

NORMAN Workshop (Hybrid)

**Artificial Intelligence (AI) for
environmental monitoring, assessment
and prioritisation of chemicals and their
mixtures**



Date: 21-22 October 2024

Venue: Helmholtz Centre for
Environmental Research – UFZ,
Kubus - Hall 1
Permoserstr. 15 - 04318 Leipzig,
Germany

21 October 2024 – Day 1

12h00 – 12h45	Registration and coffee	
12h45 – 13h00	Opening and Welcome (Werner Brack, Steering committee)	
13h00 – 15h00	Presentations on AI- based methods and use cases in support of environmental monitoring and assessment (Chairs: Juliane Hollender, Jan Koschorreck)	
	13h00 – 13h15	The Norman Network, Valeria Dulio, INERIS, France
	13h15 – 13h30	A small thought on combining expertise – a big step for Component-Based biodiversity impact assessments of chemical pollution? Leo Posthuma, RIVM, The Netherlands
	13h30 – 13h45	The use of AI to predict chemical toxicity - Erik Kristiansson, Chalmers Univ. of Technology, Sweden
	13h45 – 14h00	AI-driven Chemical-effect association with deepFPlearn, including enhanced credibility measures, graph neural networks, classification, and regression - Jana Schor, UFZ, Germany
	14h00 – 14h15	First results from ML based toxicity prediction trial in NORMAN, Nikiforos Alygizakis - Environmental Institute, Slovakia
	14h15 – 14h30	ML based methods to support suspect and non-target data - Anneli Kruve, Stockholm University, Sweden
	14:30 – 14:45	Data Science approaches to uncover contamination sources from Rhine Monitoring Data - Teofana Chonova, Eawag, Switzerland
15h00 – 15h30	Coffee break	
15h30 – 17h30	Presentations on AI- based methods and use cases in support of environmental monitoring and assessment (Chairs: Valeria Dulio, Werner Brack)	
	15h30 – 15h45	Chemical space mapping to model LCMS amenability predictions - Nate Charest, US EPA

	15h45 – 16h00	Deep learning models to predict physico-chemical properties for risk assessment of chemicals - Nadin Ulrich, UFZ, Germany
	16h00 – 16h15	Probabilistic approaches to mapping the exposome chemical space - Saer Samanipour, University of Amsterdam, The Netherlands
	16h15 – 16h30	NTS use case for UBA application lab for AI and Big Data, Jan Siegismund, German environment agency, Germany
	16h30 – 16h45	Automated Curation of Spatial Data in Environmental Monitoring: Enhancing the NORMAN Chemical Occurrence Database for Big Data Analytics and AI Applications - Ilhan Mutlu, UFZ, Germany
	16h45 – 17h00	Using innovative ML techniques to predict the risk of chemicals for multiple species - Reza Aalizadeh, NKUA, Greece and Peter von der Ohe, UBA, Germany
	17h00 – 17h15	Workshop participants pitch questions for discussions on day 2
19h30	Dinner together at „Auerbach’s Keller“ (Mädler Passage, Grimmaische Straße 2-4, 04109 Leipzig). Attendees will be responsible for covering the cost of the dinner.	

22 October 2024 – Day 2	
9h00 – 9h15	Welcome and distribution into discussion groups
9h15 – 10h15	World café with 8 tables (around the following list of 4 topics) Toxicity & AI; HRMS & AI; Source tracking & AI (potentially part of HRMS); Chemical space & AI; Data curation/databases for AI
10h15 – 10h45	Coffee break
10h45 – 11h30	World café with 8 tables (around the following list of 4 topics) Toxicity & AI; HRMS & AI; Source tracking & AI (potentially part of HRMS); Chemical space & AI; Data curation/databases for AI
11h30 – 12h30	Feedback from world café (each rapporteur reports to the plenary the main outcomes) Discussion
12h30 – 13h00	General discussion - Fields of application of AI tools in NORMAN (upcoming NORMAN JPAs) - Collaboration with additional experts/networks beyond NORMAN? - NORMAN AI strategy (a new working group?)
13h00 – 14h00	Lunch