NORMAN Workshop (Hybrid)

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

Date: 21-22 October 2024 (CET)

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**	
	13h00 – 13h15	ECHA /DG ENV/EU AI lab (EU perspective) representative
	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 quantification of 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**	
	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	AI lab UBA (tbc)
	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	Discussion (gathering input for discuss on the next day)
19h30	**Dinner together. Please indicate in the registration form if you wish to participate. 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 (3-5 tables around the following topics):** Toxicity & AI; HRMS & AI; Source tracking & AI (potentially part of HRMS); Chemical space & AI; Data curation/databases for AI Important points to include in the discussion: Harmonisation, benchmarking, evaluation, needs, limitations
10h15 – 10h45	**Coffee break**
10h45 – 11h30	Feedback from the discussion groups (each rapporteur reports to the plenary the main outcomes of the discussions) Discussion
11h30 – 12h30	**World café session (3 tables around the following topics):** - 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?)
12h30 – 13h00	Feedback from the discussion groups (each rapporteur reports to the plenary the main outcomes of the discussions) Discussion **Wrap-up and goodbye**
13h00 – 14h00	**Lunch**