Prediction of polycyclic aromatic hydrocarbons toxicity using Online CHEmical database and Modeling environment

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Data Note

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Abstract

The purpose of this computational study was to determine the aquatic toxicity of polycyclic aromatic hydrocarbons (PAHs). In PAHs two or more aromatic rings are fused in linear, angular, or clustered patterns. The ciliated protozoan *Tetrahymena pyriformis* is the most often utilised ciliate for laboratory study among the numerous animal models. From this computational risk assessment only two compounds shows 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.*

Introduction

Anthropogenic chemcial compounds may enter into the water environment and it can affect the food chain and become threaten to pristine ecology and aquatic life (Singh and Chandra, 2019). Polycyclic aromatic hydrocarbons (PAHs) are a group of organic molecule made up entirely of carbon and hydrogen atoms in aromatic ring structures. Such a chemicals attracted great concern as global environmental pollutants (Cheng et al., 2018). Chemicals are synthesized by various manufacturer because of wide application in the field of agriculture, industry, medicine, and military operations. These checmcials may released into the aquatic environment during the prodcution and usage. The United States Environmental Protection Agency (USEPA) has declared that the Sixteen PAHs would be regulated because to their possible negative effects on humans and the environment (LaGoy and Quirk 1994). Low and high molecular weight PAHs are the two types of PAHs. Low molecular weighted (LMW) PAHs are those with less than four aromatic rings, such as naphthalene, acenaphthene, fluorene, and phenanthrene. And PAHs with four or more rings, such as pyrene, chrysene, benzo[a]pyrene, and dibenz[a,h]anthracene). When compared to LMW PAHs, The vapour pressures, Henry's constants, and water solubility of high molecular weight PAHs are all lower (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 database and Modeling environment (OCHEM) predictor.

Methodology

Data collection

Chemical structure and SMILES of PAHs obtained from the OPSIN - Open Parser for Systematic IUPAC Nomenclature and shown in **Table 1** (Lo we 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 tool for simplify and automate the typical aspects of QSAR modelling. Dr. Igor V. Tetko created the OCHEM platform, which is available for free at http://www.ochem.eu (Oprisiu et al., 2013; Sushko et al., 2011). It is made up of two key subsystems that operate along with the modelling

framework. Also covers all processes necessary to develop a predictive model, including data search, computation and selection of a wide range of chemical descriptors, model analysis, machine learning methods and data validation.

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. 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.

Declarations

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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US, EPA, United States. Environmental Protection Agency. Environmental Criteria and Assessment Office (Cincinnati, 1993. Provisional guidance for quantitative risk assessment of polycyclic aromatic hydrocarbons (Vol. 600). Environmental Criteria and Assessment Office, Office of Health and Environmental Assessment, US Environmental Protection Agency.

Table 1

Table 1 is not available with this version