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Review Article

Prediction of Ciliate toxicity to the Polycyclic aromatic hydrocarbons

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Abstract

Current study aimed to assess the aquatic toxicity of Polycyclic aromatic hydrocarbons (PAHs). These organic compounds consist two or more aromatic rings fused in linear, angular, or clustered arrangements (Harvey 1991). Among the various animal model, protozoa - *Tetrahymena pyriformis* is the most commonly used ciliate for the laboratory research. From this computational risk assessment only two compounds show low log $(IGC_{50})^{-1}$ value, such as 1H-Indole and Phenazone log $(IGC_{50})^{-1}$ value predicted as 0.1 to 0.11 -log(mmol/L) ± 1.07 against the T*etrahymena pyriformis.* All the predicted values of log $(IGC_{50})^{-1}$ are accessible from the www.chemdata.dev without any restriction and charges.

Keywords: turner syndrome; parathyrodism; osteoporosis; sudan

Introduction

Chemcial compounds may enter into the water environment or bio-accumulate. Entering toxic chemcials in aquatic environemnt can affect the food chain and become threaten to pristine ecology and aquatic life (Singh and Chandra, 2019). Anthropogenic Chemicals are synthesized by various manufacturer because of wide application in the field of agriculture, industry, medicine, and military operations. These checmcials may release into the environment during the prodcution and usage (Agrawal, 2010). Polycyclic aromatic hydrocarbons (PAHs) are a class of organic compounds that consist solely of carbon and hydrogen atoms in aromatic ring structures. Such a chemicals attracted great concern as global environmental pollutants (Cheng et al., 2018). The U.S. Environmental Protection Agency (USEPA) announced regulation on the Sixteen PAHs based on their potential adverse effects on human nad our environemnt. PAHs ranked 9th on the 2015 Agency for Toxic Substances and Disease Registry (ATSDR) Priority List of Hazardous Substances (PLHS) based on their toxicity, frequency of occurrence at USEPA National Priorities List (NPL) sites, and potential for human exposure (ATSDR, 2015) (LaGoy and Quirk 1994). PAHs can be divided into two categories as low and high molecular weight. The PAHs composed of less than four aromatic rings are low molecular weighted (LMW) for example naphthalene, acenaphthene, fluorene, phenanthrene. And high molecular weight PAHs composed of four or more rings for example pyrene, chrysene, benzo[a]pyrene, dibenz[a,h]anthracene). Compared with LMW PAHs High molecular weight PAHs has lower vapor pressures, Henry's constants and less water soluble. Also, PAHs are hydrophobic and do not readily dissolve in water or volatilize to the atmosphere. The chemical stability, low water solubility, and high sorption capacity of PAHs contribute greatly to their persistence in the environment (Kanaly and Harayama 2000; Hamme et al 2003). Computational risk assessments are acquiring recognition for the evaluation of environmental toxicants. To study the aquatic toxicity of PAHs we used Online Chemical Modeling Environment (OCHEM) predictor.

Methodology

Data collection

Chemical structure and SMILES of PAHs was retrieved from the OPSIN - Open Parser for Systematic IUPAC Nomenclature and shown in **Table 1** (Lowe et al., 2011). Web server of OPSIN can be accessed from the https://opsin.ch.cam.ac.uk/.

Toxicity Prediction

The OCHEM is a web-based platform that aims to automate and simplify the typical steps required for QSAR modeling. The OCHEM is free for web users and it is available online at http://www.ochem.eu. It consists of two major subsystems and integrated with the modeling framework. Also supports all the steps required to create a predictive model along with data search, calculation and selection of a vast variety of molecular descriptors, application of machine learning methods, validation, analysis of the model and assessment of the applicability domain.

Results and Discussion

From the result of OCHEM prediction to know the log $(IGC_{50})^{-1}$ value of test compounds. Currently there is no database to share the toxicity profile of the PAHs. And this research provides a new database named CDD and it is accessible from www.chemdata.dev. From this *in silico* risk assessment, 1H-Indole and Phenazone log $(IGC_{50})^{-1}$ value predicted as 0.1 to 0.11 -log(mmol/L) ± 1.07 against the T*etrahymena pyriformis* (**Table 1**). Also, log $(IGC_{50})^{-1}$. All the predicted values of log $(IGC_{50})^{-1}$ are accessible from the www.chemdata.dev.

Conflict of interest

Declarations of interest: none

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Supporting Material

Supporting material accessible from the web link www.chemdata.dev.

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