INTEGRATING AI INTO CHEMICAL SAFETY ASSESSMENT
OPPORTUNITIES, CHALLENGES, AND THE PATH FORWARD

Workshop background and objectives

Chemical safety assessment is the systematic analysis of scientific data to characterize the potential adverse effects resulting from human or environmental exposure to chemicals. Safety assessment relies on a wide variety of data sources of both qualitative and quantitative nature.

The capacity and advancement of Artificial intelligence (AI) to process and analyse vast datasets with complex relationships, and also unstructured data types (like images, text), has opened new possibilities for chemical safety assessment, including predictive toxicology and hazard identification. AI offers advantages in terms of efficiency, scale, and the ability to interrogate large datasets, for example in the areas of screening, predictive (eco)toxicology and omics data assessment. AI can be applied both retrospectively, on already generated/historical data, as well as prospectively, using newly generated data. Both applications require application of FAIR principles[1].

However, the rapid integration of AI technologies into chemical safety assessment presents significant challenges including considerations on the quality of training data, the dynamic nature of learning algorithms, and the implications for regulatory assessments. For example, AI technology learns regardless of the quality of the training set, so issues such as poor training sets could lead to low quality applications and interpretations. In addition, as AI is a learning system, it is challenging to ensure that assessments or conclusions drawn in the past are still valid in the future. As technology continues to advance, the integration of AI in chemical safety assessment is likely to expand, providing opportunities for innovative solutions to complex challenges.

This workshop aims to leverage the collective expertise of scientists, technologists, regulators, and industry leaders in the application of AI in chemical safety assessment.

The workshop objectives are to:

1. Give an overview of the "state of the art" of AI technologies relevant chemical safety assessment, as well as Success Stories and Lessons Learned, including opportunities and risks
2. Discuss how AI could be applied in mainstream chemical safety assessment, both with respect to hazard identification and safety assessment, while minimizing risks
3. Review and discuss the challenges associated with application of AI in chemical safety assessment

It is intended that this workshop be a first step towards developing a road map for the application of AI in mainstream chemical safety assessment.

A workshop write-up will be prepared and submitted for publication in a peer reviewed journal.

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[1] Findable, Accessible, Interoperable, and Reusable

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Draft Agenda

Day 1: 16 October — Setting the scene [F2F participants and online]		
Time	**Agenda item**	**Who**
12:00-1:00 PM	*Arrival, registration and lunch*	
1:00-1:10 PM	**Welcome, introduction and workshop objectives**	
1:10-1:40 PM	**From Data to Decisions: AI's Role in Modern Toxicology**	**Nicole Kleinstreuer (National Institute of Environmental Health Sciences; NIEHS, US**
1:40-2:05 PM	**Artificial intelligence in science: recent developments and policy implications**	**Alistair Nolan (OECD)** Online
2:05-2:20 PM	**FAIR data and data that is Fully AI Ready**	**Erik Schultes (GO FAIR Foundation, NL)** Online
2:20-2:35 PM	**FAIR Knowledge enabling FAIR Risk Assessment**	**Barry Hardy (Edelweiss Connect GmbH, CH)**
2:35-2:40 PM	FAIR principles Q&A	**Erik Schultes & Barry Hardy**
2:40-3:00 PM	*Coffee break*	
3:00-3:35 PM	**Application of AI to cell imaging for drug discovery and diagnosis**	**Paul Rees (Swansea University, UK)**
3:25-3:50 PM	**AI in toxicology – the now, the new and the next**	**Thomas Hartung (John Hopkins University, US)**
3:50-4:15 PM	**Generative AI for Toxicology and Drug Safety**	**Weida Tong (US FDA)**
4:15-4:40 PM	**Cell painting and cell image analysis**	**David Rouquie (Bayer, FR)**
4:40-5:00 PM	*Coffee break*	

Day 1: 16 October — Setting the scene [F2F participants and online]

Time	Agenda item	Who
5:00-5:25 PM	**Leveraging the use of AI in the Virtual Human Platform for Safety Assessment (VHP4Safety) project**	**Anne Kienhuis (RIVM, NL)**
5:25-5:50 PM	**Applications of machine learning and AI approaches to develop PBPK and QSAR models to predict ADMET properties to aid chemical safety assessment**	**Zhoumeng Lin (University of Florida, US)**
5:50-6:15 PM	**Introducing AI in EFSA systematic reviews**	**Fulvio Barizzone (EFSA)**
6:15-6:25 PM	**Summarise and closing remarks**	
7:00-9:00 PM	***Networking event***	

Day 2: 17 October — [F2F participants only]

Time	Agenda item	Who
9:00-9:20 AM	**Welcome and recap, and introduction on the breakout groups and of day 2**	
9:20-9:30 AM	**Lessons learnt from genomics**	**Tim Gant (Imperial College London)**
9:30-10:40 AM	**Breakout Group Discussions: First Round**	
10:40-10:55 AM	***Coffee break***	
10:55-12:05 AM	**Breakout Group Discussions: Second Round**	
12:05-1:15 PM	**Breakout Group Discussions: Third Round**	
1:15-2:30 PM	***Lunch***	
2:30-3:15 PM	**Plenary feedback from breakout groups**	
3:15-3:30 PM	**Summarise and closing remarks**	

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Organising Committee

Alistair	Boxall	University of York
Tim	Gant	Imperial College London
Przemyslaw	Piechota	Nestle
Hua	Qian	ExxonMobil
David	Rouquie	Bayer
Ben	van Ravenzwaay	Wageningen University and Research
Maryam	Zare Jeddi	Shell
Blanca	Serrano	ECETOC
Andrea	Salvadori	ECETOC
Lucy	Wilmot	ECETOC
Francesca	Uguccioni	ECETOC
Sergio	Perez	ECETOC

PRACTICALITIES

Venue

Bayer SAS
355 rue Dostoïevski
06550 Sophia Antipolis
France

Where to stay

Mouratoglou Hotel & Resort
3550 Rte des Dolines
06410 Biot
France
(book using this reservation link before 6 July to benefit from the negotiated rate of 165€/night including breakfast)

Contact

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