

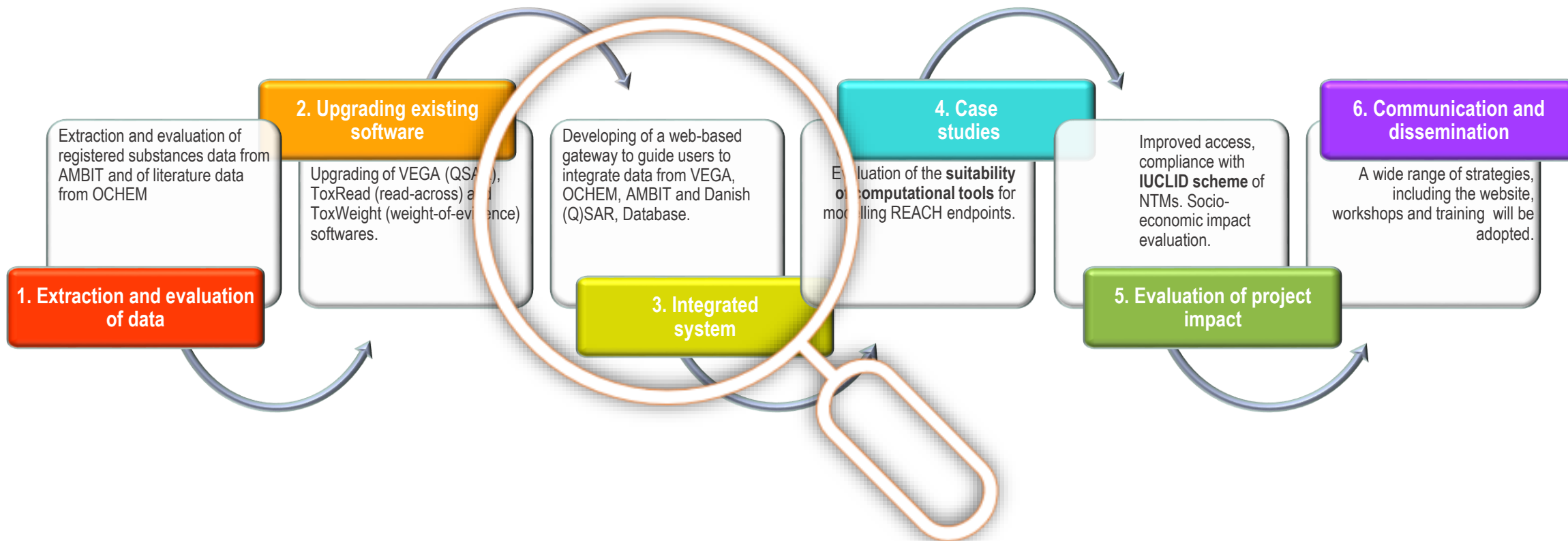
Un grande network di metodi in silico al servizio dell'utente: introduzione al "gateway" virtuale di CONCERT REACH

Nelly Giuseppa Raitano

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



PROJECT ACTIVITIES

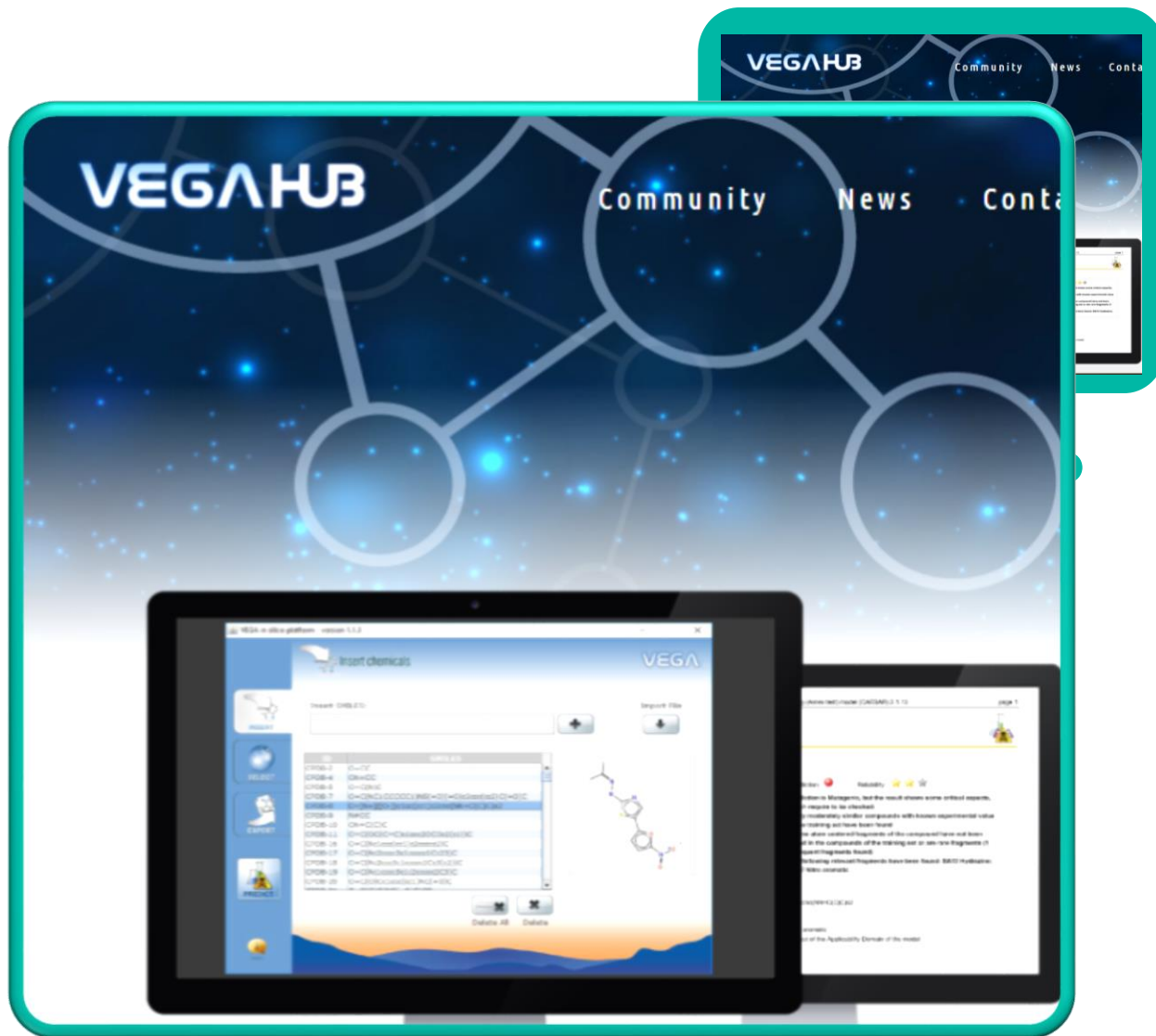


THE TOOLS



The network is composed of **VEGA**, the **Danish (Q)SAR Database**, **OCHEM** for the *in-silico models*, and for the read across workflow and data from the registered substances, of **ToxRead** and **AMBIT**.

THE TOOLS



110 (Q)SAR freely available models for regulatory purposes.

Different areas:

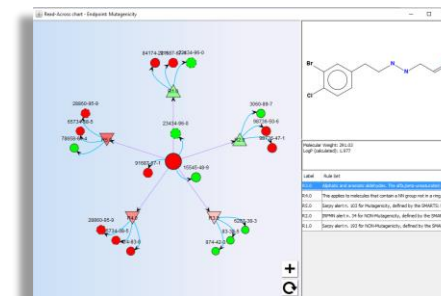
- Human toxicity
- Eco-toxicity
- Environmental
- Physico-chemical
- Toxicokinetics

VEGA




Reproducible read-across evaluation for 25 endpoints showing similar compounds and SAs in common between chemicals.

TOXREAD



THE TOOLS



DQ DATABASE

Estimates for **more than 650,000 substances** obtained with **more than 200 (Q)SARs** from free and commercial platforms.

DQ MODELS

New portal to access some of the models of the database directly, also for new substances.

Downloadable QPRF report is generated.

THE TOOLS



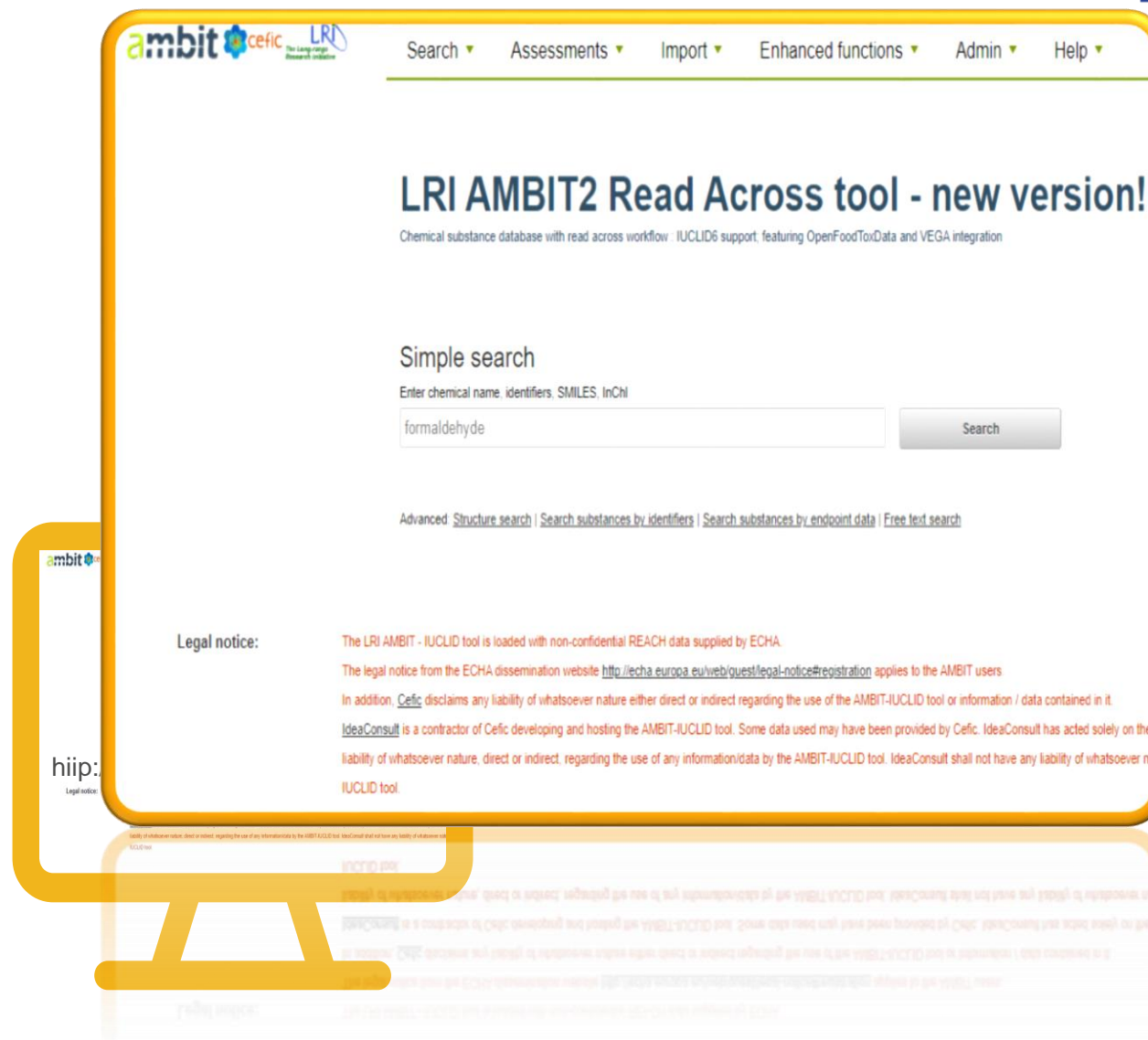
LIFE17 GIE/IT/000461

The OCHEM package offers a database of molecules and their ADMET properties.

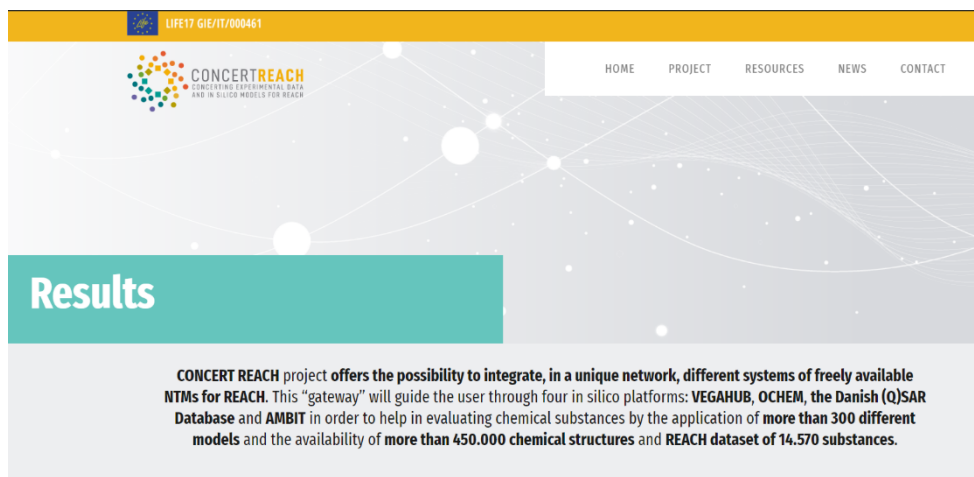
OCHEM contains more than **1 million** experimental records for about 499 properties collected from 12428 sources

THE TOOLS

The AMBIT system consists of a database including more than **450.000 chemical** structures and REACH data on **14.570 substances**



The GATEWAY

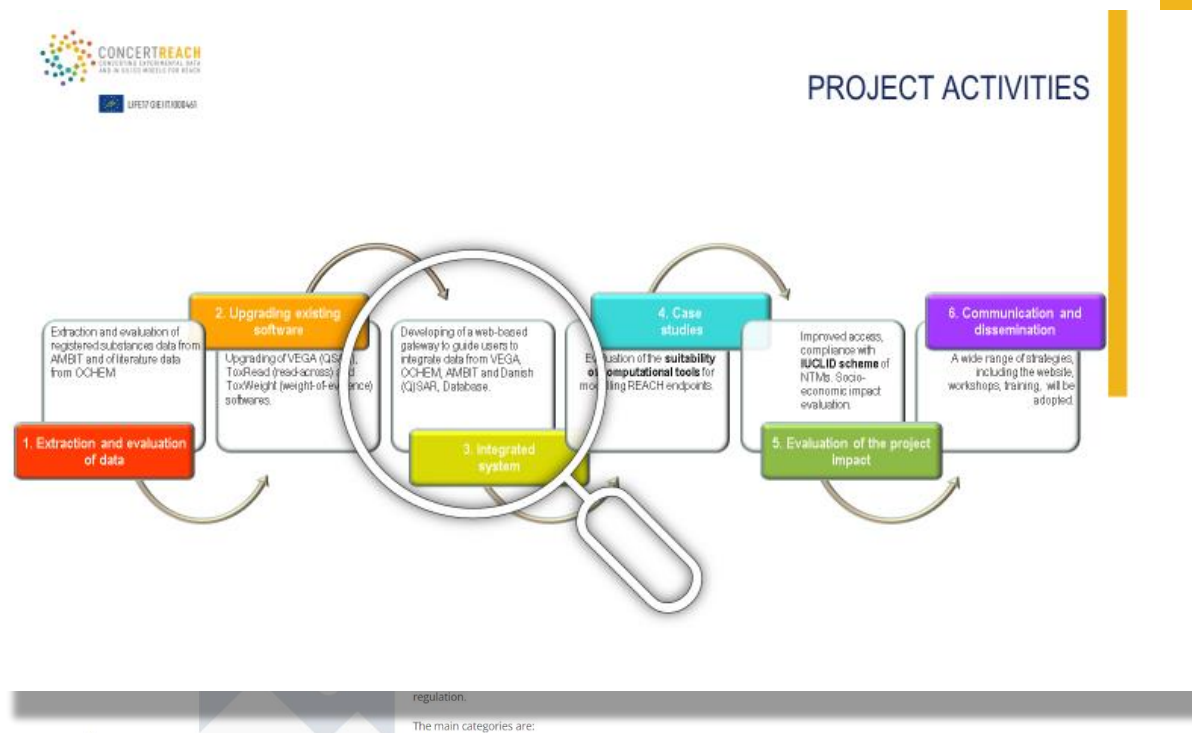


Results

CONCERT REACH project offers the possibility to integrate, in a unique network, different systems of freely available NTMs for REACH. This "gateway" will guide the user through four in silico platforms: VEGA HUB, OCHEM, the Danish (Q)SAR Database and AMBIT in order to help in evaluating chemical substances by the application of more than 300 different models and the availability of more than 450.000 chemical structures and REACH dataset of 14.570 substances.

The "gateway" reports all the predictive software available in the four platforms relative to REACH endpoints.

However, please consider that we cannot guarantee that they are correct and usable for the REACH legislation. Additionally, if industry wants to use the result from a certain model, it has to verify if this is legally legitimate. For certain very specific endpoints we have reported models that may have been developed using more general data. These models may not perfectly adhere to the endpoint.



<https://www.life-concertreach.eu/results/>



HOME

PROJECT

RESULTS

RESOURCES

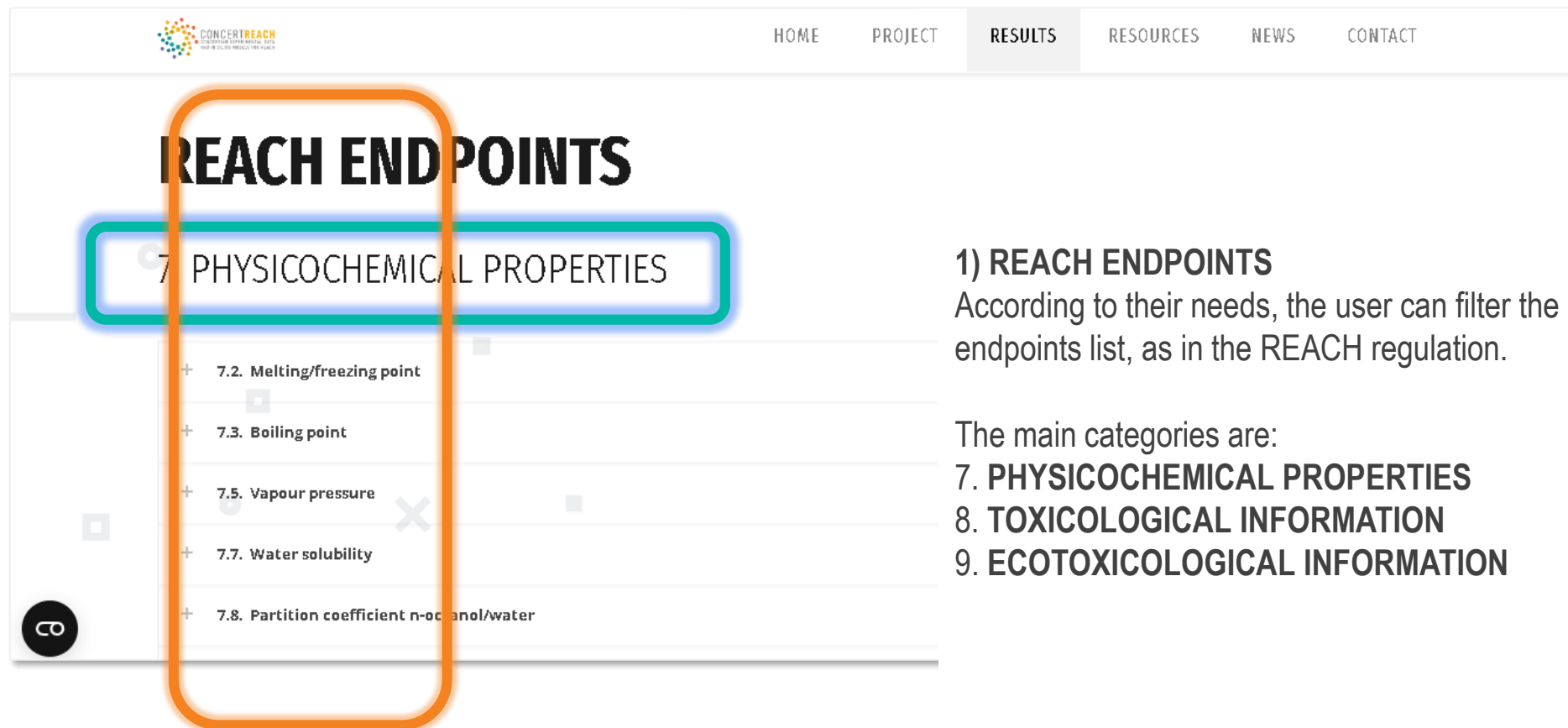
NEWS

CONTACT



WHIDE ENGAGEMENT
OF
AUTHORITIES AND INDUSTRY

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HOME PROJECT **RESULTS** RESOURCES NEWS CONTACT

REACH ENDPOINTS

7. PHYSICOCHEMICAL PROPERTIES

- + 7.2. Melting/freezing point
- + 7.3. Boiling point
- + 7.5. Vapour pressure
- + 7.7. Water solubility
- + 7.8. Partition coefficient n-octanol/water

1) REACH ENDPOINTS

According to their needs, the user can filter the models by the endpoints list, as in the REACH regulation.

The main categories are:

- 7. PHYSICOCHEMICAL PROPERTIES
- 8. TOXICOLOGICAL INFORMATION
- 9. ECOTOXICOLOGICAL INFORMATION

2) SELECTION OF THE SUITABLE MODEL

<https://www.life-concertreach.eu/results/>



REACH ENDPOINTS

7. PHYSICOCHEMICAL PROPERTIES

+ 7.2. Melting/freezing point

+ 7.3. Boiling point

+ 7.5. Vapour pressure

+ 7.7. Water solubility






+ 7.8. Partition coefficient n-octanol/water

+ 7.16. Dissociation constant

+ 7.5. Vapour pressure

- 7.7. Water solubility

All **VEGA AND ToxRead** DANISH QSAR DATABASE **AMBIT** OCHEM

End Point	Model	Type	Dataset size	Training set size	Test set size	Platform	Remarks
P-CHEM 4.8. Water solubility	Dataset		18126			AMBIT	
P-CHEM, 4.8 water solubility, OECD 105	Water solubility model (IRFMN)	continuous	5018	4014	1004	VEGA	
P-CHEM, 4.8 water solubility, OECD 105	Water solubility from Kow (mg/L) (EPI)	continuous				DanishQSARDatabase	
P-CHEM, 4.8 water solubility, OECD 105	Water solubility from Fragments (mg/L) (EPI)	continuous				DanishQSARDatabase	
Water solubility	ASNN	continuous		1311		OCHEM	 

3) PREDICTING

Once selected the model of interest, click on the link present in the “model” column; you will be redirected to the access page of the models.

3) PREDICTING

Once selected the model of interest, click on the link present in the “model” column; you will be redirected to the access page of the models.



4) INTERPRETATION OF THE RESULTS

The user can consult all the available documentation of the *in silico* tools in the dedicated section.



Environment International

Volume 131, October 2019, 105060



Review article

Integrating *in silico* models and read-across methods for predicting toxicity of chemicals: A step-wise strategy

Emilio Benfenati ^a  , Qasim Chaudhry ^b, Giuseppina Gini ^c, Jean Lou Dorne ^d

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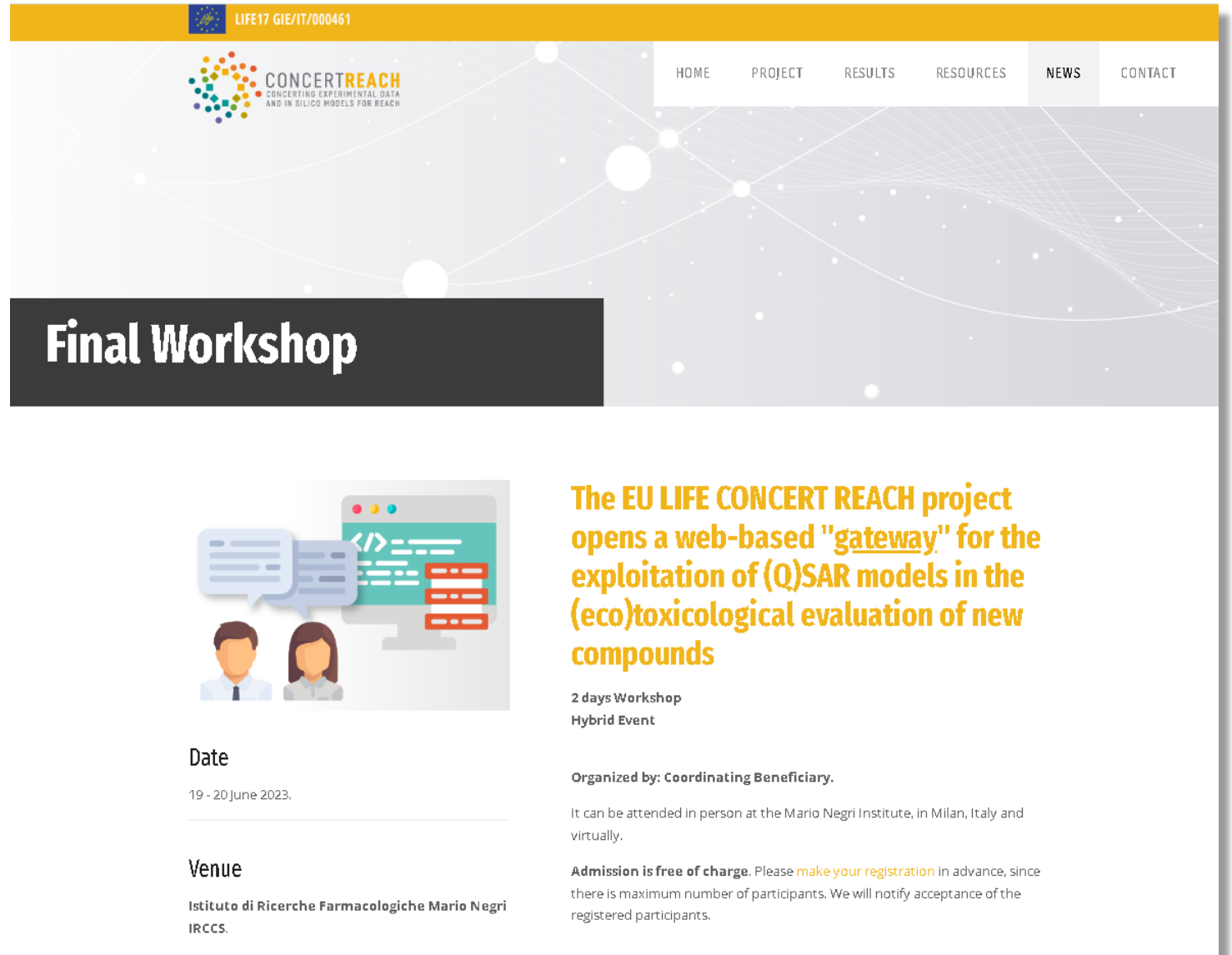
2-day workshop

Monday 19/06, full day

Workshop presentations

Tuesday 20/06, morning

Training sessions




The screenshot shows the website for the ConcertReach project. At the top, there is a yellow header with the European Union flag and the text 'LIFE17 GIE/IT/000461'. Below this is the ConcertReach logo, which consists of a colorful circular pattern of dots and the text 'CONCERTREACH CONCERTING EXPERIMENTAL DATA AND IN SILICO MODELS FOR REACH'. To the right of the logo is a navigation menu with links for 'HOME', 'PROJECT', 'RESULTS', 'RESOURCES', 'NEWS', and 'CONTACT'. The main content area features a large black banner with the text 'Final Workshop' in white. Below the banner is an illustration of two people (a man and a woman) looking at a computer screen displaying code and data. To the right of the illustration is the text: 'The EU LIFE CONCERT REACH project opens a web-based "gateway" for the exploitation of (Q)SAR models in the (eco)toxicological evaluation of new compounds'. Below this text are the details: '2 days Workshop Hybrid Event', 'Organized by: Coordinating Beneficiary.', and a paragraph stating that the event can be attended in person at the Mario Negri Institute in Milan, Italy, and virtually. It also mentions that admission is free of charge and that registration is required in advance.

LIFE17 GIE/IT/000461

CONCERTREACH
CONCERTING EXPERIMENTAL DATA
AND IN SILICO MODELS FOR REACH

HOME PROJECT RESULTS RESOURCES NEWS CONTACT

Final Workshop



The EU LIFE CONCERT REACH project opens a web-based "gateway" for the exploitation of (Q)SAR models in the (eco)toxicological evaluation of new compounds

2 days Workshop
Hybrid Event

Organized by: Coordinating Beneficiary.

It can be attended in person at the Mario Negri Institute, in Milan, Italy and virtually.

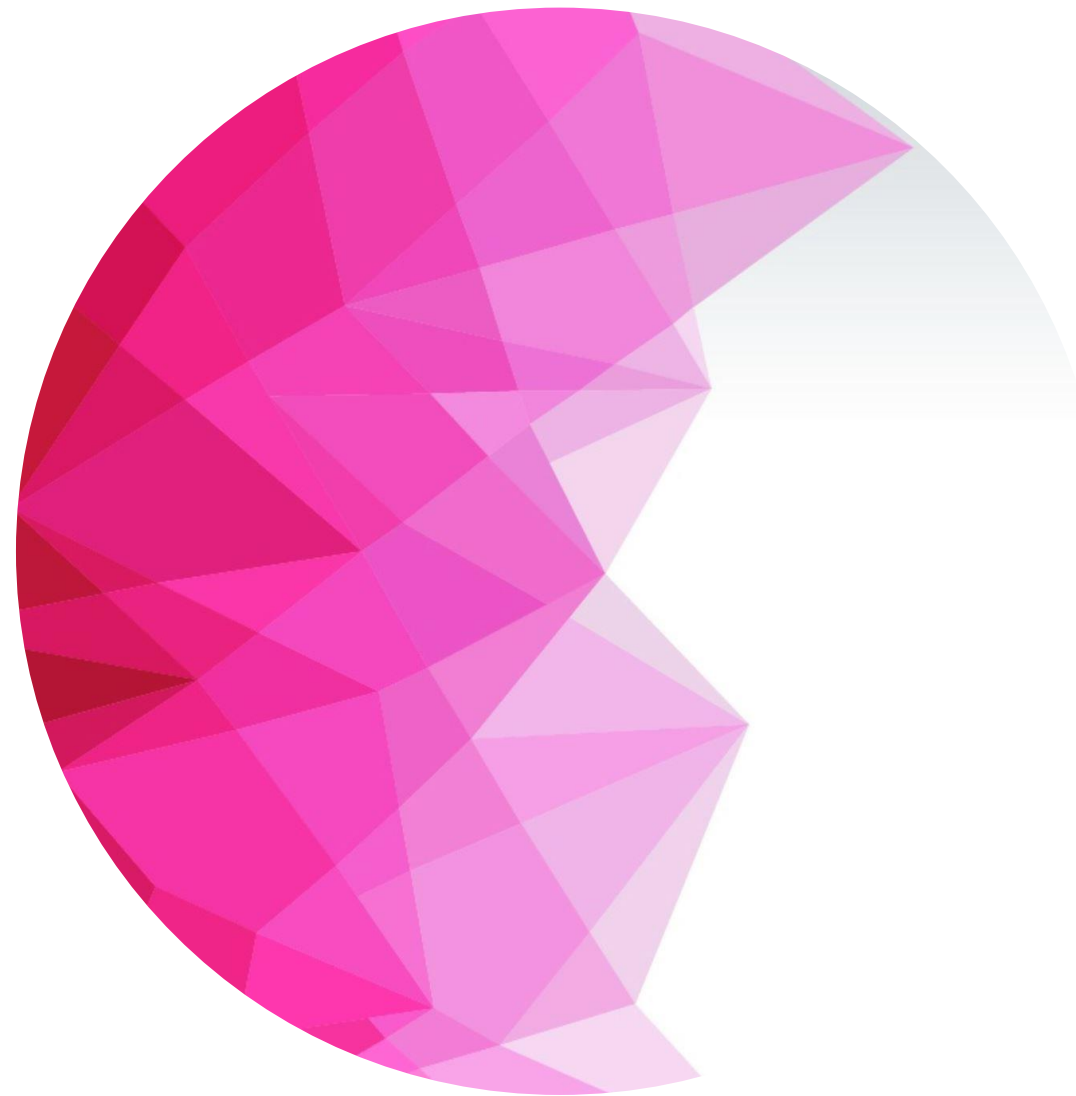
Admission is free of charge. Please [make your registration](#) in advance, since there is maximum number of participants. We will notify acceptance of the registered participants.

Date
19 - 20 June 2023.

Venue
Istituto di Ricerche Farmacologiche Mario Negri
IRCCS.

<https://www.life-concertreach.eu/final-workshop-19-and-20-june-2023/>

- 17&31/05/2023 webinars German industry
- 4-9/06/2023 QSAR2023
- 13/06/2023 Workshop Italian industry
- 19-20/06/2023 Final workshop



THANKS

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



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