## BTS Annual Congress 2025 symposium report – Olivia Harris

I attended the British Toxicology Society (BTS) Annual Congress held from the 7th until the 9th of May at Spaces at The Spine in Liverpool. The BTS Pre-Doctoral Student bursary allowed me to attend the congress and present an oral communication on a portion of my PhD project, furthering my academic development. The congress helped to broaden my understanding of the latest developments in toxicology; introducing me to a variety of topics that go beyond the focus of my own project.

A highlight of the congress was Symposium 3: Large Language Models in Risk Assessment, chaired by Susy Brescia (Health & Safety Executive) and Ciarán Fisher (GSK). This session focused on hot topics within in silico modelling, looking at the integration of artificial intelligence (AI) and machine learning within toxicology and safety science. Due to my project combining mathematical modelling and experimental work to better understand the dynamics of the oxidative stress response in drug-induced liver injury, this session was of particular interest to me.

Thierry Hanser from Lhasa Ltd started off the session with a talk entitled 'Artificial Intelligence, Machine Learning and Large Language Models (LLMs): What's What.' He gave a clear and engaging timetable of how AI has evolved, starting with early rule-based systems and leading up to today's generative models. The talk helped to outline the differences between AI, machine learning (ML), and LLMs. Dr. Hanser also highlighted how LLMs are being used more often in multiple areas such as: molecular informatics, predictive toxicology, and chemical safety. The part of the talk that was particularly interesting and important was how these tools can be used to speed up discovery, and support both decision-making and planning across a wide range of fields. I also valued the point he made about using LLMs responsibly, ensuring that scientific rigor and context stay front and centre when applying them to real-world toxicology challenges.

The second talk was given by Sebastian Lobentanzer from Helmholtz Munich and was titled 'Trustworthy AI: Constraining and Validating LLMs in Preclinical Safety'. He explored how LLMs are being used within biomedical research for tasks such as summarising scientific literature, generating new hypotheses, and supporting regulatory work. He discussed agentic systems (LLMs that can plan and carry out complex tasks on their own), highlighting the importance of pairing these models with the right tools and well-curated datasets to make sure their outputs are reliable and consistent. His take on the limitations of LLMs, especially when it comes to working with complex biological data and the struggles of data formatting, was important to consider. He recommended using stable and open-source frameworks that can help guide the models' behaviour, making the models more suitable for use in regulatory and preclinical safety work.

The final presentation in this symposium was given by Darren Green of DesignPlus Cheminformatics Consultants, titled "The future of artificial intelligence in human safety assessment". Dr. Green outlined the rapid development of AI technologies driven by investments in non-scientific fields, and the potential, that when suitably adapted, these advances hold for toxicology. He stressed the need for the explainable use of predictive models used within safety assessments. Effective integration of AI requires a mechanistic understanding of biological systems and not just statistical optimisation. Knowledge-based systems, adverse outcome pathways, and foundation models were covered in their use interpreting complex biological data. The need for transfer learning to make meaningful predictions from limited datasets, a persistent challenge in toxicology, was emphasised. Dr. Green concluded, reducing reliance on animal testing and improving human health outcomes using AI-driven approaches must ultimately support confident and defensible safety decisions.

This symposium was overall very informative and interesting, with relevance towards my project, covering topics such as AI, computational tools in safety science, and LLMs in risk assessment and showing how mechanistically informed AI is starting to shape regulatory decision-making, which aligns closely with the systems toxicology approach I use. Emerging AI tools can improve the translational relevance of in vitro systems and are potentially something that could be used to strengthen my modelling work. I'm grateful to the BTS for awarding me the Pre-Doctoral Student Bursary and making it possible for me to attend this conference.