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CHEMICAL EFFECTS

Evaluation of the cytotoxicity and genotoxicity of glufosinate-ammonium at technical and commercial grades in HepG2 cells

2023-07-30

Exposure to genotoxic agents is associated with the development of cancer and related diseases. For this reason, assessing the genotoxicity of chemical compounds is necessary. In this line, information about the genotoxic effect of glufosinate-ammonium (GLA) has been reported only for the technical grade. However, humans are frequently exposed to commercial formulations of pesticides. Commercial formulations are characterized by using inner agents that increase toxicity compared to pesticides in technical grade. This study aimed to determine the cytotoxic and genotoxic effects of GLA on HepG2 cells. MTT and comet assays were performed to evaluate cell viability and DNA damage, respectively. HepG2 cells were exposed for 24 h to different concentrations of GLA (at 0.01 µg/mL; 0.04 µg/mL; 0.1 µg/mL; 0.24 µg/mL; 0.52 µg/mL; 1.25 µg/mL; 2.62 µg/mL and 13.12 µg/mL) in commercial- (Finale Ultra®) or technical-grade (GLAT). The results indicated that only Finale Ultra® induced a reduction in cell viability at 13.12 µg/mL. Furthermore, exposure to Finale Ultra® or GLAT was associated with increased DNA damage at concentrations from 0.52-13.12- µg/mL. This study shows the genotoxic effect of GLA on HepG2 cells.

Authors: Ezeidy Denisse Gallardo-Valle, Dayanne Carbajal-Nogueda, Ma Elena Moreno-Godínez, Eugenia Flores-Alfaro, Isela Parra-Rojas, Gerardo Huerta-Beristain, Teresa Domínguez-Reyes, Marco Antonio Ramírez-Vargas

Full Source: Journal of environmental science and health. Part. B, Pesticides, food contaminants, and agricultural wastes 2023 Jul 30;1-6. doi: 10.1080/03601234.2023.2241322.

Exposure to genotoxic agents is associated with the development of cancer and related diseases.

Investigation of Damage and Creep for Bedding's Carbonaceous Slate with Chemical Erosion Effect

2023-07-22

Tunnel projects in the southwestern mountainous area of China are in full swing. According to the tunnel burial depth, structural characteristics, and chemical erosion environments of the Lixiang railway tunnel, carbonaceous slate specimens obtained in the field were taken to experimentally investigate the physical, mechanical, and creep characteristics of the bedding's slate specimens after chemical erosion.

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The results of scanning electron microscopy (SEM) indicate that chemical erosion leads to internal damage in the carbonaceous slate specimens, and the internal damages are increasing with the increase of erosion days. Moreover, the specimens' ultrasonic test (UT) results prove that specimens with smaller bedding angles suffer a more serious erosion and induce more internal cracks. Under conventional triaxial compression conditions with 40 MPa of confining pressures, the conventional triaxial compressive strength (σs) decreases with the decrease of the bedding angle and the increase of erosion days, and the failure modes of the specimens are mainly controlled by oblique shear fractures and accompanied by the occurrence of slip dislocation fractures between the bedding inclination. Under creep conditions with 40 MPa of confining pressures, the final deformations of specimens are increasing with the increase of erosion days, which means the longer the erosion days, the greater the deformations. The failure modes of the specimens under creep conditions are controlled by shear fractures, and for the specimen with a 60° bedding angle and long-term erosion, there are block separations and many cavities along the shear planes. Therefore, more attention should be paid to prevent serious failure of the surrounding rock if the surrounding rock has a bedding angle of 60° or suffers long-term erosion.

Authors: Weihao Zeng, Zhenghong Chen, Yunpeng Xie, Qiunan Chen

Reactive Palladium-Ligand Complexes for 11C-Carbonylation at Ambient Pressure: A Breakthrough in Carbon-11 Chemistry

2023-07-03

The Pd-Xantphos-mediated 11C-carbonylation protocol (also known as the "Xantphos- method"), due to its simplistic and convenient nature, has facilitated researchers in meeting a longstanding need for preparing 11C-carbonyl-labeled radiopharmaceuticals at ambient pressure for positron emission tomography (PET) imaging and drug discovery. This development could be viewed as a breakthrough in carbon-11 chemistry, as evidenced by the rapid global adoption of the method by the pharmaceutical industry and academic laboratories worldwide. The method has been fully automated for the good manufacturing practice (GMP)-compliant production of novel radiopharmaceuticals for human use, and it has been adapted for "in-loop" reactions and microwave technology; an impressive number of 11C-labeled compounds (>100) have been synthesized. Given the simplicity and efficiency of the method, as well as the abundance of carbonyl groups in bioactive drug molecules,

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we expect that this methodology will be even more widely adopted in future PET radiopharmaceutical research and drug development.
Authors: Kenneth Dahl, Anton Lindberg, Neil Vasdev, Magnus Schou
Full Source: Pharmaceuticals (Basel, Switzerland) 2023 Jul 3;16(7):955. doi: 10.3390/ph16070955.

ENVIRONMENTAL RESEARCH

2023-07-23
Plastic materials that are less than 5 mm in size are defined as Microplastics (MPs). MPs that are intentionally produced are called primary MPs; however, the most abundant type in the environment consists of the remainder created by the fragmentation of large plastic debris through physical, chemical, and oxidative processes, which are called secondary MPs. Due to their abundance in the environment, poor degradability, toxicological properties, and negative impact on aquatic and terrestrial organisms, including humans, MP pollution has become a global environmental issue. Combatting MP pollution requires both remediation and preventive measures. Although remediation is a must, considering where the technology stands today, it may take long time to make it happen. Prevention, on the other hand, can be and should be done now. However, the effectiveness of preventive measures depends heavily on how well MP escape routes are researched and understood. In this research, we argue that such escape routes (rather, loopholes) exist not only due to mismanaged plastic waste, but also due to cracks in the current waste management systems. One known MP loophole is facilitated by wastewater treatment plants (WWTP). The inability of existing WWTP to retain finer MPs, which are finally released to water bodies together with the treated wastewater, along with the return of captured larger MPs back to landfills and their release into the environment through land applications, are a few examples. Organic waste composting and upcycling of waste incineration ash provide other MP escape pathways. In addition, it is important to understand that the plastics that are in current circulation (active use as well as idling) are responsible for producing MPs through regular wear and tear. Closing these loopholes may be best attempted through policy interventions.
Authors: Hiroshan Hettiarachchi, Jay N Meegoda
Full Source: International journal of environmental research and public health 2023 Jul 23;20(14):6434. doi: 10.3390/ijerph20146434.

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Mechanism of bonding, surface property, electrical behaviour, and environmental friendliness of carbon/ceramic composites produced via the pyrolysis of coal waste with polysiloxane polymer

2023-07-29
A simple mixing-pressing followed by thermal curing and pyrolysis process was used to upcycle coal waste into high-value composites. Three coal wastes of different physicochemical properties were investigated. The hypothetical mechanisms of bonding between the coal particles and the preceramic polymer are presented. The textural properties of the coals indicated that the lowest volatile coal waste (PCD) had a dense structure. This limited the diffusion and reaction of the preceramic polymer with the coal waste during pyrolysis, thereby leading to low-quality composites. The water contact angles of the composites up to 104° imply hydrophobic surfaces, hence, no external coating might be required. Analysis of the carbon phase confirmed that the amorphous carbon structure is prevalent in the composites compared to the coal wastes. The dc volume resistivity of the composites in the range of 22 to 82 Ω-cm infers that the composites are unlikely to suffer electrostatic discharge, which makes them useful in creating self-heating building parts. The leached concentrations of heavy metal elements from the composites based on the end-of-life scenario were below the Toxicity Characteristic Leaching Procedure regulatory limits. Additionally, the release potential or mobility of the metals from the composites was not influenced by the pH of the eluants used. On the basis of the reported results, these carbon/ceramic composites show tremendous prospects as building materials due to these properties.
Authors: Orevaoghene Eterigho-Ikelegbe, Ryan Trammell, Emmanuel Ricohermoso 3rd, Samson Bada
Full Source: Environmental science and pollution research international 2023 Jul 29. doi: 10.1007/s11356-023-28661-z.

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Practical application guide for the discovery of novel PFAS in environmental samples using high resolution mass spectrometry

2023-07-29
Background: The intersection of the topics of high-resolution mass spectrometry (HRMS) and per- and polyfluoroalkyl substances (PFAS) bring together two disparate and complex subjects. Recently non-targeted analysis (NTA) for the discovery of novel PFAS in environmental and biological media has been shown to be valuable in multiple applications.

Classical targeted analysis for PFAS using LC-MS/MS, though growing in compound coverage, is still unable to inform a holistic understanding of the PFAS burden in most samples. NTA fills at least a portion of this data gap.
Objectives: Entrance into the study of novel PFAS discovery requires identification techniques such as HRMS (e.g., QTOF and Orbitrap) instrumentation. This requires practical knowledge of best approaches depending on the purpose of the analyses. The utility of HRMS applications for PFAS discovery is unquestioned and will likely play a significant role in many future environmental and human exposure studies.
Methods/results: PFAS have some characteristics that make them standout from most other chemicals present in samples. Through a series of tell-tale PFAS characteristics (e.g., characteristic mass defect range, homologous series and characteristic fragmentation patterns), and case studies different approaches and remaining challenges are demonstrated.
Impact statement: The identification of novel PFAS via non-targeted analysis using high resolution mass spectrometry is an important and difficult endeavor. This synopsis document will hopefully make current and future efforts on this topic easier to perform for novice and experienced alike. The typical time devoted to NTA PFAS investigations (weeks to months or more) may benefit from these practical steps employed.
Authors: Mark Strynar, James McCord, Seth Newton, John Washington, Krista Barzen-Hanson, Xenia Trier, Yanna Liu, Ian Ken Dimzon, Boris Bugsel, Christian Zwiener, Gabriel Munoz
Full Source: Journal of exposure science & environmental epidemiology 2023 Jul 29. doi: 10.1038/s41370-023-00578-2.

PHARMACEUTICAL/TOXICOLOGY

Current Review of Increasing Animal Health Threat of Per- and Polyfluoroalkyl Substances (PFAS): Harms, Limitations, and Alternatives to Manage Their Toxicity

2023-07-20
Perfluorinated and polyfluorinated alkyl substances (PFAS), more than 4700 in number, are a group of widely used man-made chemicals that accumulate in living things and the environment over time. They are known as "forever chemicals" because they are extremely persistent in our environment and body. Because PFAS have been widely used for many decades, their presence is evident globally, and their persistence and

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potential toxicity create concern for animals, humans and environmental health. They can have multiple adverse health effects, such as liver damage, thyroid disease, obesity, fertility problems, and cancer. The most significant source of living exposure to PFAS is dietary intake (food and water), but given massive industrial and domestic use, these substances are now punctually present not only domestically but also in the outdoor environment. For example, livestock and wildlife can be exposed to PFAS through contaminated water, soil, substrate, air, or food. In this review, we have analyzed and exposed the characteristics of PFAS and their various uses and reported data on their presence in the environment, from industrialized to less populated areas. In several areas of the planet, even in areas far from large population centers, the presence of PFAS was confirmed, both in marine and terrestrial animals (organisms). Among the most common PFAS identified are undoubtedly perfluorooctanesulfonate (PFOS) and perfluorooctanoic acid (PFOA), two of the most widely used and, to date, among the most studied in terms of toxicokinetics and toxicodynamics. The objective of this review is to provide insights into the toxic potential of PFAS, their exposure, and related mechanisms.
Authors: Alessio Filippo Peritore, Enrico Gugliandolo, Salvatore Cuzzocrea, Rosalia Crupi, Domenico Britti
Full Source: International journal of molecular sciences 2023 Jul 20;24(14):11707. doi: 10.3390/ijms241411707.

Isolation of Pseudomonas oleovorans Carrying Multidrug Resistance Proteins MdtA and MdtB from Wastewater

2023-07-14
The pollution of industrial wastewater has become a global issue in terms of economic development and ecological protection. Pseudomonas oleovorans has been studied as a bacterium involved in the treatment of petroleum pollutants. Our study aimed to investigate the physicochemical properties and drug resistance of Pseudomonas oleovorans isolated from industrial wastewater with a high concentration of sulfate compounds. Firstly, Pseudomonas oleovorans was isolated and then identified using matrix-assisted flight mass spectrometry and 16S rDNA sequencing. Then, biochemical and antibiotic resistance analyses were performed on the Pseudomonas oleovorans, and a microbial high-throughput growth detector was used to assess the growth of the strain. Finally, PCR and proteomics analyses were conducted to determine drug-resistance-related genes/proteins. Based on the results of the spectrum diagram and sequencing, the isolated bacteria were identified as Pseudomonas oleovorans and were positive to reactions of ADH, MTE, CIT, MLT,

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ONPG, and ACE. Pseudomonas oleovorans was sensitive to most of the tested antibiotics, and its resistance to SXT and CHL and MIN and TIM was intermediate. The growth experiment showed that Pseudomonas oleovorans had a good growth rate in nutrient broth. Additionally, gyrB was the resistance gene, and mdtA2, mdtA3, mdtB2, mdaB, and emrK1 were the proteins that were closely associated with the drug resistance of Pseudomonas oleovorans. Our results show the biochemical properties of Pseudomonas oleovorans from industrial wastewater with a high concentration of sulfate compounds and provide a new perspective for Pseudomonas oleovorans to participate in biological removal of chemical pollutants in industrial wastewater.

Authors: Haifeng Wang, Chenyang Sun, Xing Chen, Kai Yan, Hongxuan He

Full Source: Molecules (Basel, Switzerland) 2023 Jul 14;28(14):5403. doi: 10.3390/molecules28145403.

Rapid Detection of Volatile Organic Metabolites in Urine by High-Pressure Photoionization Mass Spectrometry for Breast Cancer Screening: A Pilot Study

2023-07-21

Despite surpassing lung cancer as the most frequently diagnosed cancer, female breast cancer (BC) still lacks rapid detection methods for screening that can be implemented on a large scale in practical clinical settings. However, urine is a readily available biofluid obtained non-invasively and contains numerous volatile organic metabolites (VOMs) that offer valuable metabolic information concerning the onset and progression of diseases. In this work, a rapid method for analysis of VOMs in urine by using high-pressure photon ionization time-of-flight mass spectrometry (HPPI-TOFMS) coupled with dynamic purge injection. A simple pretreatment process of urine samples by adding acid and salt was employed for efficient VOM sampling, and the numbers of metabolites increased and the detection sensitivity was improved after the acid (HCl) and salt (NaCl) addition. The established mass spectrometry detection method was applied to analyze a set of training samples collected from a local hospital, including 24 breast cancer patients and 27 healthy controls. Statistical analysis techniques such as principal component analysis, partial least squares discriminant analysis, and the Mann-Whitney U test were used, and nine VOMs were identified as differential metabolites. Finally, acrolein, 2-pentanone, and methyl allyl sulfide were selected to build a metabolite combination model for distinguishing breast cancer patients from the healthy group, and the achieved sensitivity and specificity were 92.6% and 91.7%, respectively, according to the receiver operating characteristic

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curve analysis. The results demonstrate that this technology has potential to become a rapid screening tool for breast cancer, with significant room for further development.

Authors: Ming Yang, Jichun Jiang, Lei Hua, Dandan Jiang, Yadong Wang, Depeng Li, Ruoyu Wang, Xiaohui Zhang, Haiyang Li

Full Source: Metabolites 2023 Jul 21;13(7):870. doi: 10.3390/metabo13070870.
Full Source: Materials (Basel, Switzerland) 2023 Jul 22;16(14):5163. doi: 10.3390/ma16145163.

Bacteriophage-based biosensors for detection of pathogenic microbes in wastewater

2023-07-27

Wastewater is discarded from several sources, including industry, livestock, fertilizer application, and municipal waste. If the disposed of wastewater has not been treated and processed before discharge to the environment, pathogenic microorganisms and toxic chemicals are accumulated in the disposal area and transported into the surface waters. The presence of harmful microbes is responsible for thousands of human deaths related to water-born contamination every year. To be able to take the necessary step and quick action against the possible presence of harmful microorganisms and substances, there is a need to improve the effective speed of identification and treatment of these problems. Biosensors are such devices that can give quantitative information within a short period of time. There have been several biosensors developed to measure certain parameters and microorganisms. The discovered biosensors can be utilized for the detection of axenic and mixed microbial strains from the wastewaters. Biosensors can further be developed for specific conditions and environments with an in-depth understanding of microbial organization and interaction within that community. In this regard, bacteriophage-based biosensors have become a possibility to identify specific live bacteria in an infected environment. This paper has investigated the current scenario of microbial community analysis and biosensor development in identifying the presence of pathogenic microorganisms.

Authors: Karthik Basthi Shivaram, Pankaj Bhatt, Mohit S Verma, Kari Clase, Halis Simsek

Full Source: The Science of the total environment 2023 Jul 27;165859. doi: 10.1016/j.scitotenv.2023.165859.

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