

A New Network of *In Silico* Models - LIFE CONCERT REACH Project

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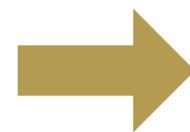
CONCERT REACH – EU project with the following main goals:

- Establishing an **integrated network of systems** offering non-testing methods (NTM) for REACH: **more than 300 *in silico* models will be linked**
- *In silico* models accompanied with **appropriate documentation structure (QMRF and QPRF)**
- Integration of an **easy to use read across tool**
- **Automated weight-of-evidence** evaluation tool
- Evaluation of **stakeholders' needs** (targeted workshops)

Important milestones so far:

- Integration of **VEGA with OECD QSAR Toolbox**
- **40 new models** developed
- Improved **rules** for ToxRead (**automated read-across**)
- **Weight of evidence**: first case study of automated WoE carcinogenicity evaluation of botanicals (collaboration on going with EFSA)
- **Workshops organized**: for EU regulators (Oct 2021) and for chemical industries (Dec 2021)

Experimental data gathering



Model development and/or validation



Integration (QSAR & read-across)



One network integrating > 300 models

Industry stakeholder feedback:

- 1) Need of **clearer guidance**
 - List of **recommended models**,
 - **Guidance** in selection of the **most appropriate models** for the substance to be predicted
 - Illustrative **examples**
 - **Successful cases** of *in silico*-generated results accepted by ECHA
- 2) **Practical demonstrations / trainings**

What's coming next:

- A web-based **gateway** guiding the user through the **network of *in silico* tools** available in the project
- **Further integration of new models / endpoints** into VEGA and ToxRead
- Integration of **VEGA in Danish (Q)SAR database**
- VERA: a **new tool for automated read-across** and grouping based on **multiple similarity metrics**
- A **new tool for weight-of-evidence** evaluation (tested in collaboration with EFSA)

