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Predictive in vitro methods: How to address current problems?

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Predictive *in vitro* methods are crucial for 21st century toxicology. Currently, most *in vitro* methods are not predictive or their predictivity has not been determined. With respect to predictive assays there is often substantial confusion about the question what an assay actually predicts, and the way how results are presented is often not helpful. Crucial for developing predictive methods is pre-validation with a statistically robust set of compounds, and proper compound annotation and classification require careful consideration. Whereas most discussions focus on selection of proper cell and tissue models, little attention is paid to endpoint selection. Examples will be discussed how bioinformatics methods can be used for the identification of proper endpoints. In addition, the analysis of high-throughput data will be addressed.

Recent Publications:

1. Su R, Xiong S, Zink D and Loo L H (2016) High-throughput imaging-based nephrotoxicity prediction for xenobiotics with diverse chemical structures. Arch Toxicol. 90:2793-2808.
2. Chuah J K and Zink D (2017) Stem cell-derived kidney cells and organoids: recent breakthroughs and emerging applications. Biotechnology Advances. 35(2):150-167.
3. Kandasamy K et al. (2015) Prediction of drug-induced nephrotoxicity and injury mechanisms with human induced pluripotent stem cell-derived cells and machine learning methods. Sci Rep. 5:12337.
4. Li Y et al. (2014) Identification of nephrotoxic compounds with embryonic stem cell-derived human renal proximal tubular-like cells. Molecular Pharmaceutics. 11(7):1982-1990.
5. Li Y et al. (2013) An in vitro method for the prediction of renal proximal tubular toxicity in humans. Toxicol Res. 2(5):352-362.

Biography

Daniele Zink earned her PhD from the University of Heidelberg, Germany in 1995 and completed her Habilitation (2001) at the Ludwig Maximilian University of Munich. In 2001, she was awarded funding of a Junior Group from the Volkswagen-Foundation, which she led until she moved to the Institute of Bioengineering and Nanotechnology (IBN) in Singapore in 2007. Her work on predictive in vitro models has been awarded by Merck Millipore and the US Society of Toxicology. She has won the prestigious LUSH Prize (2016, Science Category). She holds 10 patents/patent applications, is Editorial Board Member of Scientific Reports, has more than 70 peer reviewed publications and is Co-Founder and Director of the spin-off company Cellbae.

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