In silico models for the REACH and the food regulation: perspectives for the near future

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In silico models can and should provide tools to reduce the impact of chemical substances in our life, minimizing the risk for the human health and the environment. These tools should be cheap and interconnected. The policy and society require documentation and transparency. The in silico models should cope with multiple features, since they should explore toxicodynamic and toxicokinetic properties, related to human and environment, within the One Health strategy. At the same time, these tools should be linked with tools used by industry, with approaches suitable to address functional use, to investigate in the same system both adverse and beneficial properties.

We will provide examples of tools able to deal with tens of models simultaneously, addressing hazard and exposure at the same time, merging numerical models and predictive ones. The JANUS software for instance integrates 48 models for prioritization, the VERMEER tools predict risks for specific scenarios, and the ToxEraser tools suggest safer substances, to replace the riskiest ones.

The specific regulatory thresholds are incorporated into the tools, which apply batteries of the VEGA models, depending on the needs. The VEGAHUB system offers these solutions (ww.vegahub.eu). However, the challenges are many more, and networking solutions have to be planned, facilitating links between different platforms. These are explored within the CONCERT REACH and the OptiTox projects, for instance, addressing the REACH and the food regulations.