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CHEMICAL EFFECTS

Ecotoxicological QSAR modeling of the acute toxicity of organic compounds to the freshwater crustacean Thamnocephalus platyurus

2021-10
Growing interest in environmental toxicity assessment using Thamnocephalus platyurus as organism has led to an increased availability of acute toxicity data. Despite this growing interest in tests with this organism, however, to the best of our knowledge there are no computational models to predict the acute toxicity in T. platyurus. In view of the limited number of in silico models for this crustacean, we developed Quantitative Structure-Activity Relationship (QSAR) models for the prediction of acute toxicity towards T. platyurus, reflected by the 24h LC50, using publicly available data according to the ISO 14380:2011 guideline. Two models were developed following the principles of QSAR modeling recommended by the Organization for Economic Cooperation and Development (OECD). We used partial least squares and gradient boosting machine techniques, which gave encouraging statistical quality in our data set.
Authors: Giovanna J Lavado, Diego Baderna, Domenico Gadaleta, Marta Ultre, Kunal Roy, Emilio Benfenati
Full Source: Chemosphere 2021 Oct;280:130652. doi: 10.1016/j.chemosphere.2021.130652.

In silico prediction of chemical-induced hematotoxicity with machine learning and deep learning methods

2021-07-01
Chemical-induced hematotoxicity is an important concern in the drug discovery, since it can often be fatal when it happens. It is quite useful for us to give special attention to chemicals which can cause hematotoxicity. In the present study, we focused on in silico prediction of chemical-induced hematotoxicity with machine learning (ML) and deep learning (DL) methods. We collected a large data set contained 632 hematotoxic chemicals and 1525 approved drugs without hematotoxicity. Computational models were built using several different machine learning and deep learning algorithms integrated on the Online Chemical Modeling Environment (OCHEM). Based on the three best individual models, a consensus model was developed. It yielded the prediction accuracy of 0.83 and balanced accuracy of 0.77 on external validation.

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The consensus model and the best individual model developed with random forest regression and classification algorithm (RFR) and QNPR descriptors were made available at https://ochem.eu/article/135149 , respectively. The relevance of 8 commonly used molecular properties and chemical-induced hematotoxicity was also investigated. Several molecular properties have an obvious differentiating effect on chemical-induced hematotoxicity. Besides, 12 structural alerts responsible for chemical hematotoxicity were identified using frequency analysis of substructures from Klekota-Roth fingerprint. These results should provide meaningful knowledge and useful tools for hematotoxicity evaluation in drug discovery and environmental risk assessment.
Authors: Yuqing Hua, Yinping Shi, Xueyan Cui, Xiao Li
Full Source: Molecular diversity 2021 Jul 1. doi: 10.1007/s11030-021-10255-x.

An Overview on the Potential Hazards of Pyrethroid Insecticides in Fish, with Special Emphasis on Cypermethrin Toxicity

2021-06-25
Pesticides are chemicals used to control pests, such as aquatic weeds, insects, aquatic snails, and plant diseases. They are extensively used in forestry, agriculture, veterinary practices, and of great public health importance. Pesticides can be categorized according to their use into three major types (namely insecticides, herbicides, and fungicides). Water contamination by pesticides is known to induce harmful impacts on the production, reproduction, and survivability of living aquatic organisms, such as algae, aquatic plants, and fish (shellfish and finfish species). The literature and information present in this review article facilitate evaluating the toxic effects from exposure to various fish species to different concentrations of pesticides. Moreover, a brief overview of sources, classification, mechanisms of action, and toxicity signs of pyrethroid insecticides in several fish species will be illustrated with special emphasis on Cypermethrin toxicity.
Authors: Mayada R Farag, Mahmoud Alagawany, Rana M Bilal, Ahmed G A Gewida, Kuldeep Dhama, Hany M R Abdel-Latif, Mahmoud S Amer, Nallely Rivero-Perez, Adrian Zaragoza-Bastida, Yaser S Binnaser, Gaber El-Saber Batiha, Mohammed A E Naiel
Full Source: Animals : an open access journal from MDPI 2021 Jun 25;11(7):1880. doi: 10.3390/ani11071880.

Pesticides are chemicals used to control pests, such as aquatic weeds, insects, aquatic snails, and plant diseases.

Tradeoffs of chemicals regulation - The science and tacit knowledge of decisions

2021-06-25

In this paper, we want to shed light on the tradeoffs of chemicals regulation. We will discuss two types of tradeoffs: the social-economic impacts of regulation such as cost-induced fatalities and the tradeoffs between 'old' and 'new' chemicals, that is the established chemicals in industry and society deemed in need of replacement with 'new' chemicals. We will show that the progression from the science of chemicals risk assessment to regulation requires the science of regulatory (economic) analyses, with added insight from the philosophy of science. Indeed, risk assessment as such, which is significantly driven but is not limited to the broad toxicological context, does not unescapably dictate regulatory choices. The science of regulatory and economic analyses, we believe, could add considerably to the science of toxicology in a combined effort to improve upon the protection of public health and the environment.

Authors: Jaap C Hanekamp, Edward J Calabrese

Full Source: The Science of the total environment 2021 Jun 25;794:148566. doi: 10.1016/j.scitotenv.2021.148566.

ENVIRONMENTAL RESEARCH

Features and Practicability of the Next-Generation Sensors and Monitors for Exposure Assessment to Airborne Pollutants: A Systematic Review

2021-06-30

In the last years, the issue of exposure assessment of airborne pollutants has been on the rise, both in the environmental and occupational fields. Increasingly severe national and international air quality standards, indoor air guidance values, and exposure limit values have been developed to protect the health of the general population and workers; this issue required a significant and continuous improvement in monitoring technologies to allow the execution of proper exposure assessment studies. One of the most interesting aspects in this field is the development of the "next-generation" of airborne pollutants monitors and sensors (NGMS). The principal aim of this review is to analyze and characterize the state of the art and of NGMS and their practical applications in exposure assessment studies. A systematic review of the literature was performed analyzing outcomes from three different databases (Scopus, PubMed, Isi Web of Knowledge); a

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total of 67 scientific papers were analyzed. The reviewing process was conducting systematically with the aim to extrapolate information about the specifications, technologies, and applicability of NGMSs in both environmental and occupational exposure assessment. The principal results of this review show that the use of NGMSs is becoming increasingly common in the scientific community for both environmental and occupational exposure assessment. The available studies outlined that NGMSs cannot be used as reference instrumentation in air monitoring for regulatory purposes, but at the same time, they can be easily adapted to more specific applications, improving exposure assessment studies in terms of spatiotemporal resolution, wearability, and adaptability to different types of projects and applications. Nevertheless, improvements needed to further enhance NGMSs performances and allow their wider use in the field of exposure assessment are also discussed.

Authors: Giacomo Fanti, Francesca Borghi, Andrea Spinazzè, Sabrina Rovelli, Davide Campagnolo, Marta Keller, Andrea Cattaneo, Emanuele Cauda, Domenico Maria Cavallo

Full Source: Sensors (Basel, Switzerland) 2021 Jun 30;21(13):4513. doi: 10.3390/s21134513.

Environmental Factors Affecting Thyroid-Stimulating Hormone and Thyroid Hormone Levels

2021-06-17

Thyroid hormones are necessary for the normal functioning of physiological systems. Therefore, knowledge of any factor (whether genetic, environmental or intrinsic) that alters the levels of thyroid-stimulating hormone (TSH) and thyroid hormones is crucial. Genetic factors contribute up to 65% of interindividual variations in TSH and thyroid hormone levels, but many environmental factors can also affect thyroid function. This review discusses studies that have analyzed the impact of environmental factors on TSH and thyroid hormone levels in healthy adults. We included lifestyle factors (smoking, alcohol consumption, diet and exercise) and pollutants (chemicals and heavy metals). Many inconsistencies in the results have been observed between studies, making it difficult to draw a general conclusion about how a particular environmental factor influences TSH and thyroid hormone levels. However, lifestyle factors that showed the clearest association with TSH and thyroid hormones were smoking, body mass index (BMI) and iodine (micronutrient taken from the diet). Smoking mainly led to a decrease in TSH levels and an increase in triiodothyronine (T3) and thyroxine (T4) levels, while BMI levels were positively correlated with TSH

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and free T3 levels. Excess iodine led to an increase in TSH levels and a decrease in thyroid hormone levels. Among the pollutants analyzed, most studies observed a decrease in thyroid hormone levels after exposure to perchlorate. Future studies should continue to analyze the impact of environmental factors on thyroid function as they could contribute to understanding the complex background of gene-environment interactions underlying the pathology of thyroid diseases.
Authors: Mirjana Babić Leko, Ivana Gunjača, Nikolina Pleić, Tatijana Zemunik
Full Source: International journal of molecular sciences 2021 Jun 17;22(12):6521. doi: 10.3390/ijms22126521.

OCCUPATIONAL

Damage to the Testicular Structure of Rats by Acute Oral Exposure of Cadmium

2021-06-04
Cadmium (Cd) is one of the most important heavy metal toxicants, used throughout the world at the industrial level. It affects humans through environmental and occupational exposure and animals through the environment. The most severe effects of oral exposure to Cd on the male reproductive system, particularly spermatogenesis, have not been discussed. In this study, we observed the damage to the testes and heritable DNA caused by oral exposure to Cd. Adult male Sprague-Dawley rats were divided into four groups: a control group and three groups treated with 5, 10, and 15 mg Cd/kg/day for 17 days by oral gavage. Our results revealed that Cd significantly decreases weight gain in 10 and 15 mg/kg groups, whereas the 5 mg/kg groups showed no difference in weight gain. The histopathology showed adverse structural effects on the rat testis by significantly reducing the thickness of the tunica albuginea, the diameter of the tubular lumen, and the interstitial space among seminiferous tubules and increasing the height of the epithelium and the diameter of the seminiferous tubules in Cd treated groups. Comet assay in epididymal sperms demonstrated a significant difference in the lengths of the head and comet in all the 3 Cd treated groups, indicating damage in heritable DNA, although variations in daily sperm production were not significant. Only a slight decrease in sperm count was reported in Cd-treated groups as compared to the control group, whereas the tail length, percentage of DNA in head, and tail showed no significant difference in control and all the experimental groups. Overall, our findings indicate that Cd toxicity must be controlled using natural sources, such as herbal

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medicine or bioremediation, with non-edible plants, because it could considerably affect heritable DNA and induce damage to the reproductive system.
Authors: Tariq Iqbal, Maosheng Cao, Zijiao Zhao, Yun Zhao, Lu Chen, Tong Chen, Chunjin Li, Xu Zhou
Full Source: International journal of environmental research and public health 2021 Jun 4;18(11):6038. doi: 10.3390/ijerph18116038,

Asbestos Exposure Level and the Carcinogenic Risk Due to Corrugated Asbestos-Cement Slate Roofs in Korea

2021-06-28
Asbestos-cement slate roofs are one of the most common environmental causes of asbestos exposure. However, few studies have examined residential asbestos-cement slate-related exposure and its effects on human health. This study was performed to evaluate cumulative asbestos exposure levels and to calculate the Excess Lifetime Cancer Risk (ELCR) of residents of asbestos-cement slate-roofed houses. We reviewed previous Korean literature to estimate the concentration of airborne asbestos from asbestos-cement slate roofed buildings. Finally, eight studies were selected, and a pooled analysis was performed. The results derived from the pooled analysis were combined with the data from a health impact survey conducted from 2009 to 2016 at the Environmental Health Center for Asbestos (EHCA) of the Yangsan Pusan National University Hospital, and a carcinogenic risk assessment was performed. As a result, the representative value of the indoor exposure concentration related to asbestos-cement slate was found to be 0.0032 f/cc on average, and the representative value of the exposure related to occupational asbestos-cement slate dismantling and demolition was found to be 0.0034 f/cc. In addition, the ELCR of asbestos-cement slate related indoor exposure and occupational dismantling and demolition was found to be of medium risk, and the ELCR of residential dismantling and demolition of asbestos-cement slate was less than 10-6, indicating that the risk was low. Since there is no threshold for carcinogenicity related to asbestos, this should not be ignored even if the risk appears low, and it would be reasonable to calculate the carcinogenic risk based on total lifetime exposure. More studies on asbestos exposure scenarios and the scope of similar exposure groups through additional data collection and further analysis of risk are needed.
Authors: Eun-Soo Lee, Young-Ki Kim
Full Source: International journal of environmental research and public health 2021 Jun 28;18(13):6925. doi: 10.3390/ijerph18136925.

Asbestos-cement slate roofs are one of the most common environmental causes of asbestos exposure.

Occupational exposures in the operating room: Are surgeons well-equipped?

2021-07-02

Background: Occupational health hazards are ubiquitously found in the operating room, guaranteeing an inevitable risk of exposure to the surgeon. Although provisions on occupational health and safety in healthcare exist, they do not address non-traditional hazards found in the operating room. In order to determine whether surgeons or trainees receive any form of occupational health training, we examine the associations between occupational health training and exposure rate. Study design: A cross-sectional survey was distributed. Respondent characteristics included academic level, race/ethnicity, and gender. The survey evaluated seven surgical disciplines and 13 occupational hazards. Multivariable logistic regression was used to examine the association between academic level, surgical specialty, and exposure rate.

Results: Our cohort of 183 respondents (33.1% response rate) consisted of attendings (n = 72, 39.3%) and trainees (n = 111, 60.7%). Surgical trainees were less likely to have been trained in cytotoxic drugs (OR 0.22, p<0.001), methylmethacrylate (OR 0.15, p<0.001), patient lifting (OR 0.43, p = 0.009), radiation (OR 0.40, p = 0.007), and surgical smoke (OR 0.41, p = 0.041) than attending surgeons. Additionally, trainees were more likely to experience frequent exposure to bloodborne pathogens (OR 5.26, p<0.001), methylmethacrylate (OR 2.86, p<0.001), cytotoxic drugs (OR 3.03, p<0.001), and formaldehyde (2.08, p = 0.011), to name a few.

Conclusion: Although surgeon safety is not a domain in residency training, standardized efforts to educate and change the culture of safety in residency programs is warranted. Our study demonstrates a disparity between trainees and attendings with a recommendation to provide formal training to trainees independent of their anticipated risk of exposure.

Authors: Wilmina N Landford, Ledibabari M Ngaage, Erica Lee, Yvonne Rasko, Robin Yang, Sheri Slezak, Richard Redett

Full Source: PloS one 2021 Jul 2;16(7):e0253785. doi: 10.1371/journal.pone.0253785.

Background: Occupational health hazards are ubiquitously found in the operating room, guaranteeing an inevitable risk of exposure to the surgeon.

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PHARAMACEUTICAL/TOXICOLOGY

Perception of risk of exposure in the management of hazardous drugs in home hospitalization and hospital units

2021-07-01

Objective: To assess the perception of risk of exposure in the management of hazardous drugs (HDs) through home hospitalization and hospital units.

Material and methods: A questionnaire was released, at the national level, to health professionals with HD management expertise. Questionnaire included 21 questions that were scored using a Likert scale: 0 (null probability) to 4 (very high probability). The internal consistency and reliability of the questionnaire were calculated using Cronbach's alpha and the intraclass correlation coefficient, respectively. Results: 144 questionnaires (response rate 70.2%) were obtained: 65 (45.1%) were nurses, 42 (28.9%) occupational physicians, and 37 (26.1%) were pharmacists. Cronbach's alpha was 0.93, and intraclass correlation coefficient was 0.94 (95% CI 0.91-0.97; p-value < 0.001). The mean probability was 1.95 ± 1.02 (median 1.9; minimum: 0.05; 1st quartile 1.1; 3rd quartile 2.6; and maximum 4). Differences were observed in scoring among professional groups (occupational physicians versus nurses (1.6/2.1, p = 0.044); pharmacists versus nurses (1.7/2.1, p = 0.05); and occupational physicians versus pharmacists (1.6/1.7, p = 0.785), due mainly to the administration stage (p = 0.015).

Conclusions: The perception of risk of exposure was moderate, being higher for nurses. It would be advisable to integrate HDs into a standardized management system (risk management model applicable to any healthcare center) to improve the safety of health professionals.

Authors: Mari Ángeles Bernabeu-Martínez, Julia Sánchez-Tormo, Pedro García-Salom, Javier Sanz-Valero, Carmina Wanden-Berghe

Full Source: PloS one 2021 Jul 1;16(7):e0253909. doi: 10.1371/journal.pone.0253909.

Objective: To assess the perception of risk of exposure in the management of hazardous drugs (HDs) through home hospitalization and hospital units.

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