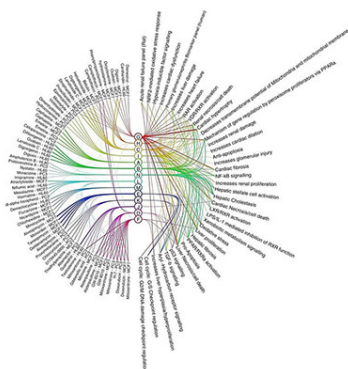


# Statistical component model to identify associations between chemicals and toxicological effects

10 August 2017



The component model describes statistical links between chemicals and the effect of their molecular toxins. Credit: Juuso Parkkinen, Aalto University

The joint Aalto University, Karolinska Institute and Institute for Molecular Medicine Finland (FIMM) study included over 1,300 known pharmaceutical molecules, on which there is a wealth of measurement data available.

'The study uses systematic data-driven analysis to combine toxicity measurements taken on cell lines with gene expression responses describing gene activation. Toxicity includes growth inhibitory and cell killing effects. The method developed in the study makes it possible to more accurately predict the toxicity of new molecules because it makes use of advanced statistical methods and much bigger datasets than before,' explains Juuso Parkkinen, who completed his doctoral dissertation at Aalto University.

At present, [toxicity](#) is primarily measured by means of animal testing. Thanks to this new method, [animal testing](#) can be partly replaced in the future by a combination of cell line testing and statistical

modelling. This would also result in considerable cost savings for pharmaceutical development.

'The new prediction [method](#) can be applied to new pharmaceutical molecules and other chemicals currently in product development to eliminate possible toxic [molecules](#),' adds Parkkinen.

Advances in statistical machine learning and [artificial intelligence](#) methods have risen to play a crucial role in many application areas in addition to medical research.

'Juuso Parkkinen is an excellent example of the usefulness of Aalto University's artificial intelligence research and doctoral studies: He wrote his dissertation on medicinal applications in my research group and then transferred to Reaktor to apply data science to a wide range of business needs,' praises Parkkinen's dissertation adviser, Professor Samuel Kaski.

**More information:** Pekka Kohonen et al. A transcriptomics data-driven gene space accurately predicts liver cytopathology and drug-induced liver injury, *Nature Communications* (2017). [DOI: 10.1038/ncomms15932](#)

Provided by Aalto University

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