

A new network of *in silico* models to cope with REACH requirements for (Q)SAR and read-across: the LIFE CONCERT REACH project



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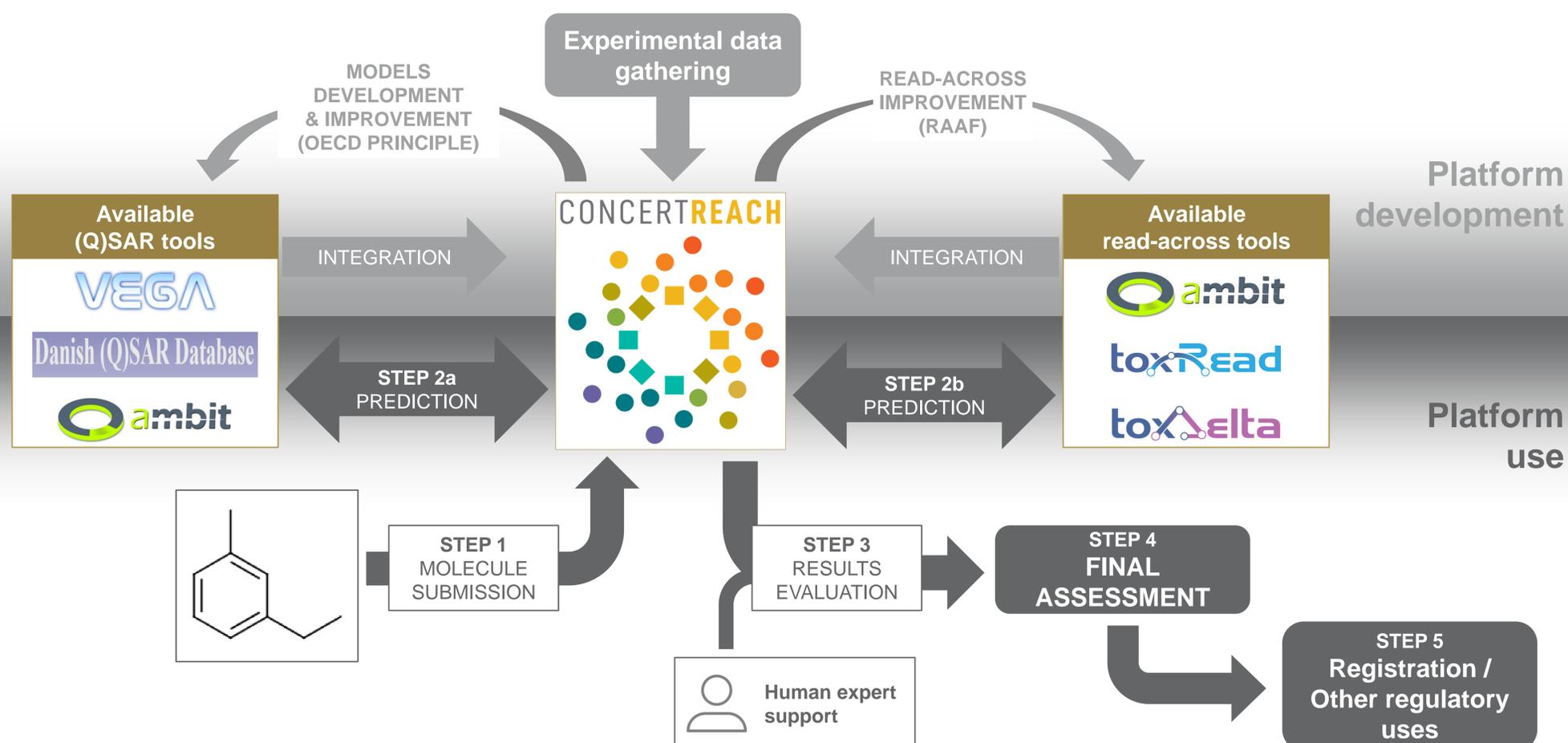
Introduction

In silico models such as (Q)SAR and read-across workflows represent nowadays widely used and increasingly accepted tools for estimation of physico-chemical, environmental fate and (eco)toxicological properties. The availability of freely accessible models to cover all possible endpoints of interest is however still limited. Moreover, the compliance of available tools and the produced results with the regulatory requirements (e.g. OECD principles for (Q)SAR validation, Read-Across Assessment Framework (RAAF)) have room for improvement.

Aims and methods

The “*Concerting experimental data and in silico models for REACH*” (CONCERT REACH) project aims at developing a new freely accessible network that will integrate regulatory-compliant (Q)SAR models and read-across automated workflows. The network will offer access to **more than 300 *in silico* models**, potentially covering all properties relevant for registration (with main focus on REACH).

Project timeline: September 2018 (start) to February 2022 (end)



Expected outcomes

- **Cost-effective** and **easy-to-use** platform for (Q)SAR and read-across evaluation
- **Fast** generation of **reliable** data for regulatory purposes
- Models' compliance with requirements (**OECD Principles**) including full documentation (**QMRF**)
- Results' compliance with regulatory requirements (e.g. REACH) including full documentation (**QPRF**)
- Generation of reports easy to integrate within dossier preparation
- Models and platform potentially usable **within different regulatory frameworks** (industrial chemicals, cosmetics, pesticides, food related substances, etc.)

Dissemination and Networking

- Key importance for the development of a useful and accepted tool
- Several activities will be organized:
 - **Webinars** for chemical industries
 - **E-meetings** with regulatory bodies
 - **International workshops**
 - **Articles**
 - **Case studies**

THE PROJECT'S CONSORTIUM



Istituto di Ricerche Farmacologiche
Mario Negri
Italy
Research institute
Developer of VEGA, toxRead, toxDelta



Technical University of Denmark
Denmark
University
Developer of Danish QSAR Database



IDEAconsult Ltd.
Bulgaria
SME for consultancy, technical services
and software development.
Developer of Ambit



knoell Germany GmbH
Germany
Consultant for chemical's registration



Kode s.r.l.
Italy
Private company active in data science
(chemometrics and chemoinformatics)



SC Sviluppo chimica S.p.A.
Italy
Service company, part of the Italian
Federation of the Chemical Industry