

# Environmental Science Processes & Impacts

rsc.li/espi

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

## IN THIS ISSUE

ISSN 2050-7887 CODEN ESPICZ 25(11) 1735–1852 (2023)



### Cover

Image credit: © Romolo Tavani/Shutterstock.

## EDITORIAL

1741

### Introduction to the "Tracking complex mixtures of chemicals in human- and eco-exposome: the nexus of models, analytics, and toxicity" themed issue

Mingliang Fang, Li Li, Zhenyu Tian and Beate Escher

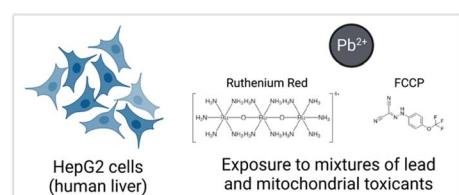


## COMMUNICATIONS

1743

### Increased cytotoxicity of $\text{Pb}^{2+}$ with co-exposures to a mitochondrial uncoupler and mitochondrial calcium uniporter inhibitor

Pooja Lalwani, Dillon E. King, Katherine S. Morton, Nelson A. Rivera, Jr, Javier Huayta, Heileen Hsu-Kim and Joel N. Meyer\*



# Environmental Science Processes & Impacts

rsc.li/espi

*Environmental Science: Processes & Impacts* is a multidisciplinary journal for the environmental chemical sciences, publishing high quality papers in areas including the chemistry of the air, water, soil and sediment.

## Editorial Board

### Editor-in-Chief

Kristopher McNeill, ETH Zürich, Switzerland

### Associate Editors

Qian Liu, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, China

Matthew MacLeod, Stockholm University, Sweden

Jasquelin Peña, University of California, Davis, USA

Paul Tratnyek, Oregon Health & Science University, USA

Cora Young, York University, Canada

### Members

Katyte Altieri, University of Cape Town, South Africa

Ludmilla Aristilde, Northwestern University, USA

Amila de Silva, Environment and Climate Change Canada, Canada

Beate Escher, Helmholtz Centre for Environmental Research, Germany

Mingliang Fang, Fudan University, China

Delphine Farmer,

Colorado State University, USA

Weihua Song, Fudan University, China

Lenny Winkel,

Swiss Federal Institute of Aquatic Science and Technology, Eawag, Switzerland

## Advisory Board

Urs Baltensperger, Paul Scherrer Institute, Switzerland

Alexandria Boehm, Stanford University, USA

Richard Brown, National Physical Laboratory, UK

Junji Cao, Institute of Earth Environment, CAS, China

Kathrin Fenner, Swiss Federal Institute of Aquatic Science and Technology, Eawag, Switzerland

Tamara Galloway, University of Exeter, UK

Philip Gschwend, Massachusetts Institute of Technology, USA

Liang-Hong Guo, China Jiliang University, China

Colleen Hansel, Woods Hole Oceanographic Institution, USA

Hans Christian Bruun Hansen, University of Copenhagen, Denmark

Stuart Harrad, University of Birmingham, UK

Heileen Hsu-Kim, Duke University, USA

Jianying Hu, Peking University, China

Young-Shin Jun, Washington University in St. Louis, USA

Andreas Kappler, University of Tübingen, Germany

Karen Kidd, McMaster University, Canada

Edward Kolodziej, University of Washington, USA

Ruben Kretzschmar, ETH Zürich, Switzerland

Derek Muir, Environment & Climate Change Canada, Canada

Kara Nelson, University of California, Berkeley, USA

Jasquelin Peña, University of California, Davis, USA

Noelle Selin, Massachusetts Institute of Technology, USA

Susan Solomon, Massachusetts Institute of Technology, USA

Elsie Sunderland, Harvard University, USA

Sachchida Nand Tripathi, Indian Institute of Technology Kanpur, India

David Waite, University of New South Wales, Australia

Frank Wania, University of Toronto at Scarborough, Canada

Guang-Guo Ying, South China Normal University, China

## Information for Authors

Full details on how to submit material for publication in *Environmental Science: Processes & Impacts* are given in the Instructions for Authors (available from <http://www.rsc.org/authors>). Submissions should be made via the journal's homepage: rsc.li/espi

Authors may reproduce/republish portions of their published contribution without seeking permission from the Royal Society of Chemistry, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation)–Reproduced by permission of the Royal Society of Chemistry.

This journal is © The Royal Society of Chemistry 2023.

Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

Registered charity number: 207890

## Editorial Staff

### Executive Editor

Neil Scriven

### Deputy Editor

Grace Thoburn

### Development Editor

Nour Tanbouza

### Editorial Production Manager

Claire Darby

### Publishing Editors

Emma Carlisle, Hannah Hamilton, Ephraim Otumudia, Irene Sanchez Molina Santos, Michael Spencelayah, Callum Woof, Lauren Yarrow-Wright

### Editorial Assistant

Kate Bandoo

### Publishing Assistant

Linda Warneke

### Publisher

Sam Keltie

For queries about submitted papers please contact Claire Darby, Editorial Production Manager, in the first instance. E-mail: [espi@rsc.org](mailto:espi@rsc.org)

For pre-submission queries please contact Neil Scriven, Executive Editor. E-mail: [espi-rsc@rsc.org](mailto:espi-rsc@rsc.org)

*Environmental Science: Processes & Impacts* (electronic: ISSN 2050-7895) is published 12 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, UK CB4 0WF.

All orders, with cheques made payable to the Royal Society of Chemistry, should be sent to the Royal Society of Chemistry Order Department, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK Tel +44 (0)1223 432398; E-mail [orders@rsc.org](mailto:orders@rsc.org)

2023 Annual electronic subscription price: £1839 US\$3301. Customers in Canada will be subject to a surcharge to cover GST. Customers in the EU subscribing to the electronic version only will be charged VAT.

If you take an institutional subscription to any Royal Society of Chemistry journal you are entitled to free, site-wide web access to that journal. You can arrange access via Internet Protocol (IP) address at [www.rsc.org/ip](http://www.rsc.org/ip)

Customers should make payments by cheque in sterling payable on a UK clearing bank or in US dollars payable on a US clearing bank.

Whilst this material has been produced with all due care, the Royal Society of Chemistry cannot be held responsible or liable for its accuracy and completeness, nor for any consequences arising from any errors or the use of the information contained in this publication. The publication of advertisements does not constitute any endorsement by the Royal Society of Chemistry or Authors of any products advertised. The views and opinions advanced by contributors do not necessarily reflect those of the Royal Society of Chemistry which shall not be liable for any resulting loss or damage arising as a result of reliance upon this material. The Royal Society of Chemistry is a charity, registered in England and Wales, Number 207890, and a company incorporated in England by Royal Charter (Registered No. RC000524), registered office: Burlington House, Piccadilly, London W1J 0BA, UK, Telephone: +44 (0) 207 4378 6556.

### Advertisement sales:

Tel +44 (0) 1223 432246; Fax +44 (0) 1223 426017; E-mail [advertising@rsc.org](mailto:advertising@rsc.org)

For marketing opportunities relating to this journal, contact [marketing@rsc.org](mailto:marketing@rsc.org)

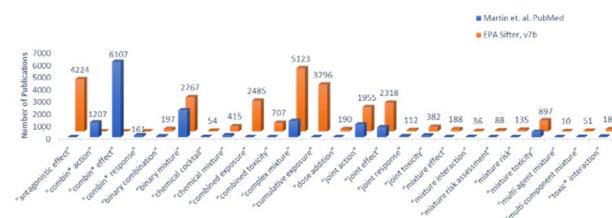


## COMMUNICATIONS

1752

## Evaluation of mixture toxicity literature and chemical space: a data centric approach

Vatsal Mehta, Mahmoud Shobair and Catherine Mahony\*

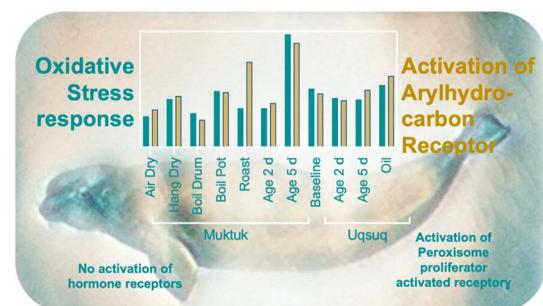


## PAPERS

1759

Mixture effect assessment applying *in vitro* bioassays to in-tissue silicone extracts of traditional foods prepared from beluga whale blubber

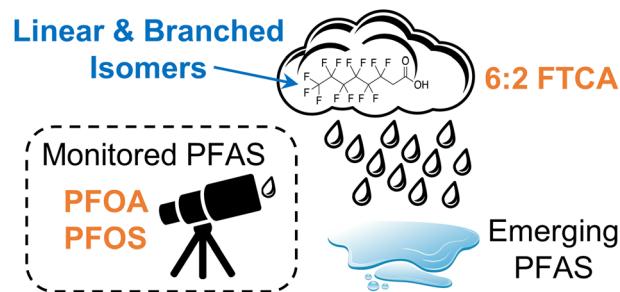
Beate I. Escher,\* Matthew J. Binnington, Maria König, Ying D. Lei and Frank Wania\*



1771

## Non-targeted identification and semi-quantitation of emerging per- and polyfluoroalkyl substances (PFAS) in US rainwater

Yubin Kim, Kyndal A. Pike, Rebekah Gray, Jameson W. Sprankle, Jennifer A. Faust and Paul L. Edmiston\*



1788

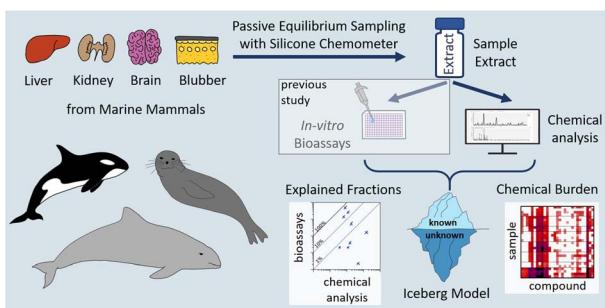
## Adding open spectral data to MassBank and PubChem using open source tools to support non-targeted exposomics of mixtures

Anjana Elapavalore,\* Todor Kondić, Randolph R. Singh, Benjamin A. Shoemaker, Paul A. Thiessen, Jian Zhang, Evan E. Bolton and Emma L. Schymanski\*

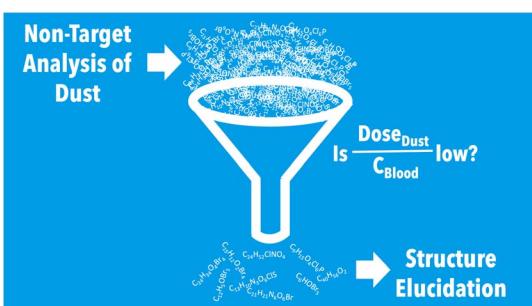


## PAPERS

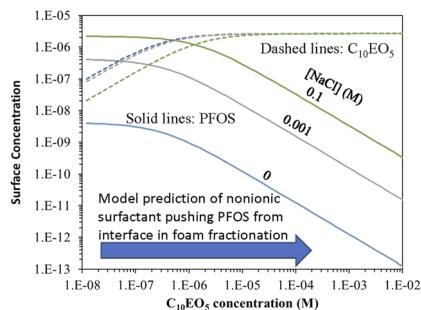
1802



1817



1830



1839



# Characterizing the marine mammal exposome by iceberg modeling, linking chemical analysis and *in vitro* bioassays

Eva B. Reiter,\* Beate I. Escher, Elisa Rojo-Nieto,  
Hannah Nolte, Ursula Siebert and Annika Jahnke\*

# Prioritizing molecular formulae identified by non-target analysis through high-throughput modelling: application to identify compounds with high human accumulation potential from house dust

Zhizhen Zhang, Li Li, Hui Peng and Frank Wania\*

# A fundamental model for calculating interfacial adsorption of complex ionic and nonionic PFAS mixtures in the presence of mixed salts

Yi Gao, Song-Thao Le, Tohren C. G. Kibbey,  
William Glamore and Denis M. O'Carroll\*

# Occurrence of emerging contaminants in pet hair and indoor air: integrative health risk assessment using multiple ToxCast endpoints

Ying Zhang, Yujun Tong, Fei Cheng,\* Jingwen Shi, Jiehui Huang, Mingqi Yu and Jing You