lower RANTES (OR = 0.65, 95%CI: (0.43, 0.95), $p = 0.03$) levels were significantly associated with an increased risk of eczema in childhood.

Conclusions

Maternal exposure to $PM_{2.5}$ was associated with neonatal cytokines and had lasting effects on eczema in childhood. IL7 and RANTES could act as mediators between $PM_{2.5}$ exposure and eczema in children.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084501: Oxidative Potential as a Health Risk Estimation of Ambient $PM_{2.5}$ in Chiang Mai City, Northern Thailand: A Study in 2021

Teetawat Santijitpakdee [1,2,3], Tippawan Prapamontol [1], Pitakchon Ponsawansong [1], Sawaeng Kawichai [1], Nichakorn Taejajai [1], Wenhuai Song [3], Fang Cao [3] and Yan-lin Zhang [3]

[1] Environment and Health Research Group, Research Institute for Health Sciences (RIHES), Chiang Mai University, Chiang Mai 50200, Thailand
[2] School of Health Sciences Research (SHSR), Research Institute for Health Sciences (RIHES), Chiang Mai University, Chiang Mai 50200, Thailand
[3] School of Applied Meteorology; Atmospheric Environment Center, Joint Laboratory for International Cooperation on Climate and Environmental Change, Ministry of Education (ILCEC), Nanjing University of Information Science & Technology, Nanjing 210044, China

This study aims to ascertain the oxidative potential (OP) of $PM_{2.5}$ in Chiang Mai (CM) City, Northern Thailand, which suffers from severe air pollution involving health risk. The dithiothreitol assay (DTT) was used to analyze the OP of 53 samples of $PM_{2.5}$ filters collected between January and April 2021 using a medium-volume air sampler with a flow rate of 100 L/minute for 24 hours every other day. We analyzed components of $PM_{2.5}$ including carbonaceous content [i.e., organic carbon (OC), elemental carbon (EC), water soluble organic carbon (WSOC)], eight water-soluble inorganic ions (WSIIs), and twenty-one metal components.

The study found that OP^{DTTv} (volume-normalized DTT activity) in $PM_{2.5}$ had an average of 0.13 ± 0.01 nmol/min/m^3 and OPDTTm (mass-normalized DTT activity) of 2.44 ± 0.24 pmol/min/μg. OP^{DTTv} was moderately correlated with carbonaceous components (r = 0.44–0.50, P 0.01), WSIIs components (r = 0.41–0.55, P 0.01), and metal components (r = 0.40–0.48, P 0.01). There is no significant positive correlation between such $PM_{2.5}$ components and the OPDTTm found in this study. Interestingly, moderate positive correlations were observed between OP^{DTTv} and potassium (K, K^+) and WSOC, indicating that these sources were primarily derived from biomass combustion tracers and secondary organic aerosols, respectively. Moderate positive correlations were also observed between OP^{DTTv} and secondary ions (NO_3^-, NH4$^+$). The redox-active nature of NO3- produced by gases and free radicals led to OP^{DTTv} associations with secondary ions. Furthermore, associations were found between OP^{DTTv} and transition metals such as copper (Cu) and iron (Fe), which contribute to generating oxidative stress.

Our study showed that the OP of $PM_{2.5}$ is dominated by carbonaceous components from burning biomass, secondary organic aerosols, and transition metals. Further OP studies of other chemical components in $PM_{2.5}$ should also be explored to estimate more potential health risks.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-082696: $PM_{2.5}$-Induced Declined Cardiac Tolerance to Ischemia-Reperfusion Injury Can Be Ameliorated by Hydrogen Sulfide

Bhavana Sivakumar and Gino Kurian

SASTRA Deemed University

Early studies have documented that $PM_{2.5}$ can not only induce cardiac tissue toxicity, but can adversely affect the performance of the myocardium and deteriorate its tolerance to withstand ischemia-reperfusion (IR) injury. The primary factor that contributes to the adverse impacts of $PM_{2.5}$ exposure on the heart is subcellular changes, with particular emphasis on mitochondrial dysfunction, inflammation, oxidative stress, and deterioration of pro-survival signaling pathways. Despite the ongoing efforts to uncover the mechanistic changes induced in the heart by $PM_{2.5}$ exposure, no studies have presented strategies for mitigating $PM_{2.5}$-induced cardiotoxicity or enhancing the tolerance of the myocardium to withstand IR injury. Considering the potential of hydrogen sulfide, a gasotransmitter known to protect the heart from pathologies linked to oxidative stress and mitochondrial dysfunction, we explored the efficacy of H2S in attenuating $PM_{2.5}$-associated increased IR injury. Female Wistar rats were exposed to 250 ug/m^3 of $PM_{2.5}$ for 3 hours daily for 21 days, after which the hearts were isolated and mounted on an isolated rat heart apparatus. H2S was administered directly to the $PM_{2.5}$-exposed hearts, after which the hearts were subjected to 30 min of ischemia and 60 min of reperfusion to induce IR injury. Our results revealed that the ability of the $PM_{2.5}$-exposed myocardium to withstand IR injury had considerably improved. The pivotal mechanism driving these beneficial changes was the preservation of mitochondrial function (improved bioenergetics, respiration) along with quality control mechanisms. The improvement in mitochondrial function was also reflected in terms of reduced oxidative stress and activation of pro-survival signaling pathways. Based on these findings, we concluded that hydrogen sulfide holds promise as a potential therapeutic agent for enhancing the myocardium's resilience to additional stressors in the form of IR injury.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085621: Plant-Based Approaches for Wastewater Management: A Comprehensive Review of Phytoremediation Techniques

Krishna Neeti, Reena Singh and Abhishek Kumar

National Institute of Technology Patna

Wastewater management is a complex issue that requires attention due to the presence of harmful pollutants, toxic particles, and emerging contaminants that originate from industrial activities. These pollutants can contaminate the soil and surface water, and infiltrate groundwater, posing health risks to humans and animals alike. The emerging contaminants in wastewater, such as pharmaceuticals, personal care products, pesticides, and flame retardants, are primarily synthetic organic compounds that pose serious risks to human health and biota. The demand for freshwater is increasing, which necessitates significant investments in capital and energy for water treatment plants. This review article explores the innovative use of plants in wastewater treatment, specifically through bioaccumulation. Various phytoremediation techniques, such as phytovolatilization, phytoextraction, phytofiltration, rhizofiltration, phytodegradation, phytostabilization, and phytoassimilation, are explored as sustainable alternatives. Aquatic plants, such as water hyacinth, duckweed, and water lettuce, stand out for their exceptional phytoremediation capabilities. These plants can be used to remove pollutants from wastewater, making it safe for reuse or discharge into the environment. The use of plants in wastewater treatment is a cost-effective and eco-friendly approach that can help address the growing water scarcity problem. By using phytoremediation techniques, we can reduce the need for expensive and energy-intensive treatment methods, while also promoting the growth of green spaces in urban areas. This article underscores the potential of plant-based strategies in wastewater management, emphasizing their role in mitigating environmental contaminants and safeguarding public health.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085657: Potential Risk of Cyclopiazonic Acid Toxicity in Kodo Millet (*Paspalum scrobiculatum* L.) Poisoning

Mamatha Bhanu L S

Yuvaraj's College, University of Mysore

Kodo millet, a staple food in North India, is frequently consumed, but its consumption can lead to intoxication and poisoning. Kodo millet is a rich source of nutrition, with anti-oxidant and medicinal properties, and is typically cultivated in dry and semi-arid regions. It is often infected by fungal species rather than bacterial and virus pathogens, causing economic crop loss and adversely affecting grain and fodder yield. Ergot, a parasitic fungal endophyte found in Kodo millet ear heads, can cause poisoning when consumed. Moreover, Kodo millet grains are frequently infested with *Aspergillus tamarii* Kita, which produces a significant amount of the mycotoxin cyclopiazonic acid (CPA). Cyclopiazonic acid (CPA) is a neurotoxin produced by certain *A. flavus* and *Aspergillus oryzae* strains, which produce aflatoxins. Mycotoxicosis outbreaks in humans are not well characterized, and the direct correlation between mycotoxin consumption and toxic effects in vivo is not well established. CPA, a specific inhibitor of sarcoplasmic reticulum $Ca2^{+-}$ATPase, can adversely affect broiler chicken health, as demonstrated by toxicological evaluation of aflatoxins and CPA alone or in combination. Most toxins have reported acute and chronic effects in prokaryotic and eukaryotic systems, including humans, despite thefact that their specific modes of action are unclear. This review explores fungal pathogens, the toxicity of CPA to animals and humans, both by itself and in combination with other mycotoxins, as well as biocontrol strategies and storage methods for better utilization of Kodo grains post harvest.

© 2024 by the author. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084409: Reuse of Wastewater: Concerns about the Effects of Mixtures of Chemical Substances on Human Health

José Cabêda [1], and Carina Ladeira [2]

[1] Guarda Nacional Republicana, Destacamento Territorial de Vila Franca de Xira, Núcleo de Proteção Ambiental
[2] H&TRC—Health & Technology Research Center, Escola Superior de Tecnologia da Saúde de Lisboa (ESTeSL), Instituto Politécnico de Lisboa, Avenida D. João II, lote 4.69.01, Parque das Nações, 1990-096 Lisboa, Portugal; NOVA National School of Public Health

Due to global warming, new practices should be adopted in the use of wastewater in the agricultural, industrial, and urban sectors. In the European context, the countries of the Southern Mediterranean are those that present the greatest vulnerabilities, and those on which inaction will take the greatest toll.

The regulation approved on 13 May 2020, by the European Parliament establishes minimum requirements for the reuse of treated urban wastewater, aiming to guarantee an alternative water supply.

Although low concentrations of chemical contaminants may be present in the environment, their effects can be exacerbated by the presence of other chemical substances, acting as chemical mixtures. In the specific case of wastewater, studies have reported the presence of biocides, pesticides, dermocosmetic products (including UV filters), pharmaceuticals, and detergents, among many others, which constitute a mixture of micropollutants with concentrations ranging between ng/L and µg/L. As individual components, all of these substances are toxic to humans. Since there is a gap in the risk assessment of chemical mixtures, an interesting proposal would be the implementation of a combined method comprising the chemical analysis of water and the study of these mixtures' potential effects through in vitro exposure to extracts isolated from different wastewaters in culture. This way, the potential genetic damage and the effects on immunomodulation, inflammation, and several other biomarkers can be studied at the chemical mixture level.

Even though these practices are not commonly adopted in Portugal and the maximum values of chemical substances are predetermined, the effects of a mixture are expected to exceed the effects of individual substances through toxicological reactions such as addition, potentiation, and synergy. Furthermore, through the phenomenon of globalization, the supply of these foodstuffs in national markets will become a reality, making food a route of exposure to these substances throughout the food chain.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084381: Spatiotemporal Gradients of PAHs in Greek Urban Environments and Subsequent Health Impacts

Irini Tsiodra [1], Kalliopi Tavernaraki [1,2], Georgios Grivas [1], Kyriaki Papoutsidaki [2], Despina Paraskevopoulou [1,2], Eleni Liakakou [1], Constantine Parinos [3], Alexandra Gogou [3], Aikaterini Bougiatioti [1] and Nikoalos Mihalopoulos [1,2]

[1] IERSD, National Observatory of Athens
[2] ECPL, Department of Chemistry, University of Crete
[3] Institute of Oceanography, Hellenic Centre for Marine Research

During seasonal campaigns in six contrasting urban environments in Greece, $PM_{2.5}$ filter samples were collected and analyzed to study the spatiotemporal variability of polycyclic aromatic hydrocarbon (PAH) levels and examine the link to toxicity and subsequent long-term health impacts expressed using carcinogenic risk estimates. Sampling sites included a variety of urban background and traffic (Athens, Heraklion, and Ioannina with approximately 3.5 M, 0.2 M, and 0.15 M inhabitants, respectively), rural (Xanthi, 0.05 M inhabitants) and port locations (Piraeus and Volos with 0.5 M and 0.15 M inhabitants respectively). When considering the 16 EPA priority PAH members, quite homogeneous levels were observed across locations during summer, almost independently of the population (from 0.4 ng m^{-3} in Xanthi and Ioannina to 0,6 ng m^{-3} in Heraklion, and 0.8 ng m^{-3} in Athens). The highest levels during summertime (2.2 ng m^{-3} and 1.2 ng m^{-3}, respectively) were observed in Piraeus and Volos, known for their industrial and harbor activities. On the other hand, during winter, levels were significantly higher compared to summer, with the enhancement ranging from ∼12 times for most of the sites to a striking 95 times for Ioannina, indicating the significant role of local emissions, especially heating. When solely considering B[a]P, an IARC Group 1 carcinogen and the only EU-regulated PAH, the winter/summer ratios were ∼22 in Athens, Volos, and Xanthi, 50 in Piraeus, and 366 in Ioannina that is afflicted by severe wood burning pollution events. The identified spatiotemporal contrasts, which are explored for the first time for PAHs at such a scale in the Eastern Mediterranean, provide important insights into sources and controlling atmospheric conditions, and reveal large deviations in exposure aggravation among cities, which also raises an issue of environmental injustice on a national level.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085608: Toxic and Essential Metals in *Stenella coeruleoalba*: Assessment of Marine Environmental Pollution and Dolphin Health Status

Clara Naccari [1], Vincenzo Ferrantelli [2], Roberto Bava [1] and Ernesto Palma [1]

[1] Department of Health Sciences, Univerisity "Magna Graecia" of Catanzaro, Italy
[2] Istituto Zooprofilattico Sperimentale della Sicilia "A. Mirri", Palermo , Italy

Introduction

Heavy metals are environmental contaminants and can easily accumulate and biomagnificate in various species (fishes and mammalians) at the top of the aquatic food chain. Among marine mammalians, the common dolphin (*Stenella coeruleoalba*) is used as a sentinel species of environmental pollution. The aim of this study was to determine the content of toxic metals in organs of *Stenella coeruleoalba* in comparison with essential elements, and to assess marine environmental pollution and dolphin health status.

Materials and Methods

Samples of liver, lung, muscle, and skin of *Stenella coeruleoalba* (n = 18 dolphins) were digested with HNO_3 (70%) and H2O2 (30%) and submitted to analysis in ICP-MS for the determination of toxic (Hg, Cd, Pb, and As) and potentially toxic (Cr and Ni) metals and essential micro (Se, Zn, Cu, Fe, and Mn) and macro (Na, Ca, K, and Mg) elements .

Results

The results showed the presence of all analyzed metals, with the highest Hg levels in all dolphin samples. The correlation between toxic (Hg, Cd, Pb, and As) and potentially toxic (Cr and Ni) metals and essential micro-elements (Zn, Se, and Cu) was expressed as molar ratios. The ratios were 1 (value considered as a protection index) for $^{66}Zn/^{201}Hg$, $^{82}Se/^{201}Hg$, and $^{63}Cu/^{201}Hg$ and for $^{66}Zn/^{52}Cr$, $^{82}Se/^{52}Cr$, and $^{63}Cu/^{52}Cr$ in all organs, showing that toxic metals cannot be detoxified by these essential metals. However, the concentrations of all micro and macro elements were normal and predictive of dolphins' health status.

Conclusions

The presence of toxic metals in organs of dolphins is correlated to marine environmental pollution and influenced by their food habits. The content of micro and macro elements, introduced through diet, informs dolphins' health status, although detoxifying essential metals are unable to carry out protective action against toxic metals, probably due to the deficiency, sequestration, or presence of other pollutants.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085504: Target Analysis and Suspect Screening of per- and Polyfluoroalkyl Substances in Maternal–Newborn Paired Samples near Fluorochemical Facilities

Xinyi Lu and Jia Bao

School of Environmental and Chemical Engineering, Shenyang University of Technology, Shenyang 110870, China

Introduction

Fuxin Fluorochemical Industrial Park is one of the main concentrated fluorochemical facilities in northeastern China. Our previous studies revealed that perfluorooctanoic acid (PFOA) and perfluorobutane sulfonate (PFBS) were the dominant PFAS contaminants determined in environmental samples around local fluorochemical facilities, and the levels of those two PFASs generally showed an increasing temporal trend over time.

Method

In this study, 50 paired samples of maternal and cord serum as well as placenta were derived from Fuxin pregnant women. Twenty-one legacy PFASs were analyzed in all the samples via high-performance liquid chromatography–tandem mass spectrometry (HPLC–MS/MS), and novel PFASs in all the samples were beneficial for the method of suspect screening.

Results

A total of 11 categories (49 species) of novel PFASs were identified in all samples, of which 4 categories (20 species) were discovered in human serum and placenta for the first time, accounting for 90% of maternal serum and 96% of placenta and umbilical cord serum. Legacy PFASs had median values of 1.2, 1.3, and 1.6 for mother–placenta transfer (Rm/p), placenta–newborn transfer (Rp/n), and mother–newborn transfer (Rm/n), respectively. Rm/p, Rp/n, and Rm/n for each novel PFAS were also able to be derived, with median values of 0.9, 1.2, and 0.8, respectively.

Conclusions

In summary, of the 11 classes (49 species) of novel PFASs detected, 4 classes (20 species) had never been reported previously in human blood and placenta samples. Different from legacy PFCAs and PFSAs, most of the novel PFASs observed in placentas and cord sera had higher levels than those in maternal sera.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084484: The Impact of Occupational Exposure on Workers' Respiratory Microbiota

Sandra Lavandeira [1], Marta Oliveira [2], Maria José Alves [3,4] and Simone Morais [1]

[1] REQUIMTE/LAQV, ISEP, Polytechnic of Porto, Porto, Portugal
[2] 1REQUIME/LAQV, ISEP, Polytechnic of Porto, Porto, Portugal
[3] AquaValor—Center for Valorization and Transfer of Water Technology, Chaves, Portugal
[4] CIMO, Polytechnic of Bragança, Bragança, Portugal

Introduction

Several recent studies have demonstrated that occupational exposure to chemical and biological pollutants alters the human microbiome. Considering that the respiratory tract is one of the main entry points for foreign substances into the body, this small review aims to explore the effects that different occupational exposures have on workers' respiratory microbiota.

Methodology

A PRISMA-based systematic review search was carried out in Scopus, Medline (PubMed), and Web of Science databases, through a combination of the following keywords utilizing the operators "AND" and "OR": "microbiome", "microbiota", "respiratory tract", "airways", "nasal", "occupational", and "worker".

Results and Discussion

Among the selected studies, exposure to biological agents via agricultural or health professionals was the most studied occupational risk factor and was found to lead to changes in the workers' microbiota. Changes in oral and nasal microbiota were also detected in workers exposed to chemical agents such as farm workers exposed to pesticides, cooks exposed to fumes, and facility workers exposed to phthalates. More studies are needed to understand the role of occupational exposure in changing the microbiota of the respiratory tract and the health risks associated with this change.

Conclusions

This review highlights how occupational exposure to different chemical or biological agents can promote the dysbiosis of the respiratory microbiota. This dysbiosis affects the host's immune response and contributes to the development of respiratory diseases.

Funding: This work was financially supported by the project PCIF/SSO/0017/2018, as well as the Fundação para a Ciência e Tecnologia (FCT) and Ministério da Ciência, Tecnologia e Ensino Superior (MCTES) through national funds.

Acknowledgments: This work received support from UIDB/50006/2020, UIDP/50006/2020, LA/P/0008/2020, PCIF/SSO/0090/2019, and 2022.05381.PTDC by FCT-MCTES. M. Oliveira and S. Lavandeira thank, respectively, the Individual Program Agreement CEECIND/03666/2017 and the PhD grant (2022.12979.BDANA), funded by the FCT-MCTES.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085718: Thiram Effects on HeLa TI Cells

Varvara Maksimova [1], Anzhelika Bukina [1,2], Guzel Khayrieva [3], Valeriia Popova [1], Marianna Yakubovskaya [1] and Kirill Kirsanov [1]

[1] N.N. Blokhin National Medical Research Center of Oncology, 115478 Moscow, Russia
[2] Lomonosov Institute of Fine Chemical Technologies, MIREA—Russian Technological University, 86 Vernadsky Ave., 119571 Moscow, Russia
[3] I.M. Sechenov First Moscow State Medical University, 8-2 Trubetskaya Str., 119991 Moscow, Russia

Introduction

Dithiocarbamate pesticides possess a diverse array of molecular mechanisms, making them multifunctional substances. Among the commonly used dithiocarbamates, there is the fungicide thiram, employed for safeguarding plants and seeds against fungal diseases. The limited solubility of thiram in water facilitates its accumulation in the soil, thereby raising concerns about its potential impact on human health. Despite the widespread use of thiram, there is still a paucity of knowledge regarding its toxic effects on humans. This study aimed to assess the genotoxic effects of thiram, its influence on cell colony formation, and its effect on the expression profile of genes associated with proliferation and repair. Additionally, we conducted an analysis of thiram's integral epigenetic activity under different time exposures.

Materials and Methods

HeLa TI cells were used in this study. DNA damage was assessed using the DNA comet assay, while the clonogenic assay was utilized to evaluate the colony-forming ability of cells after thiram treatment. Gene expression levels were measured using real-time PCR. The epigenetic activity of thiram was assessed by quantifying the reactivation level of the epigenetically silenced GFP gene utilizing flow cytometry.

Results

Using HeLa TI cells, we observed that thiram significantly increased tail moment in the DNA comet assay and caused a significant decrease in cell survival as determined by the clonogenic assay. Additionally, thiram downregulated the gene expression levels of *DDB2*, *ERCC5*, *LIG4*, and *WEE1*, while upregulating the expression levels of *MCM2*, *DDIT3*, *ERCC3*, *JUN*1, and *ESR1*. The analysis of epigenetic activity revealed that thiram induced a statistically significant increase in the GFP+ cells amount after exposures of 24, 72, and 96 hours.

Conclusions

Thus, thiram exhibits genotoxic and cytotoxic effects, influences the expression of proliferation and repair genes, and induces dose- and time-dependent epigenetic modifications in HeLa TI cells. This work was supported by RSF (23-25-00541).

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

Abstracts

Session B. Drugs Toxicity and Safety

sciforum-085716: Assessment of the Chemical Hazards in Herbs consumed in Europe: Toxins, Heavy Metals, and Pesticide Residues

M. Carpena [1], P. Barciela [1], A. Perez-Vazquez [1], K. Noras [2], J. Trafiałek [3], M. A. Prieto [1] and M. Trząskowska [3]

[1] Universidade de Vigo, Nutrition and Bromatology Group, Department of Analytical Chemistry and Food Science, Instituto de Agroecoloxía e Alimentación (IAA) – CITEXVI, 36310 Vigo, España
[2] Department of Biometry, Institute of Agriculture, Warsaw University of Life Sciences–SGGW, Nowoursynowska 159 St., 02-776 Warsaw, Poland
[3] Department of Food Gastronomy and Food Hygiene, Institute of Human Nutrition Sciences, Warsaw University of Life Sciences–SGGW, Nowoursynowska 159 St., 02-776 Warsaw, Poland

The increasing global interest in herbs and spices necessitates a thorough examination of the chemical hazards associated with their consumption. The objective of this work was to provide an understanding of the current state and prevalence of chemical contaminants (toxins, heavy metals, and pesticide residues) in herbs and spices consumed in Europe, facilitating informed decision-making in public health and regulatory frameworks [1].

Through an extensive literature search, contamination levels of chemical hazards among different herbs and spices were evaluated. The European Rapid Alert System for Food and Feed (RASFF) has shown 1133 notifications for spices and herbs in the last 10 years (2013–2023). Focusing on the chemical hazards associated with the consumption of these products, mycotoxins (especially aflatoxins and ochratoxin A) and plant-derived compounds with potential health implications (e.g., pyrrolizidine alkaloids) were the most often notified. Nevertheless, besides these naturally occurring compounds, other deliberated added substances such as artificial unauthorized dyes (e.g., Sudan I, II, III, and IV) that can pose a human health risk have been identified. Finally, environmental contaminants could be also present in herbs and spices. Pesticide residues (e.g., chlorpyrifos, carbendazim, bifenthrin) have been notified and studies in terms of their persistence and adherence to regulatory limits and heavy metals were also investigated focusing on cadmium, lead, and mercury due to the bioaccumulation abilities of plants. Other environmental contaminants such as dioxins and dioxin-like polychlorinated biphenyls (dl-PCBs) and polycyclic aromatic hydrocarbons (PAHs) were considered for the study.

In conclusion, this work contributed to identifying gaps and challenges in regulatory practices and to the dialogue on the safety and quality of herbs and spices, offering a holistic perspective on toxins, heavy metals, and pesticide residues and fostering collaboration between all stakeholders to advance in public health protection in Europe.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085555: Drug-likeness, Pharmacokinetics, and Toxicity Prediction of Phytotoxic Terpenoids

Obinna Kenneth Didigwu and Charles Okeke Nnadi

Department of Pharmaceutical and Medicinal Chemistry, Faculty of Pharmaceutical Sciences, University of Nigeria Nsukka, 410001 Enugu State, Nigeria

Terpenoids constitute one of the most widespread phytoconstituents, with complex chemical structures, a plurality of biological activities, and variable pharmacokinetic profiles. The emerging roles of terpenoids in drug design require an understanding of their ADME/T properties for structure modification and possible repurposing. This study evaluated the drug-likeness of phytotoxic terpenoids obtained from the Toxic Plants–Phytotoxins (TPPT) database via in silico prediction of their pharmacokinetic and toxicity profiles. The TPPT database, comprising 1586 phytotoxins, was filtered to 576 terpenoids. Using Swiss ADME, pkCSM, and ProTox II webserver tools, Lipinski's properties and topological polar surface area (TPSA) were predicted for drug-likeness, alongside their pharmacokinetic profiles and toxicity on various organ endpoints. In total, 9.55% of the terpenoids obeyed Lipinski's rule of five. None of the compounds inhibited hERG I, while 12.73% inhibited hERG II, implying that some were cardiotoxic. In addition, 25.45% of the compounds elicited AMES toxicity; 25.45% caused liver injury; and 32.73% caused skin sensitivity. Furthermore, 72.73% showed high Caco-2 permeability and 76.36% displayed good skin permeability, implying their suitability for transdermal drug delivery. P-glycoprotein was extruded by 29.09% of the compounds and inhibited by 34.45%; 47.27% of the compounds readily crossed the blood–brain barrier, 23.64% penetrated the central nervous system, 56.36% were sensitive to cytochrome p450 isoenzymes, 36.37% inhibited cytochrome p450 isoenzymes, 49.09% resulted in immunotoxicity, 1.82% were toxic to cells, 14.55% would cause cancer, and 21.82% showed high tolerated doses in humans. Most of them showed a high volume of distribution, were free-flowing in plasma, and demonstrated moderate bioavailability, while all had high intestinal absorption and 78.18% demonstrated good water solubility. This study identified marrubiin as a drug-like, non-toxic, and highly bioavailable terpenoid with strong potential for further optimization, and development.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084517: Enhancing Chemical-Induced Human Carcinogenic Risk Evaluation through Advanced AI Technologies

Nelly Babayan [1], Helga Stopper [2], Lusine Khondkaryan [3], Ani Tevosyan [4], Gohar Tadevosyan [3], Lilit Apresyan [3], Lusine Adunts [4] and Zaven Navoyan [4]

[1] Institute of Molecular Biology, NAS RA
[2] Institute of Pharmacology and Toxicology, University of Würzburg, Germany
[3] Institute of Molecular Biology, NAS RA, Armenia
[4] Toxometris.ai Inc., USA

Introduction

Efficient cancer risk assessment is vital for sustainable practices in pharma, agriculture, and environmental protection. Traditional animal tests for chemical carcinogenicity are time- and cost-consuming. Ongoing efforts focus on pioneering alternative approaches to improve accessibility and reliability in cancer risk assessment.

Objectives

This study aimed to develop a scoring function that can rank chemical compounds based on their potential human carcinogenicity through in silico methods.

Materials & Methods

An ensemble of diverse AI/ML models, including Boosting Machines, Graph Neural Networks, and Large Language Models was used to predict endpoints associated with carcinogenicity, including in vitro mutagenicity, in vitro and in vivo clastogenicity/aneugenicity, and rodent carcinogenicity. The risk-score function was developed by applying a weighting strategy to every endpoint. The datasets of human carcinogenic and non-carcinogenic chemicals were used to evaluate the performance of risk-score, the p-value was estimated to indicate the significance of the difference.

Results

It was shown that the mean risk-score values differ significantly (p0.0001) between human carcinogens and non-carcinogens. The accuracy to predict human carcinogens was 73%, which was slightly lower than the 76% accuracy achieved in experimental carcinogenicity studies in mice, while significantly surpassing the 65% accuracy obtained in studies with rats.

Conclusions

The devised risk score evaluates the potential of chemicals to induce cancer in humans in silico by integrating information from diverse cancer-related test results, providing an approach nearly as accurate as in vivo experiments. Due to its speed and efficiency, the developed approach can effectively be employed for screening of large quantities of chemicals. The developed risk score focuses on genotoxic carcinogens. It is anticipated to enhance the versatility and applicability of the approach through the inclusion of additional endpoints associated with non-genotoxic carcinogenesis, as well as by implementing more sophisticated AI/ML technologies, such as multi-task learning.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085658: Exploring Schiff Bases as Promising Alternatives to Traditional Drugs in the In Silico Treatment of Leishmaniasis

Diego R. Peixoto [1], Carlos Seiti H. Shiraishi [2,3,4], Rui M. V. Abreu [2,3], Osmair V. Oliveira [5], José Divino Santos [1]

[1] Laboratório de Química de Materiais e Modelagem Molecular – QMMOL, Campus Central: SEDE – CET, Universidade Estadual de Goiás
[2] Centro de Investigação de Montanha (CIMO), Instituto Politécnico de Bragança, Campus de Santa Apolónia 5300-253, Portugal
[3] Laboratório Associado para a Sustentabilidade e Tecnologia em Regiões de Montanha (SusTEC), Instituto Politécnico de Bragança, Campus de Santa Apolónia, 5300-253 Bragança, Portugal
[4] Nutrition and Bromatology Group, Universidad de Vigo, Depart of Analytical Chemistry and Food Science, Faculty of Science, E-32004 Ourense, Spain
[5] Instituto Federal de Educação, Ciência e Tecnologia de São Paulo, Campus Catanduva

Leishmaniases are complex diseases prevalent in (sub)tropical regions, caused by the protozoan Leishmania spp. and transmitted by phlebotomine sandflies. With visceral and cutaneous manifestations, they affect 2 million people annually, resulting in 70,000 deaths, classified by the WHO as a global cause of death from infectious diseases. Tripanothione Reductase (TR), EC 1.8.1.1, a crucial enzyme in the parasite's redox metabolism, emerges as a therapeutic target, and its inhibition can disrupt redox balance, leading to the parasite's death. Current treatment is based on amphotericin B, pentamidine, and meglumine antimony, with a limited understanding of its mechanism of action and severe side effects. In this context, the present study aims to explore Schiff base compounds, either found in nature or synthesized, as promising sources that need to be investigated. These compounds are characterized by a double bond between carbon and nitrogen atoms, which can combine with alkyl or aryl groups. Thirty-two structures from the PubChem database were selected and compared to commercial inhibitors. The emerging therapeutic evaluation was investigated using in silico molecular docking methods against the protein with PDB code 2JK6, employing AutoDock Vina and PLIP for interaction analysis and toxicity assessments. Virtual screening with a library of 32 Schiff base compounds showed promise, with notable compounds such as 3-Quinolinamine (δG = -10.5 kcal/mol), 1,3-bis[(E)-(2-amino-4-ethyl-5-hydroxy-phenyl)methyleneamino]urea (δG = -10.4 kcal/mol), and Naphtaldehyde disulfide Schiff base (δG of -9.8 kcal/mol) demonstrating significant affinities with *Leishmania* infantum TR, surpassing commercial inhibitors (amphotericin B with δG = -9 kcal/mol; pentamidine with δG = -8.8 kcal/mol; meglumine antimony with δG = -5.9 kcal/mol). To assess the safety of the highlighted compounds, a toxicity screening was conducted, concluding the efficacy of Schiff base compounds against TR protein as alternatives to conventional treatment for leishmaniasis based on computational studies.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-086117: Fatal Dermal Absorption of Organophosphate Insecticide

Shankar M Bakkannavar and Vinod C Nayak

Kasturba Medical College, Manipal, Manipal Academy of Higher Education, Manipal, India

Organophosphate compounds are one of the leading causes of death due to poisoning worldwide due to their easy accessibility as insectides and pesticides. Ninety-five percent of pesticide poisonings occur in developing countries, especially in the Asia–Pacific region. Moreover, in countries like India, pesticides are one of the most commonly used suicidal poisons because of their easy accessibility. Agriculture being the country's main source of occupation, pesticides are easily accessible throughout India. Organophosphorus toxicity can commonly occur due to household pesticide use or due to occupational exposure. Though rare, accidental poisoning can occur in people working in the pesticide industry, farmers, and sometimes in the general population. Organophosphorus compounds are absorbed by all routes and cause fatality unless treated with the appropriate antidote. Suicidal poisoning will usually be by ingestion, whereas accidental poisoning will be either inhalational or dermal. Homicidal poisoning cases with the use of organophosphorus compounds have also been reported in the literature. People may become unknowing victims of these chemicals. The dermal absorption of these compounds is common, but it rarely results in fatality. Acute poisoning is common after oral, respiratory, or dermal exposure to low-volatility or high-volatility pesticides. We present an accidental fatal case of organophosphorus poisoning wherein the mode of entry was through dermal absorption.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085699: Hormonal and Sperm Changes in Rats Treated with Oxycodone Hydrochloride

Archange Michel Emmanuel Mboungou Malonga [1] and Landry Martial Miguel [2]

[1] Student at the Faculty of Health Sciences of Marien NGOUABI in Congo
[2] Maître-Assistant CAMES à la Faculté des Sciences de la Santé de l'Université Marien NGOUABI au Congo

Oxycodone hydrochloride is a semi-synthetic product derived from thebaine, an alkaloid derived from poppy plants. It is indicated in cases of intense pain. These treatments are not without side effects such as sexual behavior disorders. Data on the use of oxycodone hydrochloride on reproductive functions are limited, including its effect on fertility. General objective: To evaluate the effects of oxycodone hydrochloride on hormonal and sperm parameters in male Wistar rats.

Materials and Methods

A total of 12 male Wistar rats weighing between 100 and 300 g were selected. We formed three groups, each comprising four male wistar rats: (1) control group having consumed distilled water, (2) group having received 5 mg/kg of oxycodone hydrochloride, and (3) group having received 10 mg /kg of oxycodone hydrochloride. The animals were treated for thirty days using gavage. At the end of the treatment, the animals in each group were anesthetized, followed by blood sampling (retro orbital) and organs after dissection. Then, an exploration of hormonal and sperm parameters was performed.

Results

Oxycodone hydrochloride significantly modifies the weight of the testicles, prostate, and epididymis. The results show necrospermia, with a significant difference in the batches treated with oxycodone hydrochloride at the respective doses. The presence of oligospermia, asthenospermia, and teratospermia was also observed in the batches treated at the respective doses. Our results reveal a significant decrease in testosterone levels.

Conclusions

The prolonged administration of oxycodone hydrochloride at doses of 5 and 10 mg/kg to male Wistar rats modifies testicular weight, and leads to a depletion of hormonal and sperm parameters.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085727: Hormonal and Sperm Changes in Rats Treated with Valproic Acid

Archange Michel Emmanuel Mboungou Malonga

Student at the Faculty of Health Sciences of Marien NGOUABI in Congo

The influence of valproic acid on murine fertility and offspring is well documented: VPA reduces both fertility rate (by 25%) and the number of fetuses. In addition, VPA causes behavioral alterations in rodents similar to the symptoms observed in autism.

General objective: To evaluate the effects of valproic acid on hormonal and sperm parameters in male Wistar rats. Materials and methods: A total of 24 male Wistar rats weighing between 100 and 300 g were selected. We formed three batches comprising eight male Wistar rats each: (1) a control batch that consumed distilled water; (2) a batch that received 200 mg/kg of AVP; and (3) a batch thatreceived 400 mg/kg of AVP. The animals were treated for thirty days viagavage. At the end of the treatment, the animals in each group were anesthetized, followed by blood sampling (retro-orbital) and organ dissection. Then,their hormonal and sperm parameters were explored.

Results

AVP significantly modifies the weight of the testicles, prostate, epididymis, and spermiduct. The results show necrospermia with a significant difference in the batches treated with AVP at the respective doses as well as the presence of asthenospermia and oligospermia in the batches treated with the respective doses of AVP. Our results reveal a significant decrease in testosterone levels and a non-significant decrease in FSH and LH.

Conclusions

Prolonged administration of AVP at doses of 200 and 400 mg/kg to male Wistar rats modifies the weight of the testes and the prostate, leading to a depletion of hormonal and sperm parameters.

© 2024 by the author. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085719: In Silico Discovery of Hemolytic Peptides Through a Novel Approach Based on Network Science and Similarity Searching Methods

Kevin Castillo-Mendieta [1], Yovani Marrero-Ponce [2], Guillermin Agüero-Chapin [3] and Mariela Perez Cardenas [1]

[1] School of Biological Sciences and Engineering, Yachay Tech University, Hda. San José s/n y Proyecto Yachay, Urcuquí 100119, Ecuador
[2] Universidad San Francisco de Quito (USFQ), Grupo de Medicina Molecular y Traslacional (MeM&T), Colegio de Ciencias de la Salud (COCSA), Escuela de Medicina, Edificio de Especialidades Médicas; and Instituto de Simulación Computacional (ISC-USFQ), Diego de
[3] CIIMAR, Centro Interdisciplinar de Investigação Marinha e Ambiental Universidade do Porto. Terminal de Cruzeiros do Porto de Leixões. Av. General Norton de Matos s/n, 4450-208 Matosinhos, Portugal

Peptides are promising drug development frameworks thanks to their high target selectivity, tolerability, and relatively low production cost. However, despite the fact that several thousand potentially therapeutic peptides have been reported, until 2018, only about sixty had been approved in the United States, Europe, and Japan. Toxic effects, including hemolysis, have been identified as the primary challenge that hinders the development of promising peptide drugs. To overcome this obstacle, we propose a novel approach based on complex network science, interactive data mining, and multi-query similarity searching (MQSS) to gain a better understanding of the chemical space of hemolytic peptides. By leveraging these techniques, we aim to design more effective peptide drugs with reduced hemolytic activity, thus facilitating the development of safer and more efficient therapies. Metadata networks (METNs) were used to systematically identify and characterize general patterns that are commonly associated with hemolytic peptides. In addition, half-space proximal networks (HSPNs) were constructed using five different two-way dissimilarity measures with the aim of effectively representing the hemolytic peptide space. Then, the best candidate HSPNs were used to extract various scaffolds that capture information on almost the entire chemical space while avoiding peptide overrepresentation. These scaffolds were used to develop MQSS models for predicting the hemolytic toxicity of peptide sequences. Our best model outperformed state-of-the-art machine learning (ML)-based models, achieving an MCC equal to 0.99. This model was used to characterize the prevalence of hemolytic toxicity on therapeutic peptides. We found that the number of reported hemolytic peptides might be 3.9-fold lower than their actual number. Finally, by means of an alignment-free approach, we reported 47 putative hemolytic motifs, which might provide hints about the mechanisms of hemolysis and can also be used as toxic signatures when developing novel peptide-based drugs.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085724: In Silico Toxicity and ADME Properties of New Drug Candidates Based on the 2-Quinolone Scaffold

Khadija El Gadali [1,2], Meriem Rafya [1], Az-eddine El Mansouri [3], Mohamed Maatallah [2], Arie Vanderlee [4], Ahmad Mehdi [5], Fatiha Benkhalti [1], Moha Taourirte [1] and Hassan B. Lazrek [2]

[1] Laboratoire de Recherche en développement durable et santé, Faculty of Sciences and Technology Gueliz (FSTG), BP549, Marrakech 40000, Morocco
[2] Laboratory of molecular Chemistry, Department of Chemistry, Faculty of Sciences Semlalia, Marrakech 40000, Morocco
[3] University of the free state Faculty of natural and agricultural sciences Chemistry department 205 Nelson Mandela, Bloemfontein 9301, Republic of South Africa
[4] Institut Européen des Membranes, IEM, UMR 5635, Univ. Montpellier, CNRS, ENSCM, 34095 Montpellier, France
[5] ICGM, UMR5253 1919, Route de Mende 34293 Montpellier cedex 5, France

The development of new therapeutic compounds is of great importance today due to the growing challenge of drug resistance. However, this process is complex, expensive, and time-consuming. Recently, in silico methods have been widely used to predict the toxicity of drug candidates and analyze their properties, such as Absorption, Distribution, Metabolism and Excretion (ADME), in a virtual environment, saving time and resources. This computational approach allows comprehensive evaluation of potential adverse effects and toxicity risks, enabling researchers to prioritize compounds with favorable safety profiles early in the development stage. In this study, we present an assessment of the ADME properties and toxicity of two novel hybrid molecules **A** and **B** incorporating 2-quinolone, 1,2,3-triazole and benzimidazole moieties in one scaffold, both displaying higher potency against *E. coli* compared to ampicillin. In terms of pharmacokinetics, compounds **A** and **B** have high gastrointestinal absorption and demonstrated a non-blood-brain barrier permanent, indicating low risk of neurological side effects. The *in silico* toxicity prediction showed that hybrids A and B are not cytotoxic nor carcinogenic, and don't interact with mitochondrial membrane potential (MMP). Nevertheless, both compounds were predicted to be mildly hepatotoxic and mutagenic with probabilities of 0.50–0.52. Moreover, **A** and **B** were found to be immunotoxic with the probability score of 0.97. Additionally, the tested derivatives A and B showed LD50 with 1000 mg/kg and thus belong to class IV in toxicity. The results obtained provide a foundation for advancing further research and the development of innovative antibiotic drugs with enhanced efficacy and reduced toxicity.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085726: Neurotoxicity of Valproic Acid in Wistar Rats: Effects on Memory

Archange Michel Emmanuel Mboungou Malonga

Student at the Faculty of Health Sciences of Marien NGOUABI in Congo

Introduction

Memory is the function that allows us to integrate, retain, and restore information to interact with our environment. Several neural networks are taken into account in multiple forms of memorization. The influence of valproic acid on neurodevelopment is documented. VPA causes behavioral alterations in rodents.

General Objective

To evaluate the neurotoxicity effects of valproic acid on the memory ofWistar rats. Materials and methods: A total of 48 Wistar rats were divided into three groups: (1) the distilled water group, (2) the VPA 200 mg/kg group, and (3) the VPA 400 m/kg group. The products were administered daily by gavage for thirty days. After treatment, all animals were subjected to behavioral tests, including memory tests. Rats were selected from each batch for histologically oriented necropsies and for mating with untreated rats. The young rats resulting from matings were subjected to behavioral tests.

Results

The variables of the different behavioral tests were noted. Rats exposed to VPA and the young rats born to it showed a significant decrease in success rate and performance on behavioral tests. The results revealed stress and anxiety. Histological abnormalities were observed in the VPA-exposed groups.

Conclusions

VPA administered to Wistar rats at the doses studied causes memory alterations. This exposure results in behavioral abnormalities, reduced pass rates on memory tests, stress, and seizures in VPA-treated rats.

© 2024 by the author. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084464: Review on the Toxicity and Safety of Medicinal Plants during Pregnancy

Aniket Rajesing Girase [1], Javesh Kashinath Patil [2], Devshree Yashwantbhai Patel [1], Harsha Vasudev Chaudhari [1], Sachinkumar Madhukar Mahajan [3]

[1] Department of Pharmaceutical Quality Assurance, P.S.G.V.P. Mandal's College of Pharmacy, Shahada-425409, Dist-Nandurbar, Maharashtra, India
[1] Associate Professer Department of Pharmaceutical Quality Assurance, P.S.G.V.P. Mandal's College of Pharmacy, Shahada-425409, Dist-Nandurbar,Maharashtra, India
[1] KVPS's Institute of Pharmaceutical Education, Boradi, Tal-Shirpur, Dist-Dhule, Pin 425 405 [M.S.]

Introduction

Although herbs are widely used and considered safe, they can be toxic, especially during pregnancy. Most reports of toxic plants are the result of misidentification of the plants in sales records or improper preparation and handling by untrained staff. Therefore, these plants are best managed by experienced staff. Medicinal plant uses can be particularly advantageous to low-income patients, as drug treatment is expensive. It is important for doctors to understand the composition, benefits, and potential toxic effects of the herbs that they dispense and prescribe and to provide preventive and safe treatment. Pregnant women will continue to be a major target for teratological screening for at least the next few years.

Method

Toxicology testing includes pharmacological safety, immunotoxicity and antigenicity, endocrine toxicity, gastrointestinal toxicity, enterotoxicity, nephrotoxicity, hepatotoxicity, and drug studies. Phytochemicals and their metabolites are known to cause uterine contractions and hormonal imbalances, leading to miscarriage.

Conclusions

Advances in new technologies have revolutionized our understanding of biology and may facilitate decisions regarding the identification of teratogens. Serious illnesses during pregnancy pose exceptional challenges to healthcare providers because they have the potential to harm the mother and fetus. Teratogenic effects from poisons or antibiotics can be life-threatening. Plants such as acacia, ailanthus, aloe vera, aristolochia, areca nut, bamboo, cassia, ragweed, lemongrass, and racemic black cohosh should be avoided during pregnancy.

Results

A recent international study found that only 22% of medicinal plants used by pregnant women were safe to use during pregnancy. Similarly, a study conducted in Asia found that only 39% of the most commonly used medicinal plants by pregnant women were safe to use during pregnancy

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085721: Self-Poisonings by Use of 'Suicide Kits' and a 'Home-Made' Multi-Xenobiotics Mixes: Are They a Growing Problem in Forensic Toxicology?

Karolina Nowak [1], Paweł Szpot [2], Agnieszka Chłopaś-Konowałek [3], Kaja Tusiewicz [2], Olga Wachełko [4] and Marcin Zawadzki [5]

[1] Department of Pharmacology, Faculty of Medicine, University of Opole, 48 Oleska Street, 45052 Opole, Poland
[2] Department of Forensic Medicine, Faculty of Medicine, Wroclaw Medical University, 4 J. Mikulicza-Radeckiego Street, 50345 Wroclaw, Poland
[3] Department of Forensic Medicine, Division of Molecular Techniques, Wroclaw Medical University, Skłodowskiej-Curie 52, 50369 Wrocław, Poland
[4] Institute of Toxicology Research, 45 Kasztanowa Street, 55093 Borowa, Poland
[5] Faculty of Medicine, Wroclaw University of Science and Technology, 27 Wybrzeze Wyspianskiego Street, 50370 Wroclaw, Poland

Introduction

Year by year, the field of psychiatry faces an escalating crisis, particularly concerning children and adolescents. This crisis stems from the rising prevalence of mental disorders among the population and the constrained access to professional psychiatric and psychological assistance. The global impact of the COVID-19 pandemic, coupled with the associated social isolation, has further exacerbated this trend. The surge in mental disorders has also coincided with an increase in suicide attempts. Over the past few years, scientific reports have emerged on the utilization of online-acquired 'suicide kits' for self-harm. These kits typically consist of various compounds with distinct mechanisms of action, whose simultaneous use may induce severe, life-threatening effects. Additionally, there is evidence that adolescents can learn to assemble such 'kits' through internet forums.

Method

Post-mortem biological matrices and evidence found at the scene were subjected to analysis using a variety of techniques, including LC-MS/MS, GC-MS/MS, and HS-GC-FID/FID. This comprehensive approach covered a broad spectrum of substances, encompassing drugs, illicit substances, NPS, and volatile compounds. Information pertaining to the circumstances of death was obtained from prosecutors or judicial authorities.

Results

The authors will scrutinize the causes of death concerning the composition of 'suicide kits,' explaining the mode of action, toxicity, and concentrations of the substances identified in post-mortem matrices. Challenges in interpretation arising from factors such as inappropriate collection and storage conditions of post-mortem materials and the instability of xenobiotics will be discussed.

Conclusions

The authors' toxicological findings corroborate recorded suicide cases, involving both purchased 'suicide kits' and self-composed multi-xenobiotic mixtures. In instances of suspected suicidal death resulting from xenobiotics, the authors recommend conducting potentially extensive toxicological analyses utilizing various analytical techniques. The final interpretation of toxicological results must hinge on a thorough understanding of the entire case file, underscoring the necessity for close collaboration among forensic toxicologists, pathologists, and judicial authorities.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084438: The Antibacterial Efficacy and Drug Safety Profile of *Trans*-Cinnamaldehyde against *Acinetobacter baumannii*: Bioinformatics and Cheminformatics Approach

Ivan Dolanc [1], Goran Slivšek [2], Nives Ražnjević [3], Sandra Mijač [4], Antonija Jonjić [1] and Miran Čoklo [1]

[1] Institute for Anthropological Research, Centre for Applied Bioanthropology, Zagreb, Croatia
[2] Faculty of Veterinary Medicine, University of Sarajevo, Sarajevo, Bosnia and Herzegovina
[3] University Hospital of Split, Split, Croatia
[4] Children's Hospital Srebrnjak, Zagreb, Croatia

Introduction

The discovery of antibiotics saves millions of lives worldwide, but in recent years bacterial antibiotic resistance has become a growing global problem as bacteria have become increasingly able to adapt to all known antibiotics. Projections have shown that in 2019, more than 4.9 million people worldwide died directly or indirectly as a result of antibiotic resistance. Therefore, it is crucial to discover new antibacterial agents that have therapeutic potential and are non-toxic and drug-safe so that humanity can successfully fight antibiotic resistance. Since such studies are usually very expensive and disappointing results are a waste of valuable time, the use of bioinformatics and chemoinformatics tools can help overcome these problems.

Method

SwissADME software was used to assess *trans*-cinnamaldehyde's pharmacokinetics, drug-likeness, and medicinal chemistry friendliness, while potential therapeutic targets in *Acinetobacter baumannii* were assessed using the RCSB Protein Data Bank online platform tools and evaluated with a comprehensive review of the existing literature.

Results

Trans-cinnamaldehyde fulfils the requirements for the number of rotatable bonds and proton acceptors, which should be readily absorbed in the gut and can cross the blood—brain barrier, but is not a substrate for P-gp, which contributes to its therapeutic potential as it is not immediately excreted from the body. Theoretically, it should not be hepatotoxic as it has no inhibitory effect on liver cytochromes. It meets all five of Lipinski's rules and, according to these criteria, is a molecule that could have therapeutic effects. The most promising potential targets in Acinetobacter baumannii are the proteins AbOmpA and bap, where trans-cimetaldehyde could destabilise membrane integrity and disrupt biofilm formation.

Conclusions

Bioinformatics and chemoinformatics tools can help obtain resources for developing new antibiotics. In vitro tests need to be performed to confirm the efficacy of trans-cinnamaldehyde as a potential therapeutic agent against *Acinetobacter baumannii*.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

Abstracts

Session C. Toxicological Mechanisms of Toxicants

sciforum-084136: Endogenous-Exogenous Chemicals with Neurotoxic Potential

Peter S. Spencer

Oregon Health & Science University

Introduction

While certain highly reactive chemicals are neurotoxic at high environmental concentrations, low endogenous concentrations of the same substances are required for normal neurophysiological function.

Methods/Results

Airborne pollutants carbon monoxide, hydrogen sulfide, nitric oxide and cyanide are each employed as endogenous gasotransmitters [1], while high concentrations are associated with various neurological disorders. The pyrrole-forming neurotoxic gamma-diketone metabolites of certain aliphatic (n-hexane) and aromatic solvents (1,2-diethylbenzene) cause axonal polyneuropathy, yet gamma-diketones are present in solvent-unexposed subjects, and their urinary pyrrole derivatives increase in diabetes mellitus, a major cause of polyneuropathy [2]. Formaldehyde, the common metabolite of two naturally occurring epi/genotoxic neurotoxins (MAM, L-BMAA) linked to a prototypical neurodegenerative disease (Western Pacific Amyotrophic Lateral Sclerosis and Parkinsonism-Dementia Complex) [3], is a neurotoxic and carcinogenic xenobiotic, but the substance is an indispensable component of one-carbon metabolism essential for biosynthetic reactions and epigenetic modulation [4]. Elevated levels of endogenous formaldehyde have been linked to Alzheimer disease [5].

Conclusions

Such considerations suggest that understanding the relationship between the endogenous functions and effects of such highly reactive chemicals may illuminate both how their endogenous mis-regulation may contribute to neurological disease and the mechanisms underlying their neurotoxic effects from exposure to high concentrations. As taught by Paracelsus (1491–1541), the "Poison is in everything, and no thing is without poison. *The dosage makes it either a poison or a remedy*".

References

1. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC7994231/;
   https://www.ncbi.nlm.nih.gov/pmc/articles/PMC9291117/.
2. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC7113121/;
   https://www.ncbi.nlm.nih.gov/pmc/articles/PMC9574754/
3. https://pubmed.ncbi.nlm.nih.gov/33190068/
4. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC7804977/
5. https://onlinelibrary.wiley.com/doi/full/10.1111/jnc.12356;
   https://pubmed.ncbi.nlm.nih.gov/37100142/;
   https://pubmed.ncbi.nlm.nih.gov/25282336/

© 2024 by the author. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085912: Effects of Non-Lethal Arsenic Contamination on Manifesting Fin Strokes in Zebrafish (*Danio rerio*)

Tithi Paul [1,2], Chayan Munshi [2]

[1] Department of Zoology, Visva Bharati University, Santiniketan 731235, India
[2] Ethophilia (An Autonomous Research Group), Santiniketan 731235, India

Introduction

The locomotion of fish is considered to be crucial in regulating activities such as prey predation and foraging. Understanding the swimming patterns of fishes provides deep insights into the underlying neuroethological and biomechanical mechanisms. The fish locomotion mechanism is predominantly controlled through regulated fin strokes, which involve correlation between the stroking patterns of the fins (pectoral, dorsal, anal, pelvic and caudal). However, geometric morphology and hydrodynamics also play a critical role. The aim of our study is to elucidate whether non-lethal concentrations of arsenic trioxide (As_2O_3) in the aquatic environment can affect the swimming pattern of a freshwater-habitant zebrafish (*Danio rerio*).

Method

A population of zebrafish was exposed to a 1/50 LC50 concentration of As_2O_3 for 7 days. A comparative assessment of fin stokes per minute was conducted between fishes from uncontaminated and arsenic trioxide-contaminated water. The stroking frequencies of all the fins were analysed to understand the effect of arsenic on fish locomotion.

Results

Our result demonstrates that fishes in arsenic-contaminated water manifest more frequency of all fin strokes. All of the fins move significantly more in a given time frame due to arsenic trioxide contamination. The alteration of the fin stroke pattern of fishes in a polluted environment is clearly elucidated.

Conclusions

This study clearly indicates that arsenic contamination can be a causative abiotic stressor for the alteration of neuronal activities, which in turn alters the muscular activities responsible for the movements of fins. Danio rerio is a promising model to study the environmental pollution and neurotoxicity of arsenic. It is postulated that enhanced fin activity alters the locomotion pattern as well as the velocity of fish. This study encompasses the three disciplines of behavioural ecotoxicology, neurotoxicology and biomechanics, highlighting locomotory abnormalities in fish due to environmental perturbation.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-086091: Exploring Marine-Derived Fungal Preussin Toxicity to MDA-MB-231 Cells Cultured in 2D and 3D

Rosária Seabra [1,2], Fernanda Malhão [1,2], Alexandra Correia [1,3], Carla Costa [4,5], Anake Kijjoa [1,2] and Eduardo Rocha [1,2]

[1] CBAS—Instituto de Ciências Biomédicas de Abel Salazar, Universidade do Porto, Porto, Portugal
[2] CIIMAR—Centro Interdisciplinar de Investigação Marinha e Ambiental, Universidade do Porto, Matosinhos, Portugal
[3] I3S—Instituto de Investigação e Inovação em Saúde, Universidade do Porto, Porto, Portugal
[4] INSA—National Institute of Health Dr. Ricardo Jorge, Porto, Portugal
[5] ITR—Laboratório para a Investigação Integrativa e Translacional em Saúde Populacional, EPIUnit — Instituto de Saúde Pública da Universidade do Porto, Porto, Portugal

Triple-negative breast cancer (TNBC) presents poor prognosis, early recurrence, limited therapeutic options, and high drug resistance, calling for the search of molecules that may serve as new drugs, drug adjuvants, or scaffolds for drug development. Preussin is a naturally derived compound that reduces cell viability and proliferation and promotes cell death and cell cycle arrest in 2D cultured cell lines. In this study, we investigated the effects of preussin isolated from the marine sponge-associated fungi Aspergillus candidus on the TNBC cell line MDA-MB-231, comparing 2D and 3D cell culture models. Three-dimensional cultures typically better simulate tumour behaviour in vivo and were generated here using ultra-low adhesion U bottom plates. Preussin at 25 µM or higher decreased cell viability in 2D (72 h exposure) and 3D cultured cells (96 h exposure), as assessed with MTT assay. These effects align with the observed decrease in cell proliferation (above 25 µM of preussin) in both culture models, evaluated with BrdU assay, as well as the increase in late apoptosis and necrosis at 35 µM for 2D culture and over 25 µM in 3D culture, as measured via flow cytometry using Annexin V-PI staining. In agreement with this, apoptosis and necrosis characteristics were observed in the cells' ultrastructure after exposure to preussin. With standard and enzymatic versions of the comet assay, we excluded the genotoxic effects of preussin at 25 or 35 µM after 2 h and 24 h of exposure. In an in vitro scratch assay, preussin decreased cell migration in the MDA-MB-231 cell line at a starting concentration of 5 µM. This study sheds light on the mechanisms underlying preussin's effects on a TNBC cell line, supporting its value as an antiproliferative, cytotoxic, and antimigratory agent in a dose-dependent manner in both culture models.

Funding: UIDB/04423/2020 and UIDP/04423/2020.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085655: Exploring the Role and Regulation of HIF-1 in Manganese Toxicity Using Caenorhabditis Elegans as a Model

Tao Zehua

Department of Preventive Medicine and Health Inspection, School of Medicine, Jiangsu University

Introduction

Chronic manganese exposure has been associated with multiple health consequences, including neurological, behavioral, and cognitive impairments. However, the precise mechanism of manganese toxicity remains unclear. The nematode Caenorhabditis elegans, a model organism in environmental toxicology, offers an excellent platform to investigate the role of HIF-1 in manganese-induced toxicity. HIF-1 is a transcription factor that becomes activated under hypoxic conditions and regulates genes related to cell survival, energy metabolism, and angiogenesis. In this study, we aimed to explore the involvement of HIF-1 in manganese-induced toxicity and its potential mechanism.

Methods

We used wild-type Caenorhabditis elegans (N2), HIF-1 mutant nematodes (ZG31), and DAF-16::GFP nematodes as models for manganese exposure. Low-, medium-, and high-dose groups (10, 20, 50 mM $MnCl_2$) were set up to observe the regulatory effects of manganese exposure on nematode lifespan and behavior. Quantitative real-time PCR (qPCR) was used to measure the expression levels of genes such as Daf-16 and HIF-1 to explore the relationship between HIF-1 and manganese-induced nematode toxicity.

Results

Manganese exposure significantly inhibited the growth of L1-stage nematodes, leading to increased mortality and decreased bending frequency. As manganese concentration increased, the nematodes' curvature rate decreased. Lifespan experiments demonstrated that manganese exposure shortened the nematodes' lifespan and decreased the expression of the DAF-16 gene, which is associated with lifespan and aging. Notably, manganese exposure downregulated the expression of HIF-1 and its downstream genes. However, knockout of HIF-1 genes alleviated the toxic effects of manganese exposure on the nematodes.

Conclusions

Manganese exposure can damage nematode survival and behavior, possibly through the downregulation of HIF-1 expression. The role and regulation of HIF-1 in manganese toxicity warrant further investigation.

Keywords

Caenorhabditis elegans, manganese exposure, HIF-1

© 2024 by the author. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085761: Hepatoprotective Effect of Ethyl Acetate Fraction of *Ficus carica* L. leaves against CCl4 Induced Toxicity In Vitro and In Vivo

Syeda Hira

National Skills University, Islamabad, Pakistan

Background

The purpose of this study was to isolate and identify the active components from F. carica leaves which are responsible for hepatoprotective activity.

Methods

This study was designed to identify the most active hepatoprotective sub-fractions from the ethyl acetate fraction of *Ficus carica* in an in vitro study and evaluate their in vivo hepatoprotective effect in an animal model. The ethyl acetate fraction was studied in a column, and a total of eight sub-fractions were obtained. The in vitro hepatoprotective effect of all the sub-fractions was determined on HepG2 cell lines. Toxicity was induced by CCl4 (Carbon tetrachloride), and silymarin was used as the positive control. Using the results, the most active sub-fraction was subjected to LC-MS and FT-IR analyses for the identification of bioactive compounds. The in vivo hepatoprotective effect was determined in mice. Toxicity was induced by CCl4 at the end of the experiment; the biochemical parameters, such as ALT, AST, ALP, bilirubin and total protein, were estimated in the sera. The histopathology of the liver tissues was also performed.

Results

The sub-fraction FVI exhibited more significant (P0.05) hepatoprotective activity as compared to those of the other sub-fractions, which was almost similar to the standard drug silymarin. Six known bioactive compounds were identified from this sub-fraction after LC-MS analysis. The in vivo hepatoprotective activity of sub-fraction FVI was evaluated in the CCl4-intoxicated mice. The administration of CCl4 significantly increased the levels of ALT (Alanine transaminase), AST (Aspartate aminotransferase), ALP (Alkaline phosphatase) and bilirubin and decreased the total protein content. The treatment with the sub-fraction FVI significantly (p0.05) reversed the level of these biomarkers toward a normal state at both the doses of 25 mg/kg and 50 mg/kg.

Conclusions

Our findings confirmed the hepatoprotective effect of the ethyl acetate fraction of F. carica. This could be a good candidate for the development of a natural hepatoprotective drug; the pre-clinical investigation of the ethyl acetate fraction is recommended.

© 2024 by the author. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085743: Methylmercury-Induced Ferroptosis May Be Attenuated by Vitamin K in PC12 Cells

Lin Yanli

Department of Preventive Medicine and Health Laboratory, School of Medicine, Jiangsu University, Zhenjiang 212013, China

Introduction

As a ubiquitous environmental pollutant, methylmercury (MeHg) induces toxic effects in the nervous system. However, the exact mechanism of its neurotoxicity has not been fully elucidated. Ferroptosis may be related to methylmercury toxicity and methylmercury-induced ferroptosis may be attenuated by vitamin K.

Methods

PC12 cells with neuron-like characteristics were selected and treated with different concentrations of MeHg (0, 1, 2.5, 5, and 10 μM) for 6 h. CCK8 was used to detect cell viability; a FerroOrange fluorescent probe was used to detect the level of free ferrous ions in cells; the microplate method was used to detect the level of reduced GSH in cells; FSP1, SLC7A11, and GPX4 protein expressions were detected by Western blotting; and the changes in lipid ROS content in cells were detected by flow cytometry. In the vitamin K intervention experiment, the MeHg group was treated with 5 μM MeHg for 6 h, the vitamin K + MeHg group was pretreated with vitamin K (0, 10, 20, 40, 80, and 100 μM) for 1 h and then co-treated with 5 μM MeHg for 6 h, and the changes in intracellular lipid ROS content were detected by flow cytometry.

Results

MeHg decreased the viability of PC12 cells in a dose-dependent manner. Meanwhile, the level of free ferrous ions in cells was significantly increased; the content of lipid ROS in cells was also significantly increased; the expressions of FSP1, SLC7A11, and GPX4 decreased; and the level of GSH in cells was significantly reduced. After vitamin K intervention, cell viability increased in a dose-dependent manner compared to the MeHg group, and intracellular lipid ROS content was significantly reduced after treatment with 80 μM vitamin K.

Conclusions

MeHg can induce ferroptosis in neuron-like cells, and vitamin K intervention can alleviate MeHg-induced cytotoxicity and ferroptosis; thus, its exact mechanism is worthy of further investigation.

© 2024 by the author. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085695: The Role of the HIF-1α-BNIP3 Pathway in Acrylonitrile-Induced Hippocampal Neuronal Cell Toxicity

Jing Hu

Jiangsu Univeisity

Introduction

Acrylonitrile (AN) is an important chemical raw material, and it is widely used in the production of fibers, plastics and resins. Exposure to AN occurs in occupational settings. While exposure to AN can cause neurotoxicity in bioorganisms, the exact mechanism remains unclear. Hypoxia-inducible factor (HIF) is an important transcription factor produced under hypoxia. During hypoxia, cytoplasm HIF-1α binds to stably expressed HIF-1β and is then translocated into the nucleus to bind with the hypoxia-inducible element (HRE). Multiple downstream target genes are induced.

Methods

CCK assay, LDH release rate, flow cytometry, and Western blot were used to detect the cell viability, toxicity, apoptosis and expression of related proteins in hippocampal neuronal HT22 cells after exposure to AN. Then, cells were pretreated with HIF-1α activator cobalt chloride (CoCl2) and BNIP3 overexpression, followed by the detection of relevant indicators.

Results

We found that the viability of HT22 cells treated with various concentrations of AN (0, 1, 2.5, 5 mM) was reduced, but LDH release rate, apoptosis, and ROS were significantly enhanced. The results of Western blotting showed that the expression of HIF-1α and its downstream proteins, including glucose transporter 1, erythropoietin, Bnip3 and NIX were decreased. In addition, due to HIF-1α CoCl2 pretreatment, cell viability and expression of HIF-1α and downstream proteins were increased. CoCl2 increased the expression of BNIP3, TOM20 and BCL2 and decreased the expression of the pro-apoptosis protein BAX. However, HIF-1α inhibitor dimethoxyestradiol (2MEOE2) showed opposite results. Furthermore, we found that cell viability was significantly increased after pretreatment, with BNIP3 overexpression, increased ATP content, and co-localization of BNIP3 and LC3 seen in confocal microscopy. While the expression of TOM20 decreased, the expression of LC3B and Beclin1 increased significantly, indicating that BNIP3 mitophagy may be involved in the process.

Conclusions

The HIF-1α-BNIP3 pathway may participate in the neurotoxic mechanism of AN, providing an effective treatment strategy for clinical AN poisoning.

© 2024 by the author. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084852: Thyrotropin Suppression during Intoxication Mediates a Positive Effect of Alcohol on Kidney Function in Males

Osama Ali Abulseoud [1,2], Hayrunnisa Unlu [1], Asmaa Yehia [2,3], Khalid Manji [1,4,5], Noah Manji [1,4,5], Mark Frye [6] and Leslie Thomas [7]

[1] Department of Psychiatry and Psychology, Mayo Clinic Arizona, Phoenix, AZ 85054, USA
[2] Department of Neuroscience, Graduate School of Biomedical Sciences, Mayo Clinic College of Medicine, Phoenix, AZ 58054, USA
[3] Department of Medical Physiology, Faculty of Medicine, Mansoura University, Mansoura, Egypt
[4] Barts and The London School of Medicine and Dentistry, Queen Mary University of London, UK
[5] Queen Mary University of London, Malta Campus, Malta
[6] Department of Psychiatry & Psychology, Mayo Clinic, Rochester, MN, USA
[7] Division of Nephrology and Hypertension, Department of Internal Medicine, Mayo Clinic in Arizona, Scottsdale, AZ, USA

Despite a well-established direct toxic effect on renal cells by alcohol, there is a dose-dependent positive effect of alcohol consumption salutary to common laboratory parameters related to kidney performance. Alcohol also impacts thyroid hormones, and thyroid status modulates kidney function. The modulation of kidney parameters with thyrotropin (TSH) and thyroid status indicates a possible interaction between alcohol, kidney, and thyroid functions.

This retrospective study was conducted to test the hypothesis that some portion of the positive correlation between alcohol use and estimated glomerular filtration rate (eGFR) is mediated indirectly via alcohol's effect on thyroid hormones. We reviewed the electronic medical record of 767 hospitalized adult patients free of thyroid disorders who received medical care in the Mayo Clinic Health System from June 2019 through June 2022 and had blood alcohol concentration (BAC), serum TSH, and serum creatinine measured during the hospitalization. We calculated the eGFR using both the Isotope-Dilution Mass Spectrometry (IDMS)-traceable Modification of Diet in Renal Disease (MDRD) study equation and the Chronic Kidney Disease Epidemiology Collaboration (CKD-EPI) Creatinine equation. We found in both males and females a positive correlation between BAC and eGFR and a negative correlation between BAC and TSH and between TSH and eGFR. Using mediation analysis, we found a direct effect of BAC on eGFR in both males and females (using MDRD equation: males vs. females: b = 0.047, P0.001 vs. b = 0.026, p = 0.02) (using CKD-EPI equation: males vs. females: b = 0.018, P0.001 vs. b = 0.032, p = 0.007). However, we found that TSH mediates an indirect effect of BAC on eGFR only in males (using MDRD equation: males vs. females: b = 0.01, p = 0.004 vs. b = 0.0026,p = 0.189) (using CKD-EPI equation: males vs. females: b = 0.0035, P = 0.03 vs. b = 0.003, p = 0.18). Our results demonstrate a positive direct effect of alcohol use and kidney performance. In males, this effect is partially mediated by TSH.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084294: Toxicity Mechanisms of Mixtures of Anionic and Non-Ionic Surfactants

Francisco Río, Manuela Lechuga, Ana Isabel García-López, José María Vicaria-Rivillas and Germán Luzón

University of Granada

Introduction

In recent years, several toxicological studies concerning pollutants have focused on the joint toxicological assessment of co-pollutants, revealing that multiple interactions between toxics can appear and need to be described. In the case of surfactants, while individual studies of them can provide valuable information, they may not reflect real-world exposure to multiple surfactants at once. Synergistic or antagonistic effects stem from the combined toxicity of surfactants, meaning that combined effects are greater or lower than the sum of the individual effects.

In this work, we study the joint toxicity effects of anionic and non-ionic surfactants to bacteria microcrustaceans Daphnia magna. The type of action (concentration addition or response addition) and the possible related antagonistic or synergistic toxic effects are described.

Materials and Methods

Surfactants: Anionic surfactant ether carboxylic derivatives (EC-R12-14E3, EC-R12-14E10, and EC-R8E8) and amine-oxide-based non-ionic surfactants (AO-R14, AO-R12, and AO-Cocoamido) (supplied by Kao Corporation S.A., Tokyo, Japan) were used. Individual and binary mixtures (1:1) of the surfactants were tested. Toxicity tests: Toxicity was tested using microcrustaceans D. magna and according to the guideline UNE-EN ISO 6341.

Results

The toxicity test of binary mixtures (1:1) reveals that concentration addition can be expected for mixtures of the most toxic surfactants from the same family (EC-EC-R12-14E10 + EC-R12-14E3, and AO-R14 + AO-R12), whereas response addition can be expected for the mixture EC-EC-R8E8 + EC-R12-14E3. Antagonism effects, less toxic than the expected, were identified for mixtures including AO-Cocoamido, but a synergism effect was identified for the mixture of EC-EC-R12-14E3 + AO-R14.

Conclusions

- Antagonisms effects were identified for some mixtures of ether carboxylic derivatives and amine-oxide-based surfactants.
- Mixtures showing antagonism effects are preferred for the selection of surfactants in the formulation of more eco-friendly products.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085791: Unravelling the Effects of Benzo[k]fluoranthene and Temperature on the Expression of Detoxification Genes in the Rainbow Trout Liver RTL-W1 Cell Line

Margarida Ribeiro Vilaça [1,2], Telma Esteves [1,2], Rosária Seabra [1,2], Eduardo Rocha [1,2] and Célia Lopes [2,3]

[1] Laboratory of Histology and Embryology, Department of Microscopy, ICBAS—School of Medicine and Biomedical Sciences, University of Porto (U.Porto), Rua Jorge Viterbo Ferreira 228, 4050-313 Porto, Portugal
[2] Team of Animal Morphology and Toxicology, CIIMAR/CIMAR—Interdisciplinary Centre of Marine and Environmental Research, University of Porto (U.Porto), Terminal de Cruzeiros do Porto de Leixões, Av. General Norton de Matos s/n, 4450-208 Matosinhos, Portuga
[3] Laboratory of Histology and Embryology, Department of Microscopy, ICBAS—School of Medicine and Biomedical Sciences, University of Porto (U.Porto), Rua Jorge Viterbo Ferreira 228, 4050-313 Porto, Portugal

Fish are either acutely or chronically exposed to numerous aquatic contaminants, including polycyclic aromatic hydrocarbons (PAHs), and increased water temperatures due to global warming. Both stressors may impact many of their biochemical and physiological processes, including hepatic metabolism. Combined effects of temperature and xenobiotics can exist, and little is known about these interactions. Fish liver-derived models, including well-established cell lines, can be employed to better understand these connections . The rainbow trout (Oncorhynchus mykiss) liver RTL-W1 cell line has been used to study the effects of PAHs. To test if this cell line, cultured in monolayer (2D), can be utilised as a model to study mixed effects of PAHs and temperature, we exposed RTL-W1 cells (72 h) at 18 °C and 21 °C (simulating warming) to benzo[k]fluoranthene (B[k]F), at 10 nM and 100 nM. After PAH exposures, cell density and viability were assessed (through trypan blue exclusion and LDH assays). The gene expression of detoxification targets (cytochrome P450 (CYP)1A, CYP3A27, glutathione S-transferase omega 1 (GST), uridine diphosphate (UDP)-glucuronosyltransferase (UGT), catalase (CAT), and multidrug resistance-associated protein 2 (MRP2)), was analysed using RT-qPCR. B[k]F at 10 and 100 nM reduced cell density but did not affect cell viability. Temperature did not seem to influence cell density and viability. LDH leakage was higher at 21 °C than at 18 °C. CYP1A, CYP3A27, and UGT expression was increased, compared with the control, by both concentrations of B[k]F. GST and MRP2 gene expression was increased by B[k]F100. CAT mRNA levels were higher at 21 °C than at 18 °C. There were no statistically significant interactions between PAHs and temperature over the assessed targets. Overall, the RTL-W1 in 2D culture can potentially unravel the liver effects of toxicants in a global warming scenario.

Funding: FCT strategic funding UIDB/04423/2020 and UIDP/04423/2020 to CIIMAR/CIMAR.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085327: Unravelling the Formation of a Palmelloid-like Phenotype in the Green Microalga *Raphidocelis subcapitata* When Exposed to Pollutants

Manuela Dias Machado [1,2] and Eduardo Valente Soares [2,3,4]

[1] CEB—Centre of Biological Engineering, University of Minho, Braga, Portugal
[2] LABBELS—Associate Laboratory, Braga/Guimarães, Portugal
[3] ISEP-School of Engineering, Polytechnic Institute of Porto, Porto, Portugal
[4] CEB-Centre of Biological Engineering, University of Minho, Braga, Portugal

Introduction

Unicellular microorganisms may present different defence and survival strategies, when exposed to pollutants or adverse environments. For instance, the microalgae belonging to the genera *Chlamydomonas*, *Chlorella*, and *Dunaliella*, in response to high salinity or toxics, can form a structure (comprising non-motile cells surrounded by a matrix of polysaccharides) called "palmelloid", due to its similarity with the morphology of the alga *Palmella*.

Objectives

This work aimed to verify the formation of a palmelloid-like (multinucleated) phenotype in the freshwater microalgae *Raphidocelis subcapitata* caused by exposure to inorganic or organic pollutants. The kinetics of the formation of the palmelloid-like phenotype and its reversibility were also studied.

Method

The microalga was incubated with heavy metals (Cd or Zn) and organic compounds (the antibiotic erythromycin (ERY) or the herbicide metolachlor (MET)) at various concentrations. After 24, 48, and 72 h, the palmelloid-like phenotype formation was evaluated.

Results

In the absence of stress or when exposed to ERY or Zn up to 200 μgL^{-1} (where growth was reduced or halted), R. subcapitata exhibited, primarily, a single nucleus. At sub-lethal and environmentally relevant concentrations of MET (100–200 μgL^{-1}) or Cd (200 μgL^{-1}), the alga transitioned to a multinucleated state, similar to the "palmelloid" morphology observed in different green algae. The multinucleated state was reversed when the microalgae were re-inoculated in a fresh medium (without pollutants).

Conclusions

The development of a palmelloid-like phenotype in *R. subcapitata* when exposed to sub-lethal levels of inorganic or organic pollutants is not a universal defence and response strategy to stress, as it depends on the pollutant, its concentration, and the duration of the exposure. The multinucleated state is a reversible process. The insights provided in this study contribute to increasing the knowledge of the strategies used by *R. subcapitata* to manage severe stress induced by pollutants.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084591: Unveiling the LncRNA–miRNA–mRNA Regulatory Network in Arsenic-Induced Nerve Injury in Rats Using High-Throughput Sequencing

Fang Chu, Chunqing Lu, Zhe jiao, Wenjing Yang, Xiyue Yang, Hao Ma, Hao Yu, Sheng Wang, Yang Li, Dianjun Sun and Hongna Sun

Harbin Medical University

Introduction

Arsenic is a natural toxin which is widely distributed in the environment, incurring diverse toxicities and health problems. Previous studies have shown that long non-coding RNAs (LncRNAs) are reported to contribute to As-induced adverse effects. LncRNAs are involved in the development of nerve injury, generally acting as sponges for microRNAs (miRNAs). This study aimed to investigate the competitive endogenous RNA (ceRNA) regulatory networks associated with arsenic-induced nerve damage.

Methods

A total of 40 male Wistar rats were exposed to different doses of arsenic for 12 weeks, and samples were collected for pathological observation and high-throughput sequencing. The ceRNA network was constructed using Cytoscape, and key genes were identified through the PPI network and CytoHubba methods. A real-time quantitative PCR assay was performed to validate gene expression levels.

Results

The results showed subchronic exposure to arsenic in drinking water resulted in pathological and ultrastructural damage to hippocampal tissue, including changes in neuron morphology, mitochondria, and synapses. Exposure to arsenic resulted in the dysregulation of LncRNA and mRNA expression in the hippocampal tissues of rats. These molecules participated in multiple ceRNA axes and formed a network of ceRNAs associated with nerve injury. This study also verified key molecules within the ceRNA network and provided preliminary evidence implicating the ENRNOT-00000022622-miR-206-3p-Bdnf axis in the mechanism of neural damage induced by arsenic in rats.

Conclusions

Subchronic exposure to arsenic in drinking water can cause pathological damage in hippocampal tissue, resulting in ultrastructural changes in hippocampal mitochondria and synapses. Subchronic arsenic exposure leads to altered expression of multiple LncRNA and mRNA molecules in the rat hippocampus, involved in multiple ceRNA axes forming a network associated with nerve damage. Additionally, our study preliminarily verified arsenic may be involved in the mechanism of nerve injury in rats through the ENSRNOT00000022622-miR-206-3p-Bdnf axis.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

Abstracts

Session D. Identification and Quantification of Toxicants

sciforum-084419: A Historical Drug or a Current Problem? Determination of Methaqualone and Its Analogs in Biological Material via UHPLC-QqQ-MS/MS

Kaja Tusiewicz [1], Marcin Zawadzki [2] and Paweł Szpot [1]

[1] Wroclaw Medical University, Department of Forensic Medicine, 4 J. Mikulicza-Radeckiego Street, 50345 Wroclaw, Poland
[1] Wroclaw University of Science and Technology, Faculty of Medicine, Department of Social Sciences and Infectious Diseases, 27 Wybrzeże Wyspiańskiego, 50370 Wrocław, Poland

Introduction

Methaqualone was introduced to the market in the 1960s as a sedative–hypnotic drug, intended as an alternative to compounds in the barbiturate group. Due to its side effects, as well as increasing recreational use, methaqualone and its analogs, synthesized for medical purposes, were withdrawn from the market or never appeared on the market as pharmaceutical products. Given the current state of the market for new psychoactive substances, the high level of interest in methaqualone and its analogs on dedicated online forums suggests a significant risk that their abuse could become more widespread in the coming years.

Methods

An ultra-high-performance liquid chromatography–triple quadrupole–tandem mass spectrometry (UHPLC-QqQ-MS/MS) method was developed to simultaneously determine nine compounds from the methaqualone group. Biological specimens were prepared using liquid–liquid extraction (LLE) with the use of ethyl acetate at a pH 9. The quantification of those xenobiotics was performed in blood in multiple reaction monitoring (MRM) mode. Methaqualone-d7 served as an internal standard. The limit of quantification (LOQ) of the method was 0.1 or 0.2 ng/mL depending on the substance; precision and accuracy values did not exceed ±20%. The method's recovery was in the range of 84.2–113.7%.

Results

The developed method allowed for the chromatographic separation of all nine compounds from the methaqualone group tested, with satisfactory validation parameters. Moreover, the fragmentation mass spectra presented may contribute to the ability to detect these compounds in routine toxicological analysis.

Conclusions

The described situation poses a significant problem from the analytical point of view, as well as in terms of interpretation and forensic toxicological expertise. The developed method will contribute to increased analytical capabilities and to an enhanced detection of compounds from the methaqualone group that may appear on the illicit market.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084472: Assessment of Exposure to Metals in Wheat-Based Sweets: Human Risk Evaluation

Mudassar Sanaullah

University of Education, Township, Lahore

In recent years, there has been a growing concern about the negative impact of unforeseen contaminants like metals in commonly consumed food items, posing a threat to human well-being. Globally, controlling food contamination has become a significant issue, given the potential risks it poses to human health. The goal of the current research is to determine the levels of essential (EMs: Mg, Ca, Mn, Fe, Co, Cu, and Zn) and potentially toxic metals (PTMs: Al, Cr, Ni, As, Cd, and Pb) in various brands of conventional wheat-based sweets. One hundred samples were collected and analyzed using flame atomic absorption spectrometry (FAAS) and inductively coupled plasma-optical emission spectrometry (ICP-OES). Also, the current study aimed at investigating the distribution, correlation, and multivariate analysis of 13 metals (Mg, Ca, Mn, Fe, Co, Cu, Zn, Al, Cr, Ni, As, Cd, and Pb).

The obtained metal concentrations were used to calculate the average daily intake (ADI), target hazard quotients (THQ), hazard indices (HI), carcinogenic risk (CR), and cumulative carcinogenic risk (CCR). The results also revealed that almost all sweet samples under evaluation had metal concentrations of Mn, Co, Pb, Cr, and Cd above WHO/FAO permitted levels. The estimated daily intake (EDI) of Ca (7.47×10^{-2}) and Cr (2.05×10^{-3}) was the highest among essential elements and potentially toxic elements, respectively. The THQ values were below the threshold level, i.e., 1, whereas the HI values of several sweets were found to be above the threshold level, i.e., > 1, which can lead to significant health hazards. The CR values for Cu were in the range of 1.13×10^{-4} to 2.63×10^{-4} for several samples, which is at the threshold level.

This study highlights the importance of monitoring essential and potentially toxic elements levels, and identifies the potential health risks associated with consuming contaminated wheat-based sweets.

© 2024 by the author. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-086034: Geospatial Deposition of tOxic Heavy Metals and Metalloids between a Pond and the Associated Agricultural Ecosystem in a Non-Industrialized Rural Area in West Bengal, India

Ishika Pal [1], Farhan Jamil [1], Upama Das [1], Swapnanil Mondal [1], Srinwanti Bandyopadhyay [1] and Chayan Munshi [2]

[1] Department of Zoology, Visva Bharati University, Santiniketan, 731235, India 2Ethophilia (An Autonomous Research Group), Santiniketan 731235, India
[2] Ethophilia (An Autonomous Research Group), Santiniketan 731235, India

Introduction

oxic heavy metals and metalloids are biohazards, which are known to contaminate the environment. These environmental contaminants are geologically distributed in several ecosystems and are eventually bioaccumulated in native habitats of the respective biomes. The aim of our research is to evaluate the deposition of toxic heavy metals and metalloids in the sediment/soil of a non-industrial rural area.

Methods

The concentration of heavy metals and metalloid(s) was measured from sediment/soil samples in a rural area of West Bengal, India, by using the Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) method. Sediments from a pond and the adjacent (connected) agricultural soil were compared to assess the contamination difference between the ecologically linked sub-environments.

Results

Our results reveal the considerable occurrence of the top listed toxic metalloid arsenic (As), and heavy metals lead (Pb) and cadmium (Cd) in both sub-environments. The data are analyzed in respect to the comparative concentration of these elements in the sub-environments along with the calculations of contamination factor, geo-accumulation index, pollution load index and the potential ecological risk of these elements in the soils. Our findings indicate the serious contamination of cadmium in both sub-environments; however, cadmium levels are higher in the agricultural soil.

Conclusions

Metal contamination in soil is an issue of concern for geologists, environmental biologists and ecotoxicologists. Our work concentrates on the heavy metal/metalloid contamination in the soil of a non-industrialized rural area. The experiment establishes the fact that a significant deposition of hazardous elements can not only occur in industrialized urban areas, but also that remote countryside areas are equally prone to toxic contamination. In fact, contaminated soil in the agricultural fields can create notable safety issues related to farming products. The pollution profile of non-industrial environments or apparently safe areas should be given adequate attention by researchers regarding biohazard concerns.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084916: Occurrence of tRopane Alkaloids in Teas. Effect of Tea-Making on Atropine and Scopolamine

Lorena González-Gómez [1], Sonia Morante-Zarcero [1], Jorge A.M. Pereira [2], José S. Câmara [3] and Isabel Sierra [1]

[1] ESCET—Escuela Superior de Ciencias Experimentales y Tecnología, Departamento de Tecnología Química y Ambiental, Universidad Rey Juan Carlos, C/Tulipán s/n, 28933 Móstoles, Madrid, Spain
[2] CQM—Centro de Química da Madeira, Universidade da Madeira, Campus da Penteada, 9020-105 Funchal, Portugal
[3] CQM—Centro de Química da Madeira, Universidade da Madeira, Campus da Penteada, 9020-105 Funchal, Portugal/Departamento de Química, Faculdade de Ciências Exatas e Engenharia, Universidade da Madeira, Campus Universitário da Penteada, 9000-390 Funchal, Portugal

Tropane alkaloids (TAs), particularly atropine and scopolamine, are hazardous secondary metabolites found in toxic plants such as those from the Brassicaceae and Solanaceae families. Concerns arise from reported cases of food poisoning due to these toxins, which often contaminate crops in sustainable farming with limited herbicide use. TAs, when consumed through teas and herbal teas, exhibit anticholinergic effects. Despite high contamination, data on TAs in these beverages are scarce. Thus, this study aims to evaluate the presence of atropine and scopolamine in 33 teas and herbal teas purchased in Portugal and Spain.

Infusions (black, green, white tea, and mixed herbal tea) were prepared, cooled, and purified with a method previously validated and developed by our group in similar samples [1]. This methodology involved a microextraction technique (µ-SPEed®) with a PS/DVB cartridge, where 5 × 500 µL of sample was loaded and eluted with methanol (2 × 100 µL) before analysis via HPLC-MS/MS.

Our analysis showed recoveries (at 2.5 ng/mL) of 89–109% for atropine and 73–114% for scopolamine, and good linearity (0.1–25 ng/mL, R2 0.995-0.998). The method assessed contamination levels in infusions, revealing that 63.6% of samples contained one or both analytes, with 45.5% exceeding the 0.2 ng/g limit for liquid herbal infusions.

In addition, the impact of heating conditions on standard solutions (0.2 ng/mL and 4 ng/mL) and naturally contaminated green, white, and black teas was evaluated by brewing with different boiling times (5 and 10 min) at 97 ºC. The infusion conditions described in the international standard ISO 3103 were also compared with the contaminated samples. In the experiment with standard solutions, these remained stable under boiling. In the other experiment, the results showed a higher extraction of the analytes. Overall, this study provides crucial insights into the contamination levels of TAs and demonstrates that TAs are not degraded as a result of tea-brewing.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085505: Target Analysis and Suspect Screening of Per- and Polyfluoroalkyl Substances in Tap Water Samples throughout Chinese Cities

Tieqing You and Jia Bao

School of Environmental and Chemical Engineering, Shenyang University of Technology, Shenyang 110870, China

Introduction

Per- and polyfluoroalkyl substances (PFASs) are a group of anthropogenic chemicals ubiquitously found in various water bodies around the world. The consumption of drinking water is an important pathway of human exposure to PFASs. The aim of this study was to investigate the contamination of legacy and novel PFASs in tap water samples throughout China.

Materials and Methods

Tap water samples were collected from 18 cities of China in 2022. Solid phase extraction was applied for the sample pretreatment. A target analysis of water extracts was carried out using a UPLC-QQQ-MS/MS, and a nontarget analysis of water extracts was implemented through a HPLC-QTOF-MS/MS.

Results

Overall, the recoveries of all the target PFAS analytes ranged between 80% and 110%. LODs were between 0.01 and 0.05 ng/mL, while LOQs were between 0.05 and 0.20 ng/mL. ΣPFASs in tap water were in the range of 90.2 to 473.1 ng/L (median: 193.3 ng/L). Moreover, Σ10legacy PFASs ranged between 30.1 and 131.5 ng/L (median: 64.0 ng/L). Previous studies related to Chinese tap water showed that Σ10legacy PFASs ranged from 1.4 to 175 ng/L (median: 13.5 ng/L) in 2017 and Σ17PFAA ranged from 4.49 to 174.93 ng/L (median: 22.12 ng/L) in 2019. Furthermore, 51 emerging PFASs, representing 11 distinct classes, were identified. Particularly, H-PFCAs, Cl-PFCAs, UPFCAs, FTAs, Et-PFSAs, Ke-PFSAs, and UPFAs were discovered in Chinese tap water for the first time. None of PFAS levels in the tap water samples of China exceeded the regulatory limits for PFOS (40 ng/L) and PFOA (80 ng/L) issued nationally.

Conclusions

In China, the PFAS levels of tap water were higher than those overseas. ΣPFASs in tap water ranged between 90.2 and 473.1 ng/L, with a median of 193.3 ng/L. Legacy PFASs in tap water were no longer dominated by long-chain PFASs, whereas short-chain and novel PFASs alternatives were extensively determined.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

Abstracts

Session E. Novel Methods in Toxicology Research

sciforum-086419: A New Strategy to Exploit Read-Across for Toxicity Evaluation

Emilio Benfenati, Edoardo Luca Viganò and Erika Colombo

Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Via Mario Negri 2, 20156 Milano, Italy

Read-across is becoming a more and more sophisticated technique, applying multiple metrics to identify similar substances. Recently we introduced VERA within the VEGAHUB platform (www.vegahub.eu). VERA was implemented to identify similar substances for two endpoints, carcinogenicity and fish acute toxicity. For the first endpoint VERA identifies a binary label, while for the second endpoint a continuous value is proposed. VERA, as in VEGAHUB, uses rules for the adverse effect, molecular groups and structural similarity.

In this study we extended the metrics to investigate the similarity between substances. Several features useful to compare the behaviour of the chemical compounds on a purely chemical point of view have been applied, such as polarity, reactivity, steric properties. Physico-chemical properties have been used too. Furthermore, the information about the transformation of one substance into a second one is used. These features, added to the others already present in VERA, provide a more powerful and flexible system to compare the behaviour of different substances. A large set of substances is used for the comparison, and for each feature the potency of the feature is split in three categories (high, medium, and low) and this information is combined for the different features, to identify the best similar substances. Examples have been investigated for different applications.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085694: Characterization of Rainbow Trout Hepatic 3D Spheroids for Next-Generation Ecotoxicity Testing

Prem Chand [1,2], You Song [1], Tânia Cristina Gomes [1] and Maria Thérése Hultman [1]

[1] Norwegian Institute for Water Research (NIVA), Section of Ecotoxicology and Risk Assessment, Oslo, Norway
[2] University of Oslo, Department of Biosciences, Oslo, Norway

There is an increasing demand for toxicity testing of chemicals with animal alternatives using new approach methods (NAMs). At present, there are many established in vitro tests using both primary and continuous cell cultures. However, few are suitable for evaluating chemical long-term toxicity. A recent advancement using a more complex three-dimensional (3D) spheroid model, derived from rainbow trout primary hepatocytes (RT-HEP), has shown potential as it retains physiological properties over an extended period of time.

To determine its suitability within toxicity testing, an extensive characterization of the RT-3D hepatic cell culture system is required. For this, high-resolution multiphoton fluorescence microscopy (MFM) was used to examine various parameters like morphology, DNA integrity, and inner-core hypoxia. Additionally, comprehensive characterization utilizing omics techniques and various bioassays was conducted to assess RT hepatic 3D spheroids' response to toxins.

The assessment involved exposure to model chemicals representing different modes of toxicity (MoT), such as copper, 17 β-ethinyl estradiol (EE2), pyrene, 3,4-dichloroaniline (DCA), and carbonyl cyanide m-chlorophenyl hydrazone (CCCP). One of the aims of this study was to assess the RT-3D model's sensitivity, responsiveness, and reproducibility to the above-mentioned toxins by measuring endpoints such as viability, metabolic activity, ATP synthesis, vitellogenin (Vg) induction, and oxidative stress and comparing it to in vitro literature. Furthermore, transcriptomics (RNA-seq) and untargeted metabolomics (mass spectrometry-based) approaches were employed to unravel the molecular landscape of the 3D spheroids when exposed to chemicals with diverse MoT.

Preliminary results indicate the reliability ofRT hepatic 3D spheroids in evaluating cytotoxicity, cell membrane integrity, and oxidative stress. Additionally, the absence of hypoxia at the spheroid core was confirmed. These ongoing characterizations display the potential use of RT hepatic 3D spheroids as an ecotoxicity screening tool for screening a variety of chemicals with different toxic MoT.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084207: Development of an ICP-MS/MS-Based Methodology for the Analysis of (Ultra) Trace Elements in Follicular Fluid Samples of Patients Undergoing IVF Treatment

Núria Ferrer-Cortés [1], Andrea López-Botella [1,2], María José Gómez-Torres [1,3], José -Luis Todolí-Torró [2], Raquel Sánchez-Romero [2], Sergio Rogel [4], Raiza Paul [4] and Jon Aizpurua [3,4]

[1] Biotechnology Department, Faculty of Sciences, University of Alicante
[2] Department of Analytical Chemistry, Nutrition and Food Sciences, University of Alicante
[3] Catedra Human Fertility, University of Alicante, Alicante, Carretera de San Vicente s/n, P.O. Box 99, 03080 Alicante, Spain
[4] IVF Spain Treatment Clinic, Avenida de Ansaldo 13, 03540 Alicante, Spain

Introduction

The presence of heavy metals in the environment has been linked to female infertility. Follicular fluid (FF), which surrounds the developing oocyte in the ovary, can provide valuable insights into the content of a number of elements. However, there is a lack of comprehensive studies that analyze trace elements in FF samples using standardized protocols and methods. The objective of this study was to develop a reliable method utilizing ICP-MS/MS without sample digestion to detect 22 analytes in FF samples.

Methods

Four FF samples (n = 4) were obtained from patients undergoing in vitro fertilization (IVF) treatments. These were adequately aliquoted and processed. They were subsequently analyzed via ICP-MS/MS, both in He and no-gas mode. Finally, the data of interest were compiled in a database.

Results

Analyte recovery ranged from 70% to 130%, with better results observed in no-gas mode compared to He mode. Among the 22 elements analyzed, only ^{9}Be, ^{140}Ce, ^{111}Cd, ^{139}La, ^{208}Pb, and ^{238}U were not detected. Minor concentrations were observed for ^{137}Ba, ^{209}Bi, ^{59}Co, ^{55}Mn, ^{95}Mo, ^{60}Ni, ^{121}Sb, ^{118}Sn, ^{205}Tl, and ^{51}V, while intermediate concentrations were found for ^{7}Li and ^{88}Sr. Major concentrations were identified for ^{52}Cr, ^{85}Rb, ^{47}Ti, and ^{66}Zn.

Conclusions

A new procedure was developed in this study, with several advantages. One of them is the good results in terms of the recovery of a wide variety of elements using ICP-MS/MS in thepoorly studied biological matrix that is follicular fluid. Another advantage is the low amount of sample required to perform the analysis and the development of a green method where the sample is not digested and not diluted, which allowed us to avoid the excessive dilution of the concentration of analytes. Moreover, the developed method provides a novel approach to diagnose and predict health risks in women with gynecological pathologies and to assess their overall health, including reproductive health.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084490: Development of Green(er) Cost-Effective Solvent-Based Method Coupled with Thin-Layer Chromatography Imaging System for the Determination of Allethrin in Blood and Urine

Sakshi Pandey [1] and Lalit P. Chandravanshi [2]

[1] Research Scholar, Department of Forensic Science, Sharda School of Allied Health Science, Sharda University, Greater Noida, UP, India
[2] Associate Professor, Department of Forensic Science, Sharda School of Allied Health Science, Sharda University, Greater Noida, UP, India

Introduction

In this work, a new solvent-based, environmental friendly (greener), and economically viable method was developed to detect allethrin in blood and urine samples. Allethrin is a synthetic pyrethroid insecticide commonly used in household products to control flying and mosquito species. Regulatory bodies like the Environmental Protection Agency (EPA) thoroughly evaluate the products' safety before approval, taking into account factors, such as efficacy, formulation safety, and human toxicity. Approval guarantees that the goods fulfil the safety requirements, instilling trust in their efficiency and appropriate usage. Poisoning can occur on purpose in many circumstances, including accidents and suicides.

Methodology

The aim of this research was to establish a green(er), budget-friendly, solvent-based method based on a Vortex-assisted dispersive liquid–liquid micro extraction method combined with a thin-layer chromatography imaging system. After the extraction process, 20µl extract obtained using the VA-DLLME method was spotted on a TLC plate and put into a saturated TLC chamber using ethyl acetate: benzene as a developing solvent (1:1 v/v). The developed plate was then kept in a UV chamber under 254 nm radiation and photographed by using an android phone.

Results

This method was optimized for many variables, including linearity, the limit of detection (LOD), the limit of quantification (LOQ), accuracy, precision, recovery, and enrichment factor in the urine and blood samples. This method was found to be linear, with ranges of 1–8 µg/spot in the blood sample and 8-16 µg/spot in the urine, with R2 of 0.9977 in the blood and 0.9926 in the urine, respectively. Under the optimized condition, the limit of detection and limit of quantification were found to be in the range of 0.521–0.079 µg/spot.

Conclusions

This novel method of VA-DLLME coupled with a TLC imaging system was successfully developed, and further, this method was validated. This developed method can help resource-limited laboratories in determining urine and blood samples. Also, the proposed method was successfully evaluated for its greenness.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085749: Evaluation of the Genotoxic Potential of a Flavored Oral Nicotine Pouch Product Using Integrated Approaches

Jingjie Zhang, Richard Morgan, Utkarsh Doshi, Chastain A. Anderson, Wanyoike Kangethe, Donna C. Smith and Kyeonghee Monica Lee

Altria Client Services, LLC, Richmond, VA, USA

Oral nicotine pouch (NP) products may encourage adult tobacco consumers to switch from cigarettes to potentially reduced-harm smoke-free products. These products typically consist of nicotine and flavor ingredients. While many flavor ingredients have been well studied, the data from individual ingredients could inform the toxicological profile of the product. In this feasibility study, we evaluated flavored NPs that integrated new approach methodologies (NAMs) into a standard non-clinical test battery to better understand the mechanisms of any toxicity observed and to pave the way for animal-free testing strategies that can be used for similar products.

The genotoxic potential of NPs was evaluated in the in vitro micronuclei (MN) assay and the positive response indicated a potential hazard. Based on individual ingredient assessments and supported by in vitro testing, we identified maltol and ethyl maltol ("maltols") as the driver of bioactivity in the in vitro MN assay for the whole product. Maltols, "Generally Recognized As Safe (GRAS)" for use in foods were reported to induce in vitro genotoxicity, but do not lead to in vivo sequelae. Studies also suggest that the in vivo (mouse) genotoxicity of maltols is related to the route of administration. Therefore, we hypothesized and investigated a dosimetry-based approach to interpret genotoxicity and carcinogenicity outcomes (in vitro versus in vivo) for maltols. Using open-source PBPK models, we also estimated the Cmax in the target tissue (e.g., plasma) under in vivo (rodent) exposure conditions and compared the levels to the in vitro concentrations. We also evaluated the NP in a combined in vivo MN and comet assay in rats following the ICH S2(R1) guidance and the negative in vivo results which also supported the dosimetry modeling. In summary, integrated approaches could enable a holistic evaluation of the genotoxic potential of an oral NP, building a case for NAM-based toxicological assessments without the need for confirmatory in vivo testing.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-081666: New Approach Methodologies: Physiological Responses of Daphnids to Pharmaceutical Mixtures

Emma Rowan, Anne Leung, Katie O'Rourke and Konstantinos Grintzalis

School of Biotechnology, Dublin City University

The levels of pharmaceuticals have been continuously increasing in aquatic ecosystems over the past decade due to their extensive use in human and veterinary medicine. Traditional water monitoring methods have been proven insufficient to capture pollution due to pharmaceuticals because of sensitivity limits, their inability to monitor every pollutant, and their failure to provide mechanistic insights into the actions of pollutants. To combat this, new approach methodologies (NAMs) are increasingly introduced as supplementary tools that can provide sensitive metrics for pollution assessment. In addition, NAMs can bridge the gap in ecotoxicological information regarding mixtures of pharmaceuticals, which are more commonly found in aquatic ecosystems versus pharmaceuticals existing alone. In this context, freshwater sentinel species, such as the water flea known as daphnids, were used to assess the acute effects of a typical pharmaceutical mixture on various physiological and molecular responses. In addition to mortality, phenotypic and molecular endpoints such as ingestion rate and enzyme activity were measured to determine the impact of a cocktail of commonly prescribed pharmaceuticals. Specifically, diclofenac, metformin, gabapentin, amoxicillin, trimethoprim, and erythromycin were mixed in equal amounts and tested at 0.1, 1, and 10 mg/L. Results showed differences in mortality, a decrease in feeding, and changes in enzyme activities, thus supporting a distinct pattern in the physiological responses of daphnids.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084367: ProtoPRED: An Innovative Platform for the Prediction of Toxicological Properties of Small Molecules and Nanomaterials

Martina Palomino-Schätzlein [1], Salvador Moncho [1], Jose Luis Vallés-Pardo [1], Addel Goya [1], Laureano Emilio Carpio [1], Rita Ortega-Vallbona [1], José Vicente Tarazona [1,2], Simón Perera [1], Eva Serrano-Candelas [1] and Rafael Gozalbes [1,2]

[1] ProtoQSAR S.L.
[2] MoldDrug AI Systems S.L.

Quantitative Structure-Activity Relationships (QSARs) are mathematical models relating the structure of molecules with a property, through the use of statistical tools and machine-learning algorithms.[1] They can be used to predict toxicological and environmental properties quickly and at a very low cost in comparison to in vitro and in vivo experiments. Thus, QSAR models are widely applied in different sectors, such as cosmetics and pharmaceutics.[2]

We have developed a computational platform, ProtoPRED3, that allows the reliable, easy, fast and user-friendly prediction of a wide range of toxicological properties of chemical compounds. ProtoPRED only requires the input of the chemical structure (accepting several formats) and performs predictions in seconds, for one or several substances. The predictions come along with detailed reports that provide extensive information about the training and test set, model algorithm, model validation and the quality of the prediction, required to use them for registration purposes.

ProtoPRED includes more than 50 endpoints, grouped in different modules. There are two specific regulation-focused modules (ProtoICH and ProtoREACH) which include models that are linked to the ICH-M7 and REACH regulations, respectively. Other modules are based on the type of endpoints: physicochemical properties (ProtoPHYSCHEM), human toxicity (ProtoTOX), ecotoxicity and environmental fate (ProtoECO) and pharmacokinetics (ProtoADME). In addition, there is a module dedicated to predict the properties of nanomaterials (ProtoNANO).

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

Abstracts

Session F. Toxicity Reduction and Environmental Remediation

sciforum-084499: An Overview on Toxicity Reduction and Environmental Remediation

Harsha Vasudev Chaudhari [1], Dr.Javesh Kashinath Patil [2], Devshree Yashwantbhai Patel [1], Aniket Rajesing Girase [1] and Hasni Hamid Yahiya Sayyed [3]

[1] Departments of Pharmaceutical Quality Assurance, P.S.G.V.P.Mandal's College of Pharmacy, Shahada-425409, Dist-Nandurbar, Maharashtra, India
[2] Associate Professor Departments of Pharmaceutical quality assurance, P.S.G.V.P.Mandal's College of Pharmacy, Shahada Dist-Nandurbar, India
[3] Assitant Professor DEPARTMENT OF Pharmaceutical Quality Assurance, P.S.G.V.P.Mandal's College of Pharmacy shahada-425409, Dist. Nandurbar, Maharashtra, India

Toxicity reduction and environmental remediation are crucial aspects of addressing pollution and protecting ecosystems and human health. Toxicity reduction involves implementing strategies to minimize the spread of toxic substances into the environment. This can be achieved through various means such as implementing stricter regulations on industrial processes, promoting the use of safer chemicals, and encouraging sustainable practices in sectors like agriculture and manufacturing. Environmental remediation focuses on cleaning up and restoring areas that have been contaminated by toxic substances. There are different approaches to remediation depending on the type and extent of contamination. Some common methods include soil and groundwater remediation techniques, such as excavation, bioremediation, and chemical treatment. These methods aim to remove or neutralize pollutants, allowing the environment to recover. The procedure of environmental remediation is carried out in order to protect people and the environment against the potentially dangerous impact of exposure to adulterants and contaminants. For illustration, drawing up sediments—the bottoms of gutters, lakes, morasses, and the ocean—frequently involves physically removing those sediments.

It is important to note that toxicity reduction and environmental remediation require a collaborative effort between governments, industries, and communities. By working together, we can mitigate the impact of pollution, protect ecosystems, and ensure a safer and healthier environment for all.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085790: Ecotoxicological Behavior of Functionalized Magnetic Nanohybrids in Water Flea *Daphnia magna* and Their Recovered Physicochemical Properties

Juan Adrian Ramos Guivar [1], Noemi-Raquel Checca-Huaman [2] and Edson C. Passamani [3]

[1] Universidad Nacional Mayor de San Marcos
[2] Centro Brasileiro de Pesquisas Físicas, Rio de Janeiro 22290-180, RJ, Brazil
[3] Departamento de Física, Universidade Federal do Espírito Santo -UFES, Vitória 29075-910, ES, Brazil

Magnetic nanoremediation is quite advantageous due to its fast kinetic adsorption response, high specific surface area, catalytic response, and multifaceted surface adsorption mechanism [1]. However, their industrial application will require the spread of magnetic nanohybrids into the environment. Specifically, water effluents are the main target for the final cycle of magnetic nanoadsorbents. In light of this, the ecotoxicological evaluation of nanomaterials' lines and derivatives is mandatory. The main worry is the possible source of contamination that these nanomaterials represent, despite their potential applications. In this work, the 24-hour lethal dose concentration (24h-LC50) and morphological effects produced by magnetic nanohybrids were studied in Daphnia magna (D. magna) biomarkers. For this purpose, culture optimization was carried out first. Then, 24h-LC50 values were determined for various magnetic nanohybrids and compared to other parent systems in the literature [1,2]. Morphological damage was compared to the negative control for duplicate experiments, and statistical significance was also evaluated. In addition, the after-exposure properties of magnetic nanohybrids were assessed by means of various physicochemical techniques [3], and it was observed that all of their properties remained unchanged.

References

1. Moyano-Arocutipa et al. In Situ and after Synthesis of Magnetic Nanoarchitectures Grown onto Zeolite Type 5A/CTAB Frameworks and Their Ecotoxicological Properties. *Cryst. Growth Des.* **2023**, *23*, 2951–2970.
2. Huertas-Chambilla et al. In-Field 57Fe Mössbauer study of maghemite nanoparticles functionalized multiwall carbon nanotubes and their ecotoxicological properties in young Daphnia magna. *HYperfine Interact.* **2022**, *243*, 24.
3. Ramos-Guivar et al. Raman, TEM, EELS, and magnetic studies of a magnetically reduced graphene oxide nanohybrid following exposure to Daphnia magna. *Nanomaterials* **2022**, *12*, 1805.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084443: Encapsulating UiO-66(Zr) in Polyvinyl Alcohol/Sodium Alginate Beads for Enhanced Removal of Roxarsone from Aqueous Solutions

Rui Ma [1] and Guangze Nie [2]

[1] Nanjing Tech University (Student)
[2] Nanjing Tech University (Professor)

Roxarsone (ROX) is a common organic arsenic pollutant in water which poses significant risks to human health and to the natural environment. Here, UiO-66(Zr)/polyvinyl alcohol/sodium alginate composite aerogel beads (UiO-66(Zr)@PVA/SA) were prepared as an adsorbent for enhanced removal of ROX. The composite adsorbent, uniquely characterized by high porosity and an expansive specific surface area, offers a promising yet straightforward avenue for the effective capture of ROX through inner-sphere ligand complexation and electrostatic attraction. The microstructure of the synthesized UiO-66(Zr)@PVA/SA was examined using scanning electron microscopy and X-ray diffraction. Batch adsorption experimental results confirmed that UiO-66(Zr)@PVA/SA has a remarkable adsorption capacity (88.35 mg/g, based on the Langmuir model), coupled with its rapid adsorption kinetics (250 min) for ROX removal. Moreover, UiO-66(Zr)@PVA/SA revealed exceptional selectivity toward ROX, even with high concentrations of competitive anions present in the water. A demonstration of five consecutive ROX adsorption cycles resulted in no discernable capacity loss, indicating the robust regenerability of UiO-66(Zr)@PVA/SA. Column adsorption tests further demonstrated its excellent capability (2750 mL wastewater/g adsorbent). In light of these experimental outcomes, UiO-66(Zr)@PVA/SA clearly shows potential as a future solution for ROX wastewater treatment, presenting a novel approach to developing superior adsorbents utilizing unpolluted raw materials for treating contaminated water.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085836: Environmental and Human Health Benefits of Bionematicidal Volatiles in Comparison to Commercial Synthetic Nematicides

Jorge M. S. Faria [1,2] and Tomás Cavaco [3,4]

[1] INIAV, I.P., National Institute for Agrarian and Veterinarian Research, Quinta do Marquês, 2780-159 Oeiras, Portugal
[2] GREEN-IT Bioresources for Sustainability, Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa (ITQB NOVA), Av. da República, 2780-157 Oeiras, Portugal
[3] Instituto Nacional de Investigação Agrária e Veterinária (INIAV), Quinta do Marquês, 2780-159 Oeiras, Portugal
[4] Instituto Superior de Agronomia (ISA), Universidade de Lisboa, 1349-017 Lisboa, Portugal

Modern farming is heavily dependent on the frequent application of pesticides that are known to disturb plant, animal, and microbial biodiversity (as well as accumulate in the environment and influence human health). Plant parasitic nematodes are some of the most damaging pathogens to food crops, impacting crop yield twice as much as phytophagous insects. To combat these pests, large amounts of pesticides are added to agricultural soils and eventually leach out to adjacent environments, accumulate in food and feed, and become very toxic. Volatiles produced by plants and microbes have been increasingly analysed for their anti-nematodal activities since they can present very active chemical structures suitable for developing novel biopesticides. The present study reviews the benefits of some of the most active compounds found in the literature in comparison to the most widely used commercial nematicides. By resorting to data retrieved from freely available online databases on their experimental properties, and given the use of certified software for the prediction of their environmental, toxicological, and ecotoxicological impacts, namely the US EPA Estimation Program Interface (EPI) and the Toxicity Estimation Software Tool (TEST), the advantages and disadvantages of using volatiles in the development of bionematicides are discussed. Ultimately, shifting to a more sustainable usage of pesticides and to farming practices that favor biodiversity can be beneficial to crop production.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085752: Global Measures to Stop the Exportation of Highly Hazardous Pesticides from the EU to Developing Countries

Ahmad Mahdavi

Professor Emeritus at University of Tehran, Entomologist/Ecotoxicologist/ ICT for Agriculture and Environment, Focal Point for Mountain Partnership in the University of Tehran, CMS Preventing Poisoning Group, RAMSAR, SWS, WWN, University of Tehran/and S

Addressing the exportation of highly hazardous pesticides (HHPs) from the European Union (EU) to developing countries requires a multi-faceted approach involving regulatory measures, international cooperation, and sustainable agricultural practices. Here are some strategies that could be considered.

Strengthen and Enforce Regulations: Advocate for stricter regulations within the EU regarding the exportation of HHPs, ensuring that these regulations align with international standards and prioritize human and environmental safety. Strengthen enforcement mechanisms to ensure compliance with existing regulations. Promote Safer Alternatives: Encourage the development and use of safer, less toxic alternatives to HHPs through research and development incentives.

Increase Transparency and Labeling: Enhance transparency in the supply chain by requiring clear labeling of pesticide products, including information on toxicity, environmental impact, and potential harm to human health. Capacity Building and Education: Invest in training programs and capacity building for farmers in developing countries to adopt sustainable and integrated pest management practices.

Ban or Restrict Certain Pesticides: Advocate for a ban or strict restrictions on the exportation of specific HHPs that are known to be highly toxic and that can pose significant risks to human health and the environment.

Support Integrated Pest Management (IPM): Encourage the adoption of Integrated Pest Management practices that focus on preventing and managing pests through a combination of biological, cultural, and mechanical control methods. Corporate Responsibility: Engage with agrochemical companies to promote responsible business practices, including the development and promotion of safer alternatives.

Civil Society Engagement: Mobilize civil society organizations to raise awareness, advocate for policy changes, and hold governments and corporations accountable for their actions related to pesticide exports.

However, it's important to note that addressing this issue requires collaboration between governments, international organizations, the private sector, and civil society to create a comprehensive and effective strategy.

© 2024 by the author. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084257: Green and High-Performance Magnetic Catalysts for the Toxicity-Catalytic Reduction of Nitroarene

SBIAA Salah Eddine, Aflak Noura, ESSEBBAR Fatima Ezzahraa, Elakkaoui Ahmed, Anane Hafid and Ben El Ayouchia Hicham

Laboratory of Analytical and Molecular Chemistry/LCAM, Polydisciplinary Faculty of Safi, Cadi Ayyad University, Safi 46030, Morocco

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085539: Impact of Sodium Ion Stress on the Mechanism of Lead Ion Migration in Electrochemical Treatment of Lead-Contaminated Soil

Yinyin Zhang, Jiangtao Han and Libin Zang

College of GeoExploration Science and Technology, Jilin University, Changchun 130026, China

This study specifically validates the migration patterns of lead ions under sodium ion stress in soil and concludes that a high concentration of sodium ions, when coexisting with lead ions, diminishes the migration rate of lead ions, consequently reducing the removal efficiency of lead ions.

Introduction

Treatment of lead contaminated soil has become a prominent research concern, with electrochemical treatment (ECT) technology demonstrating significant potential in this regard. ECT not only overcomes the drawbacks of traditional technology of soil remediation, such as long remediation periods, low efficiency, and high costs, but also enables in situ remediation. However, the influence of varying concentrations of non contaminant ions on the removal efficiency of heavy metal ions during electrochemical treatment remediation of different naturally polluted soils remains unclear. Therefore, investigating the impact of sodium ion stress on the migration of lead ions is essential.

Methods

This study applies a DC power supply connected to the experimental device. The device was constructed using plexiglass and consisted of three compartments: the soil compartment, two electrolytic compartments. A multimeter was installed by wire between the DC power and the soil reaction device for monitoring the current.

Results

The study indicates a significant influence of the presence of sodium ions on the migration of lead ions during ECT. The high concentration of sodium ions induces ion competition in the soil, hindering the migration of lead ions and causing a decrease in their migration rate. Additionally, the competitive interaction between sodium ions and lead ions has a pronounced effect on the efficiency of ECT, leading to a reduction in the removal efficiency of lead ions.

Conclusions

These results emphasize the importance of considering sodium ion stress in the electrochemical remediation of lead contaminated soil and provide valuable insights for optimizing electrochemical remediation strategies.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085199: Model Optimization of PPCP Removal from Simulated Wastewater via Electrocoagulation

Wenkai Zhang, Jia Bao and Yang Liu

School of Environmental and Chemical Engineering, Shenyang University of Technology, Shenyang 110870, China

Introduction

With the increasing presence of pharmaceuticals and personal care products (PPCPs) in aqueous environments, PPCPs have posed serious biological and environmental impacts and threatened human health. Due to their environmental persistence, bioaccumulation, and high toxicity, PPCPs cannot be effectively removed by conventional wastewater treatment techniques.

Methods

The present study focuses on the treatment of two typical PPCPs involving diclofenac sodium (DCF) and cefixime (CFX) via periodically reverse electrocoagulation (PREC) using Al-Zn electrodes, with an in-depth study on the treatment conditions and removal mechanisms. The aqueous samples were analyzed using a UV-vis spectrophotometer. Moreover, the response surface methodology (RSM) model was applied for the optimization and prediction of removal efficiency. In addition, the flocs produced by the reaction were analyzed by SEM-EDS, XRD, and Fourier transform infrared (FTIR) spectroscopy.

Results

The removal rates of DCF and CFX could reach 90.8% and 97.4%, respectively, after 50 min of treatment, with an initial concentration of 20 mg/L, a current intensity of 0.6 A, an initial pH of 7.0, and a stirring speed of 600 rpm. Through the optimization of RSM, the removal rates of DCF and CFX were increased to 93.7% and 98.8%, respectively. In addition, the flocs possessed significant adsorption capacity and interacted with the functional groups of DCF and CFX.

Conclusions

The present study demonstrated that the PREC technique can effectively remove PPCPs from wastewater and provide a strategy for optimizing the operating parameters.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-084516: Removal of Uranium (VI) from the Water Environment Using Mechanochemical-Activated Organoclay

Iryna Kovalchuk [1,2]

[1] Institute for Sorption and Problems of Endoecology National Academy of Science of Ukraine
[2] National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute"

The contamination of the environment in the uranium-mining region of Ukraine occurs as the result of the technological processes of mining and processing of uranium raw materials. Because of its radioactivity and toxicity, uranium is a very dangerous element, and the WHO recommends a limit of 0.015 mg/L for drinking water. It was established that the level of population morbidity in these districts exceeds the average indices in the region, especially in the endocrine system and oncology.

Natural sorbents, especially clay minerals, have been widely used for water purification. The grinding of solids with the use of energy-intensive equipment and, at the same time, the introduction of intercalates into the interlayer space of minerals prevents the destruction of the layered structure of clay during mechanochemical processing and improves the physical and chemical characteristics.

The purpose of our investigation was to obtain clay-based sorption material for application in environmental protection technologies. The montmorillonite was treated with cationic surfactant hexadecyltrimethylammonium bromide and milled at a high-energy planetary ball mill. It was established that the modification slows down the deformation and amorphization of the montmorillonite structure. In addition, the formation of two-dimensional micelles on the surface of layered silicates was accompanied by a change in surface charge from negative to positive. This makes it possible to remove not only cationic but also anionic forms of inorganic toxicants, in particular uranium (VI), from the water environment. The results indicate a significant increase in the sorption capacity and high selectivity of the synthesized materials for U(VI) ions.

Thus, the obtained sorption material with a stabilized structure and high sorption characteristics could be used in environmental protection technologies. This especially applies to surface and underground waters contaminated with uranium compounds, which are characterized by a wide variety of presence forms in the surrounding water environment.

© 2024 by the author. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

sciforum-085045: Up-the-Pipe Solutions: A Best-Practice Framework to eNgage Communities in Reducing Chemical Contamination in Waste

Louis Tremblay [1], James Ataria [2], Ian Challenger [3], Jacqui Horswell [4], Virginia Baker [4], Lisa Langer [5], Alan Leckie [5], Olivier Champeau [2], Alma Siggins [4] and Grant Northcott [6]

[1] Cawthron Institute/University of Auckland
[2] Cawthron Institute
[3] Ekos Kamahi Ltd
[4] Institute of Environmental Science and Research Limited
[5] Scion
[6] Northcott Research Consultants Limited

Introduction

Anthropogenic chemicals are fundamental for maintaining our standard of living in modern society. Unfortunately, some chemicals are persistent and can enter waste streams and, ultimately, the environment. Commonly used household products, including pharmaceuticals and personal care products, are notable sources of contaminants. There is potential to reduce the levels of contaminants in waste streams or substitute them with less harmful alternatives by raising awareness. The aim of this study was to develop an 'Up-the-Pipe Solutions' framework to raise awareness within the wider community about the presence and potential risks of the chemicals found in household products.

Methods

This framework is based on 'The Natural Step' and the concept of essentiality; it recognises the importance of engaging with communities to raise awareness of each individual's contribution to the problem.

Results and Conclusions

Our daily activities and behavioural patterns can have adverse consequences, including the release of persistent contaminants into main waste streams from our kitchens, bathrooms, and green wastes. The 'Up-the-Pipe Solutions' framework was successfully used in a small community to engage with school children, local authorities, and Māori leaders to raise awareness of chemical pollution. The framework provides an opportunity to incorporate social input in the community by empowering their ability to manage pollution on an individual scale.

© 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

MDPI AG
St. Alban-Anlage 66
4052 Basel
Switzerland
www.mdpi.com

Toxics Editorial Office
E-mail: toxics@mdpi.com
www.mdpi.com/journal/toxics

Disclaimer/Publisher's Note: The title and front matter of this book are at the discretion of the Guest Editor. The publisher is not responsible for their content or any associated concerns. The statements, opinions and data contained in this book are solely those of the individual Editor and contributors and not of MDPI. MDPI disclaims responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.

Academic Open Access Publishing
since 1996