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FSA-funded Computational Toxicology Fellowship and LIDo PhD student in AI

16. The FSA and COT have been reviewing New Approach Methodologies (NAMs) to scope the best scientific methodologies available to be used in risk assessment of chemicals in foods and the environment and understand how these can be incorporated in a regulatory context with validation approaches.

17. The FSA have recruited a computational toxicology fellow at the University of Birmingham and a PhD Student (London Interdisciplinary Doctoral Program-LIDo- TOX AI) at King's College London. The aims of the projects are to develop *in silico* tools (*i.e.* artificial intelligence machine learning) for toxicological prediction of

chemicals through case studies and proof of concept studies. The fellow and student will also work alongside other government departments to understand how NAMs will improve indicative levels of safety in chemical risk assessment.

18. In addition, these new partnerships will help with networking, research collaboration, training opportunities and further our knowledge in this area. The

fellowship and studentship also compliment the work set out in our UK Roadmap towards using new approach methodologies in chemical risk assessment.

19. The programme of work in the fellowship consists of (i) scoping the FSA's problem space in chemical risk assessment and mapping this to our computational NAMs solution space, thereby aiding the FSA to develop a strategy for the utilisation of NAMs; (ii) ensuring that the FSA is trained in the use of computational NAMs by delivering training courses, including an introduction to existing and emerging NAM technologies, and topics selected from the FSA's NAM strategy; (iii) developing and evaluating confidence in a new hazard assessment workflow that integrates in vitro omics toxicity data, benchmark dose modelling and PBPK modelling to serve as the basis for quantitative risk assessment for human health, i.e., towards generating human health-based safety thresholds for FSA and other regulators; and (iv) developing and delivering a second case study that fortifies the community-wide acceptance of 21st century methods in risk assessments, to accelerate the successful application of NAMs within the FSA.

20. The postdoctoral fellow case study on a perfluorinated substance, perfluorooctanoic acid (PFOA) has now been completed and published. The NAMs employed include:

- NAMs in relation to the type of testing platform - in vitro hepatic microtissues;
- NAMs in relation to the type of data/read-outs - transcriptomics data, providing an untargeted measurement of extensive gene expression;
- NAMs in relation to data analysis - PBPK modelling.

21. Our recent work on PFOA (Silva et al., 2024) has been presented on several occasions. To list a few, PARC Science Day (poster presentation), NURA Dynamic Discussions (oral presentation, online), HSE's workshop (oral presentation, online), EFSA's workshop (oral presentation, online), EUROTOX 2023 (poster presentation), ASPIS Open Symposium 2023 (poster presentation). The PFOA work was submitted as a nomination to the Lush Prize under the Young Researcher category and was one of the five projects awarded in 2022.

22. The third case study is now under consideration by the supervisory team, which is keen to work with tropane alkaloids as this class of substances is of high interest to the FSA.

23. The programme of work in the PhD up to the present is composed of three parts: (1) Exploration of dimensionality reduction algorithms, for powering

QSAR models of mutagenicity, constructed of simple feed-forward Deep Neural Networks (DNNs) (Kalian et al., 2023, Kalian et al., 2023) (This article belongs to the Collection Artificial Intelligence and Data Mining for Toxicological Sciences and is a Feature Paper and Editor’s Choice); (2) Development of Graph Convolutional Networks (GCNs) to improve mutagenicity predictions, via graph classification of molecules, while also allowing for mining of structural alerts (SAs).

24. The PhD student current program of work consists of graph attention networks using knowledge graphs, for predicting novel points of departure for brominated flame retardants (BFRs) by the development of Graph Neural Networks (GNNs) for node classification of molecules, in order to predict toxicological properties of BFRs (Kalian et al., 2024). This won the **Toxics Travel Award 2024** and was presented at Eurotox 2024.

25. The postdoctoral fellow and PhD student are working on a case study together.