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Mathematical modelling in preclinical drug development in oncology: A perspective from the industry side

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The integration of mathematical modelling in preclinical drug development has profoundly impacted the pharmaceutical industry, enabling more precise and predictive insights into drug behavior. This approach is particularly transformative in the development of Proteolysis-Targeting Chimeras (PROTACs), a novel therapeutic modality that leverages the ubiquitin-proteasome system for targeted protein degradation. By employing mathematical models, we can simulate the pharmacokinetics and pharmacodynamics of PROTACs, optimizing their design and efficacy in cancer research and immunology, and other therapeutic areas. These models facilitate the prediction of PROTAC behaviour in complex biological systems, enhancing our understanding of their therapeutic potential and accelerating their transition to clinical use. In this presentation, we will cover various aspects of these mathematical models, including their application in optimizing PROTAC design and predicting therapeutic in-vivo outcomes, such as target engagement and tumour growth inhibition.