

**LIFE CONCERT REACH:**  
novità e benefici attesi  
dall'implementazione degli "in  
silico tools" per le imprese  
chimiche

**Nelly Giuseppa Raitano**

National event SC del 13/6 (in Italian) – @FED-COSP (online)

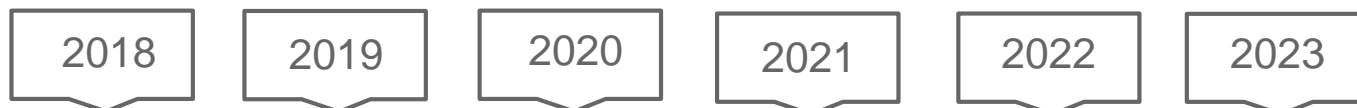


# THE PROJECT



September

June



Istituto di Ricerche Farmacologiche Mario Negri, Italy  
Research institute, **Coordinator**

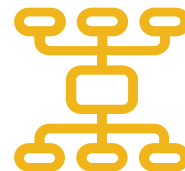
Associated Beneficiaries



External supporting

Evaluate the **potential impact** of CS in the  
EU by *exp + in silico*

**A big network** of systems offering non-  
testing methods (NTM) useful both for  
authorities and industries.



# THE *IN SILICO* MODELS IN A NUT-SHELL

## **(Q)SAR**

Quantitative Structure-Activity

Relationship,

**READ ACROSS,**

**GROUPING...**

# THE *IN SILICO* MODELS IN A NUT-SHELL

**(Q)SAR**

Quantitative Structure-Activity  
Relationship



***Endpoint***

*pharmacological effect  
(eco)toxicity  
physico-chemical property*

***Molecular***

***descriptors***



# THE *IN SILICO* MODELS IN A NUT-SHELL

## Read-across

It is a method of filling in data gaps for a substance by using **surrogate data from another substance**.

## Chemical Categories

A group of chemicals that have **some features that are common** (structure, property, behavior, functionality)



# Seven Reasons *to use QSAR*



Innovation

Time for experiments



Occurrence of enough laboratories/resources

Reduction of costs



Use of animals

Prioritization needs



Pro-active approach for greener chemicals



# THE PROJECT

01

## Policy landscape.

EU chemicals regulation, the so-called **REACH** regulation.

02

## Non-testing methods - NTMs

- Alternative methods to protect environmental and human health
- Non-testing methods (NTMs)
- Impact of substances

03

## REACH experimental data

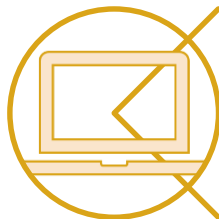
Since May 2018, a huge amount of REACH experimental data has become available, which can be better exploited, especially through NTMs.

04

## Integrated network of systems

VEGA, the Danish (Q)SAR Database, OCHEM and AMBIT are the main components of this new network offering an improved version of these tools for the in silico and read-across evaluation of chemicals.

# Results



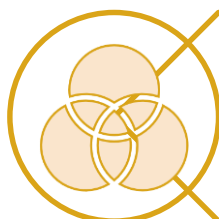
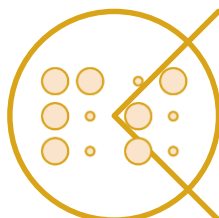
The network offers more than 450 *in silico* tools



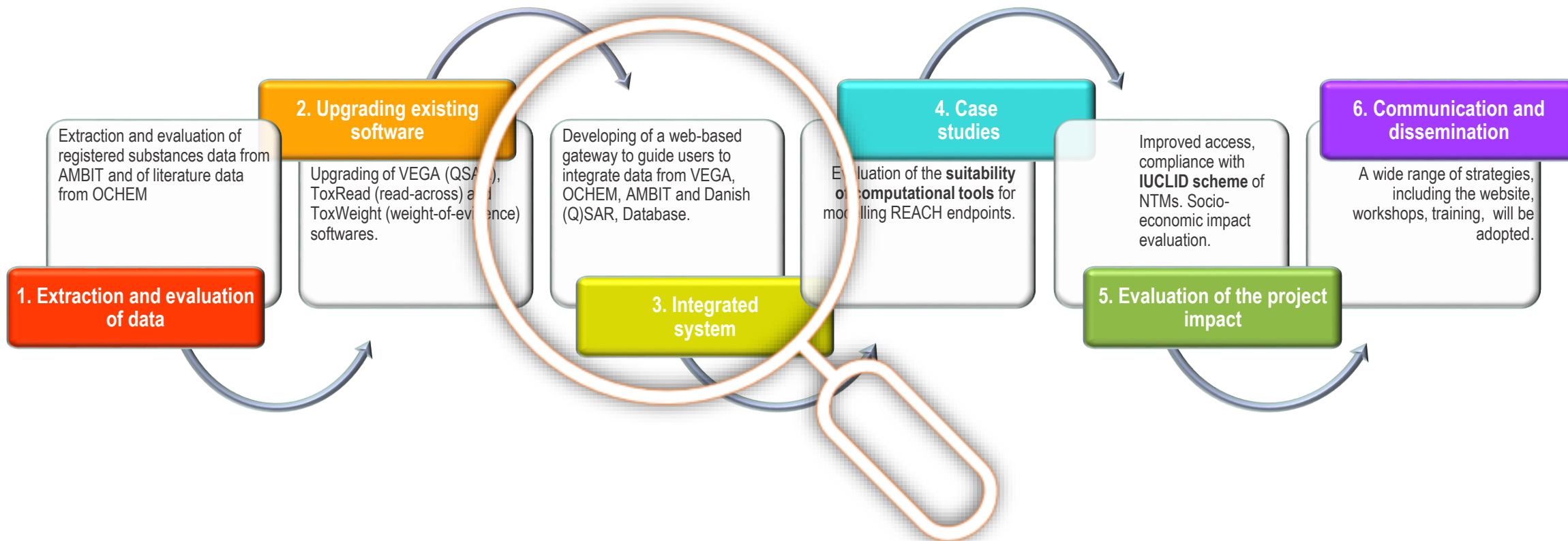
42 new *in silico* models



A new tool for grouping



# PROJECT ACTIVITIES



# THANKS

Does anyone have any questions?  
<https://www.life-concertreach.eu/>



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