

08.10.2019

+++ News Ticker Science #6 +++ Chemoinformatics +++



The screenshot shows the article page on the Environmental Science: Processes & Impacts website. The article title is 'Exploring open cheminformatics approaches for categorizing per- and polyfluoroalkyl substances (PFASs)'. The authors listed are Bo Sha, Emma L. Schymanski, Christoph Ruttkies, Ian T. Cousins, and Zhenyuan Wang. The article is categorized as a 'PAPER'. The abstract discusses the challenge of categorizing PFASs and the development of a 'spitfire' approach to systematically subdivide PFASs for chemical categorization. The article was received on 16 July 2019 and accepted on 19 September 2019. The DOI is 10.1039/c9em00321e.

Exploring open cheminformatics approaches for categorizing per- and polyfluoroalkyl substances (PFASs).

Per- and polyfluoroalkyl substances (PFASs) are a large and diverse class of chemicals of great interest due to their wide commercial applicability, as well as increasing public concern regarding their adverse impacts. Recent advancements in chemical analysis allow identification of a wide variety of PFASs that are, however, not covered by the common terminology recommended in 2011. The resulting inconsistency in categorizing and naming of PFASs is preventing efficient assimilation of reported information. In this article a team of researchers from the University of Luxembourg, University of Stockholm, ETH Zürich and IPB Halle explores how a combination of expert knowledge and cheminformatics approaches could help address this challenge in a systematic manner. The structure-based cheminformatics tool provided is implemented flexibly, interpreting structures quickly and has the potential to help scientists, regulators and other interested parties categorize, and thus assess, PFASs.

Original publication:

Sha B, Schymanski EL, Ruttkies C, Cousins IT, Wang Z. Exploring open cheminformatics approaches for categorizing per- and polyfluoroalkyl substances (PFASs). *Environ. Sci.: Processes Impacts*, 2019, DOI: [10.1039/c9em00321e](https://doi.org/10.1039/c9em00321e)