Bulletin Board

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CHEMICAL EFFECTS

A multi-residue method by supercritical fluid chromatography coupled with tandem mass spectrometry method for the analysis of chiral and non-chiral chemicals of emerging concern in environmental samples

2020-07-09

This manuscript presents the development, validation and application of a multi-residue supercritical fluid chromatography coupled with tandem mass spectrometry method for the analysis of 140 chiral and non-chiral chemicals of emerging concern in environmental samples, with 81 compounds being fully quantitative, 14 semi-quantitative and 45 qualitative, validated according to European Medicine Agency (EMA) guidelines (European Medicines Agency 2019). One unified LC-MS method was used to analyse all analytes, which were split into three injection methods to ensure sufficient peak resolution. The unified method provided an average of 113% accuracy and 4.5% precision across the analyte range. Limits of detection were in the range of 35 pg L-1-0.7 µg L-1, in both river water and wastewater, with an average LOD of 33 ng L-1. The method was combined with solid-phase extraction and applied in environmental samples, showing very good accuracy and precision, as well as excellent chromatographic resolution of a range of chiral enantiomers including beta-blockers, benzodiazepines and antidepressants. The method resulted in quantification of 75% of analytes in at least two matrices, and 56% in the trio of environmental matrices of river water, effluent wastewater and influent wastewater, enabling its use in monitoring compounds of environmental concern, from their sources of origin through to their discharge into the environment.

Authors: Jack Rice, Anneke Lubben, Barbara Kasprzyk-Hordern
Full Source: Analytical and bioanalytical chemistry 2020 Jul 9. doi: 10.1007/s00216-020-02780-9.

Current mechanistic perspectives on male reproductive toxicity induced by heavy metals

2020-07-10

Environmental and occupational exposures to heavy metals have led to various deleterious damages to the biological system of which infertility is one of them. Infertility is a global public health concern, affecting 15% of all couples of reproductive age. Out of the 100% cases of reported infertility

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among couples, 40% of the cases are related to male factors; including decreased semen quality. This review focuses on the recent mechanistic perspectives of heavy metal-induced male reproductive toxicity. The associated toxic metal-mediated mechanisms of male reproductive toxicity include ion mimicry, disruption of cell signaling pathways, oxidative stress, altered gene expression, epigenetic regulation of gene expression, apoptosis, disruption of testis/blood barrier, inflammation and endocrine disruption. The current literature suggests that non-coding RNAs (ncRNAs) mediate paternal intergenerational epigenetic inheritance and thus has a direct functional importance, as well as possess novel biomarker potential, for male reproductive toxicity. To identify the specific ncRNAs with the most profound impacts on heavy metal-induced male reproductive toxicity should be thrust of further research.

Authors: Brilliance Onyinyechi Anyanwu, Orish Ebere Orisakwe
Full Source: Journal of environmental science and health. Part C, Toxicology and carcinogenesis 2020 Jul 10;1-41. doi: 10.1080/26896583.2020.1782116.

Towards a Computational Ecotoxicity Assay

2020-07-10

Thousands of anthropogenic chemicals are released into the environment each year, posing potential hazards to human and environmental health. Toxic chemicals may cause a variety of adverse health effects, triggering immediate symptoms or delayed effects over longer periods of time. It is thus crucial to develop methods that can rapidly screen and predict the toxicity of chemicals, to limit the potential harmful impacts of chemical pollutants. Computational methods are being increasingly used in toxicity predictions. Here, the method of molecular docking is assessed for screening potential toxicity of a variety of xenobiotic compounds, including pesticides, pharmaceuticals, pollutants and toxins deriving from the chemical industry. The method predicts the binding energy of pollutants to a set of carefully selected receptors, under the assumption that toxicity in many cases is related to interference with biochemical pathways. The strength of the applied method lies in its rapid generation of interaction maps between potential toxins and the targeted enzymes, which could quickly yield molecular-level information and insight into potential perturbation pathways, aiding in the prioritisation of chemicals for further tests. Two scoring functions are compared, Autodock Vina and the machine-learning scoring function RF-Score-VS. The results are promising, though hampered by the accuracy of the scoring functions. The strengths and weaknesses of the docking protocol are discussed, as well

Thousands of anthropogenic chemicals are released into the environment each year, posing potential hazards to human and environmental health.

as future directions for improving the accuracy for the purpose of toxicity predictions.
Authors: Natasha Kamerlin, Mickaël G Delcey, Sergio Manzetti, David van der Spoel
Full Source: Journal of chemical information and modeling 2020 Jul 10. doi: 10.1021/acs.jcim.0c00574.

ENVIRONMENTAL RESEARCH

Environmental Exposures and Hearing Loss
2020-07-07
Pollutants that contaminate the natural or built environment adversely affect the health of living organisms. Although exposure to many of them could be avoided or minimized by careful preventive measures, it is impossible to totally avoid exposure to all pollutants. Ototraumatic agents, such as noise, chemicals, and heavy metals, are pervasive pollutants, mostly produced by human activity, and are critical factors in inducing acquired hearing loss. More importantly, exposure to these pollutants often occurs concurrently and, therefore, the synergistic interactions potentiate auditory dysfunction in susceptible individuals. Epidemiological studies have provided compelling data on the incidence of auditory dysfunction after exposure to a number of ototraumatic agents in the environment, while animal studies have offered crucial insights for understanding the underlying molecular mechanisms. Together, they provide a framework for developing effective interventional approaches for mitigating the adverse impacts of environmental or occupational exposure to ototraumatic agents. This article provides a brief overview of the common pollutants that cause hearing loss.
Authors: Rita Rosati, Samson Jamesdaniel
Full Source: International journal of environmental research and public health 2020 Jul 7;17(13):E4879. doi: 10.3390/ijerph17134879.

Suspect screening based on market data of polar halogenated micropollutants in river water affected by wastewater
2020-07-04
Wastewater treatment plants (WWTPs) are known point sources of contaminants of emerging concern (CECs) to the aquatic environment, but current knowledge is mostly limited to well-known chemical structures. In this study, we sought to identify unknown CECs polluting

> **Pollutants that contaminate the natural or built environment adversely affect the health of living organisms.**

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the aquatic environment through a novel suspect screening approach for organohalogens, i.e. organic halogenated molecules often toxic and resistant to transformation and characterised as persistent organic pollutants (POPs). Surface water samples were collected with passive samplers in the Fyris River catchment (Uppsala, Sweden), analysed using liquid chromatography high-resolution mass spectrometry (LC-HRMS) and screened for organohalogens using a suspect screening approach based on market data obtained from a regulatory authority. Thirteen suspects from very different application areas were confirmed or tentatively identified with high confidence, including seven previously unknown structures (diflufenican, chlorzoxazone, 3-(3,4-dichlorophenyl)-1,1-dimethylurea, 2,4-disulfamyl-5-trifluoromethylaniline, 5-amino-2-chlorotoluene-4-sulfonic acid, perfluoropentane-1-sufonic acid, (2-chlorophenyl)(hydroxy)methanesulfonic acid). Spatiotemporal occurrence patterns were detected, which helped to understand the usage pattern of the chemicals and pinpoint potential pollution sources, e.g. specific WWTPs in the catchment. Several of the newly identified structures had virtually no information publicly available and were detected years after their last registered use, which highlights the knowledge gaps and concerns about POPs.
Authors: Frank Menger, Lutz Ahrens, Karin Wiberg, Pablo Gago-Ferrero
Full Source: Journal of hazardous materials 2020 Jul 4;401:123377. doi: 10.1016/j.jhazmat.2020.123377.

Environmental contaminants in coastal populations: Comparisons with the National Health and Nutrition Examination Survey (NHANES) and resident dolphins
2019-12-15
Background: People living in coastal communities are at risk for exposure to environmental hazards, including legacy chemicals. We can use databases such as NHANES to assess whether contaminants in coastal communities are present in higher levels than in the United States overall. We can use information from studies of local animal populations to assess which of these contaminants could have been transferred to people from their shared environment.
Objective: Our objectives were to examine the POP profiles in human populations in areas where there are published POP profiles in resident dolphins and to compare our results with data from NHANES and the dolphin studies.
Methods: We identified three areas where POPs have been analyzed in local resident dolphin populations (total N =73). We identified human

> **Background: People living in coastal communities are at risk for exposure to environmental hazards, including legacy chemicals.**

communities in the same areas, and asked 27 eligible adults to read and sign a consent form, complete a questionnaire about demographics and seafood consumption, provide nine 10-mL blood samples, and provide one sample of seafood (N = 33). Blood and seafood were analyzed for a suite of POPs similar to those analyzed in published dolphin population studies. We compared the results from human blood analyses with NHANES and with data from the published reports of dolphin studies.

Results: Levels and proportions of specific POPs found in people and animals reflect POPs found in the local environment. Compared with the nationally representative data reported in NHANES, the levels of many POPs found in high levels in dolphins were also higher in the corresponding human communities. Conclusions: Contaminants measured in marine animals, such as dolphins, can be used to identify the types and relative levels of environmental contaminants expected to occur in people sharing the same environment. Likewise, contaminants measured in coastal human populations can provide insight into which contaminants may be found in nearby animal populations.

Authors: Lorraine C Backer, Birgit Bolton, Jenny A Litz, Jennifer Trevillian, Stephanie Kieszak, John Kucklick
Full Source: The Science of the total environment 2019 Dec 15;696:134041. doi: 10.1016/j.scitotenv.2019.134041.

OCCUPATIONAL

Neuropsychological effects of long-term occupational exposure to mercury among chloralkali workers

2020-07-09
Background: Mercury is one of the most well-known toxic metals for humans. Chloralkali workers are exposed to mercury vapours extensively, which may be associated with neurotoxicity.
Objective: The aim of this study was to determine the associations between mercury concentration in blood and air samples, and mercury's neuropsychological effects among chloralkali workers.
Methods: This study was conducted on 50 chloralkali workers as the exposed group and 50 non-industrial office workers as the unexposed group. All subjects were assessed using the Hamilton Depression Rating Scale, Piper Chronic Fatigue Scale and Essential Tremor Rating Scale. Mercury concentration was measured in blood and air samples using cold vapour atomic absorption spectrometry.
Results: There were significant correlations between severity of fatigue, depression and tremor in the exposed group compared with

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the unexposed group. The mean concentration of blood mercury in the exposed group was 22.59±12.5µgL-1 which was significantly higher than the unexposed group (1.28±1.05µg L-1). Based on multiple linear regression, shift work, smoking, fatigue, depression and tremor were predictor variables for blood mercury concentration.
Conclusions: This study indicated that this sample of chloralkali workers suffered from neuropsychological problems such as fatigue, depression and tremor, which is probably related to mercury exposure.
Authors: Majid Bagheri Hosseinabadi, Narges Khanjani, Mostafa Dehghani Mobarake, Hamid Shirkhanloo
Full Source: Work (Reading, Mass.) 2020 Jul 9. doi: 10.3233/WOR-203194.

Relationship between butyrylcholinesterase activity and lipid parameters in workers occupationally exposed to pesticides

2020-07-09
Exposure to organophosphate pesticides (OP) has been associated with the inhibition of cholinesterase enzymatic activity, such as butyrylcholinesterase (BuChE). Changes in BuChE activity have been associated with obesity, diabetes, hyperthyroidism, and metabolic syndrome. However, few studies have evaluated the effects of pesticides on both BuChE and lipid parameters. The aim of this study was to evaluate lipid parameters in urban sprayers and their association with BuChE activity. An analytical cross-sectional study was conducted in workers exposed to pesticides. The pesticide exposures were evaluated by the measurement of urinary dialkylphosphates. BuChE activity was determined spectrophotometrically in serum, and biochemical parameters were determined at a certified laboratory. Information regarding general characteristics, lifestyle, and other aspects was obtained from a structured questionnaire. The results showed variations in glucose, cholesterol, albumin, atherogenic index, creatinine, LDL, VLDL, triglycerides, and total lipids according to the level of exposure to pesticides in individuals with overweight and obesity. Furthermore, positive correlations between BuChE activity and lipid parameters were observed; these effects were associated with the body mass index. More studies are

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needed in human population to better elucidate the role of BuChE in lipid metabolism.

Authors: Iris Betzaida Molina-Pintor, Aurora Elizabeth Rojas-García, Yael Yvette Bernal-Hernández, Irma Martha Medina-Díaz, Cyndia Azucena González-Arias, Briscia Socorro Barrón-Vivanco

Full Source: Environmental science and pollution research international 2020 Jul 9. doi: 10.1007/s11356-020-08197-2.

PHARMACEUTICAL/TOXICOLOGY

Lung Cancer Occurrence-Correlation with Serum Chromium Levels and Genotypes

2020-07-09

Lung cancer is the leading cause of cancer-related death worldwide. Exposure to environmental and occupational carcinogens is an important cause of lung cancer. One of these substances is chromium, which is found ubiquitously across the planet. The International Agency for Research on Cancer has classified chromium(VI) as a human carcinogen. The aim of this study was to assess whether serum chromium levels, as well as DNA variants in selected genes involved in carcinogenesis, xenobiotic-metabolism, and oxidative stress could be helpful in the detection of lung cancer. We conducted a study using 218 lung cancer patients and 218 matched healthy controls. We measured serum chromium levels and genotyped ten genetic variants in ERCC2, XRCC1, MT1B, GSTP1, ABCB1, NQO1, CRTC3, GPX1, SOD2 and CAT. The odds ratios of being diagnosed with lung cancer were calculated using conditional logistic regression with respect to serum chromium level and genotypes. The odds ratio for the occurrence of lung cancer increased with increasing serum chromium levels. The difference between the quartiles with the lowest vs. highest chromium level was more than fourfold in the entire group (OR 4.52, CI 2.17-9.42, $p < 0.01$). This correlation was significantly increased by more than twice when specific genotypes were taken into consideration (ERCC-rs12181 TT, OR 12.34, CI 1.17-130.01, $p = 0.04$; CRTC3-rs12915189 non GG, OR 9.73, CI 1.58-60.10, $p = 0.01$; GSTP1-rs1695 non AA, OR 9.47, CI 2.06-43.49, $p = < 0.01$; CAT-rs1001179 non CC, OR 9.18, CI 1.64-51.24, $p = 0.01$). Total serum chromium levels > 0.1 μg/L were correlated with 73% (52/71) of lung cancers diagnosed with stage I disease. Our findings support the role of chromium and the influence of key proteins on lung cancer burden in the general population.

Authors: Piotr Baszuk, Beata Janasik, Sandra Pietrzak, Wojciech Marciniak, Edyta Reszka, Katarzyna Białkowska, Ewa Jabłońska, Magdalena

Lung cancer is the leading cause of cancer-related death worldwide.

Muszyńska, Monika Lesicka, Róża Derkacz, Tomasz Grodzki, Janusz Wójcik, Małgorzata Wojtyś, Tadeusz Dębniak, Cezary Cybulski, Jacek Gronwald, Bartosz Kubisa, Norbert Wójcik, Jarosław Pieróg, Darko Gajić, Piotr Waloszczyk, Rodney J Scott, Wojciech Własowicz, Anna Jakubowska, Jan Lubiński, Marcin R Lener

Full Source: Biological trace element research 2020 Jul 9. doi: 10.1007/s12011-020-02240-6.

Recent Advances in the Electrochemical Sensing of Venlafaxine: An Antidepressant Drug and Environmental Contaminant

2020-06-30

Venlafaxine (VEN), as one of the popular anti-depressants, is widely utilized for the treatment of major depressive disorder, panic disorder, as well as anxiety. This drug influences the chemicals in the brain, which may result in imbalance in depressed individuals. However, venlafaxine and its metabolites are contaminants in water. They have exerted an adverse influence on living organisms through their migration and transformation in various forms of adsorption, photolysis, hydrolysis, and biodegradation followed by the formation of various active compounds in the environment. Hence, it is crucial to determine VEN with low concentrations in high sensitivity, specificity, and reproducibility. Some analytical techniques have been practically designed to quantify VEN. However, electroanalytical procedures have been of interest due to the superior advantages in comparison to conventional techniques, because such methods feature rapidity, simplicity, sensitivity, and affordability. Therefore, this mini-review aims to present the electrochemical determination of VEN with diverse electrodes, such as carbon paste electrodes, glassy carbon electrodes, mercury-based electrodes, screen-printed electrodes, pencil graphite electrodes, and ion-selective electrodes.

Authors: Somayeh Tajik, Hadi Beitollahi, Zahra Dourandish, Kaiqiang Zhang, Quyet Van Le, Thang Phan Nguyen, Soo Young Kim, Mohammadreza Shokouhimehr

Full Source: Sensors (Basel, Switzerland) 2020 Jun 30;20(13):E3675. doi: 10.3390/s20133675.

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