Mario Negri Institute of Pharmacological Research - IRCCS

31/05/2023, LIFE CONCERT REACH Web-Seminars

QSAR models under REACH: Practical Examples

Nelly Giuseppa Raitano

CONCERTREACH
CONCERTING EXPERIMENTAL DATA AND IN SILICO MODELS FOR REACH

LIFE17 GIE/IT/000461

THE PROJECT

September — June

2018 | 2019 | 2020 | 2021 | 2022 | 2023

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

Associated Beneficiaries

big chem

DTU

knoell worldwide registration

kode from data to knowledge

Sviluppo chimica spa

IOEA consult

External supporting

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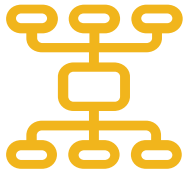
THE PROJECT
Sept 2018 - June 2023

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.



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Results

VERA
VIRTUAL EXTENSIVE READ-ACROSS

SWAN

- The network offers **more than 450 *in silico* tools**
- **42 new *in silico* models**
- A **new tool** for **grouping**
- Updated version of **read-across tools**, freely available and user-friendly
- New strategy integrating the results of read-across and *in silico* models (**weight-of-evidence**).

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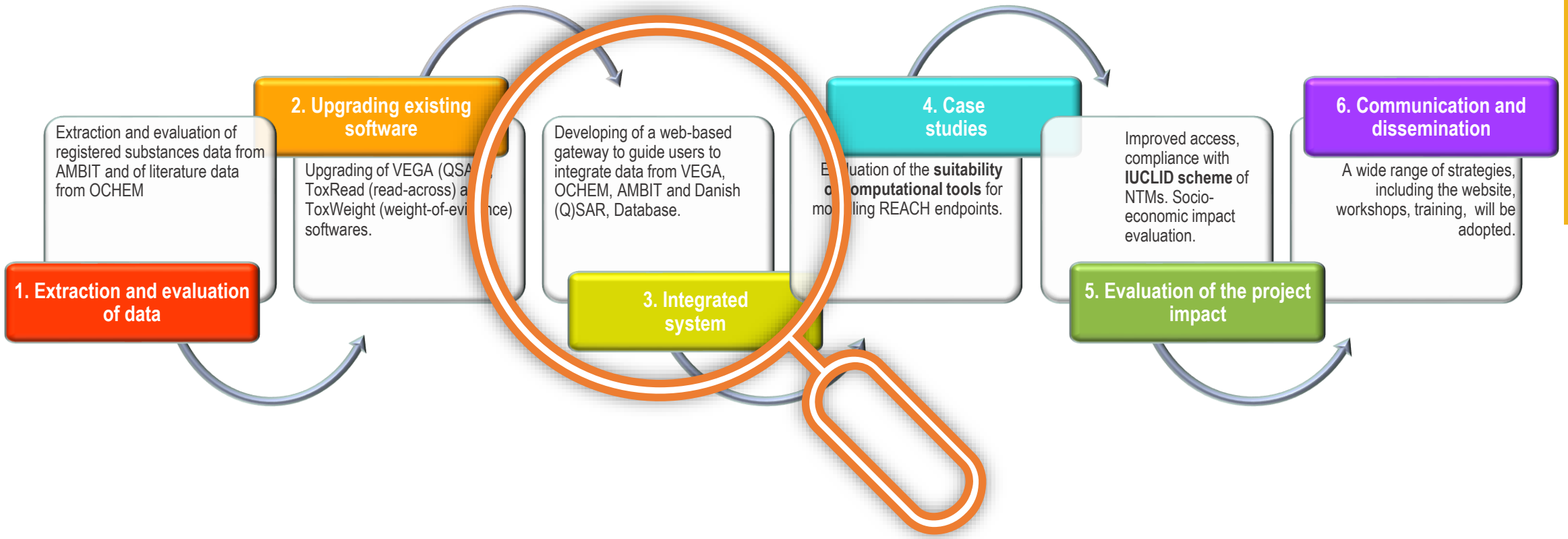
PROJECT ACTIVITIES



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

THE TOOLS

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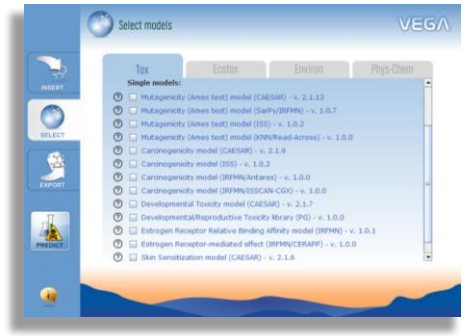
110 (Q)SAR freely available models for regulatory purposes.

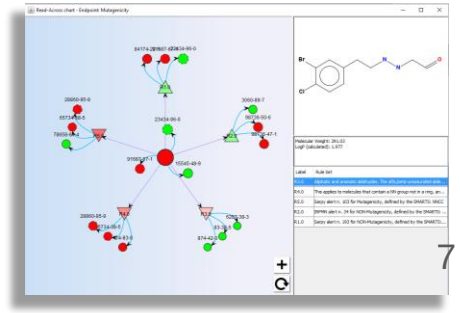
VEGA

Different areas:
-Human toxicity
-Eco-toxicity
-Environmental
-Physico-chemical
-Toxicokinetics



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.

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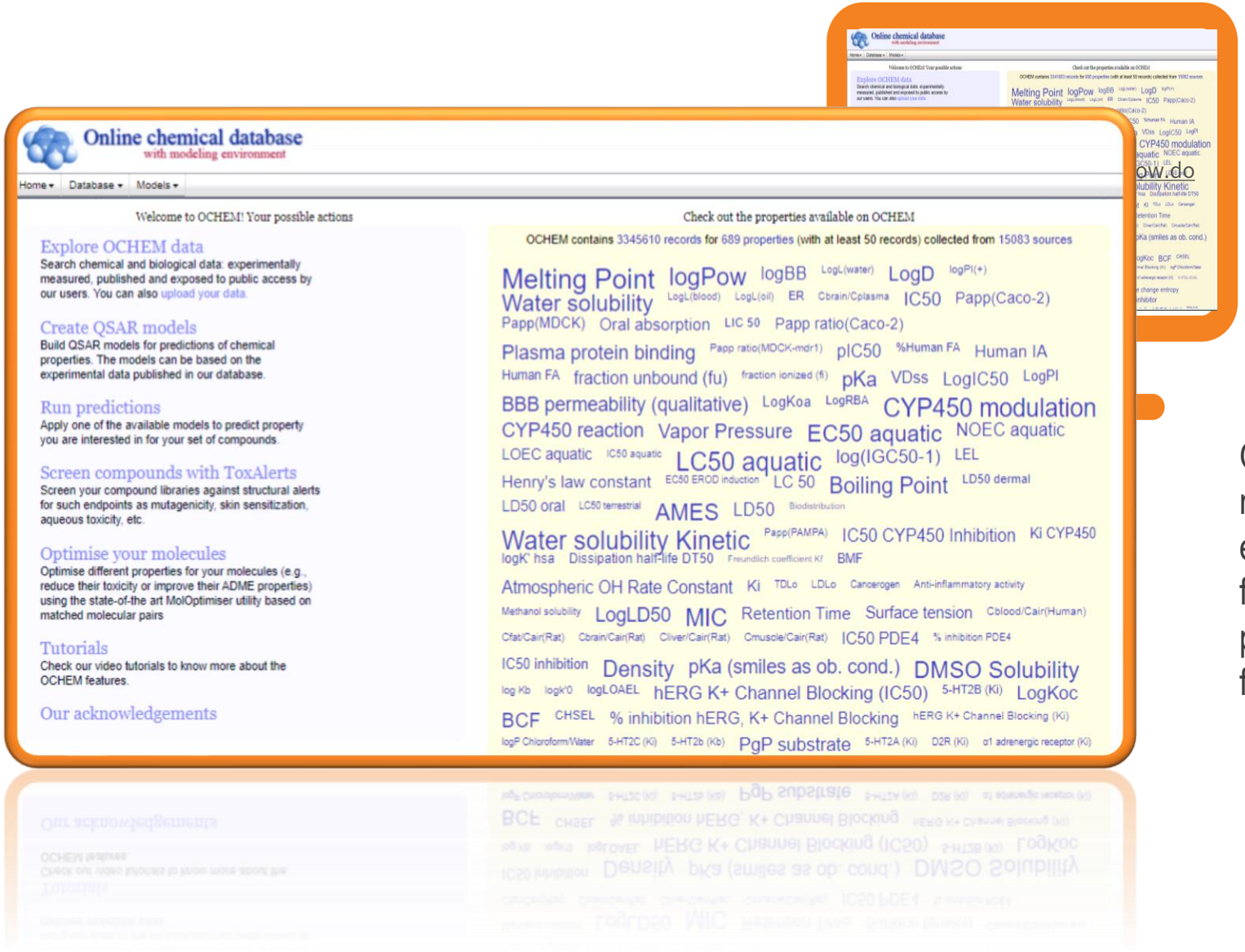

The OCHEM package offers a **database of molecules** and their **ADMET properties.**

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

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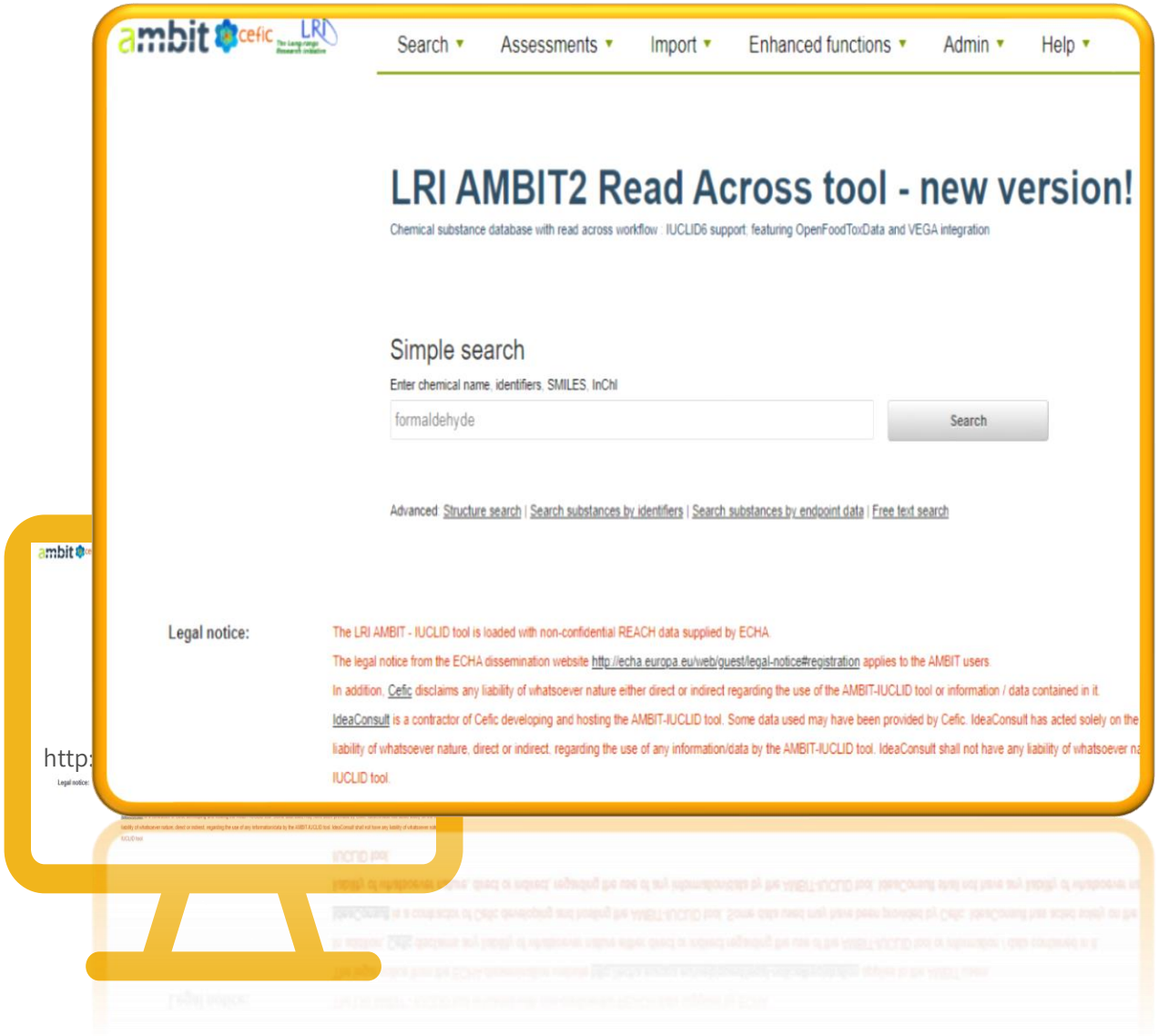
The AMBIT system consists of a database including more than **450.000 chemical** structures and REACH data on **14.570 substances**



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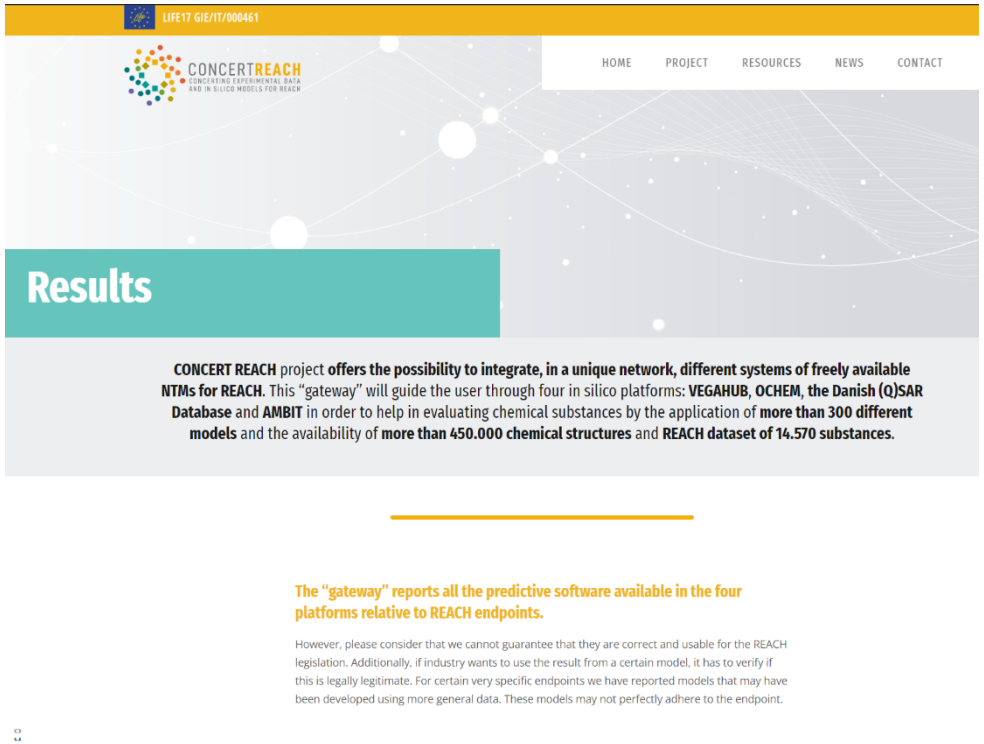
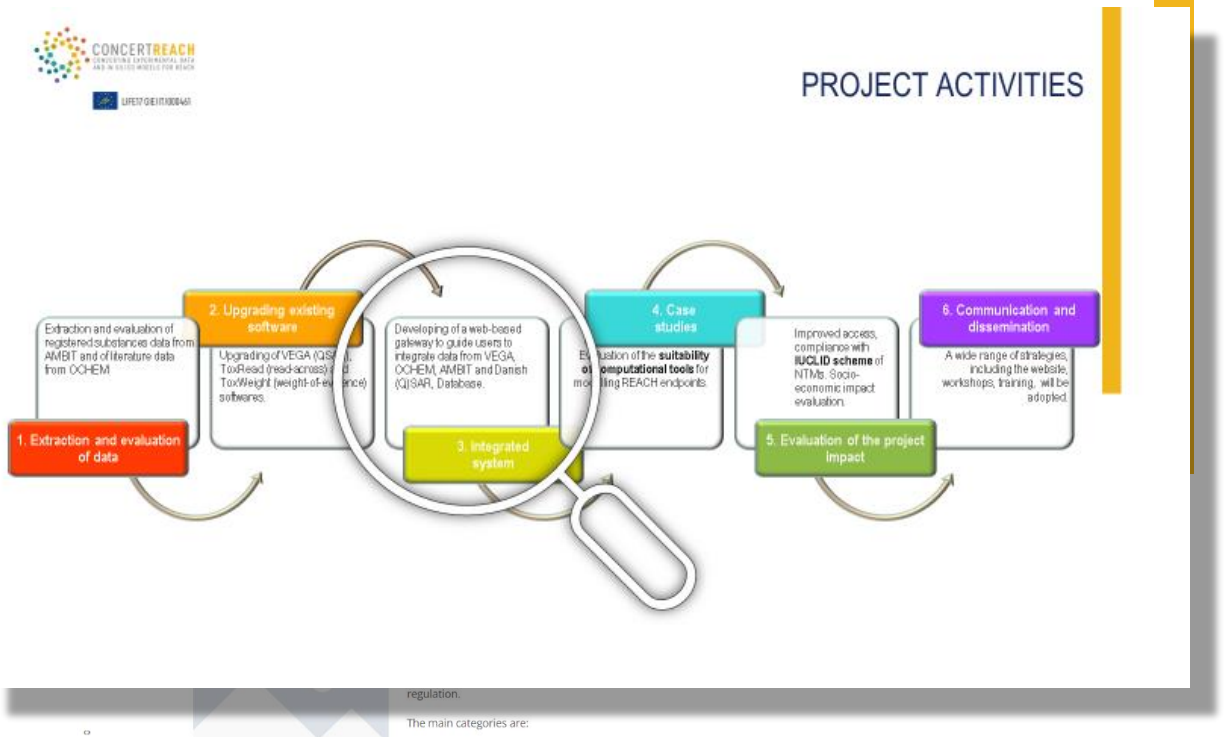
The GATEWAY





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

The GATEWAY

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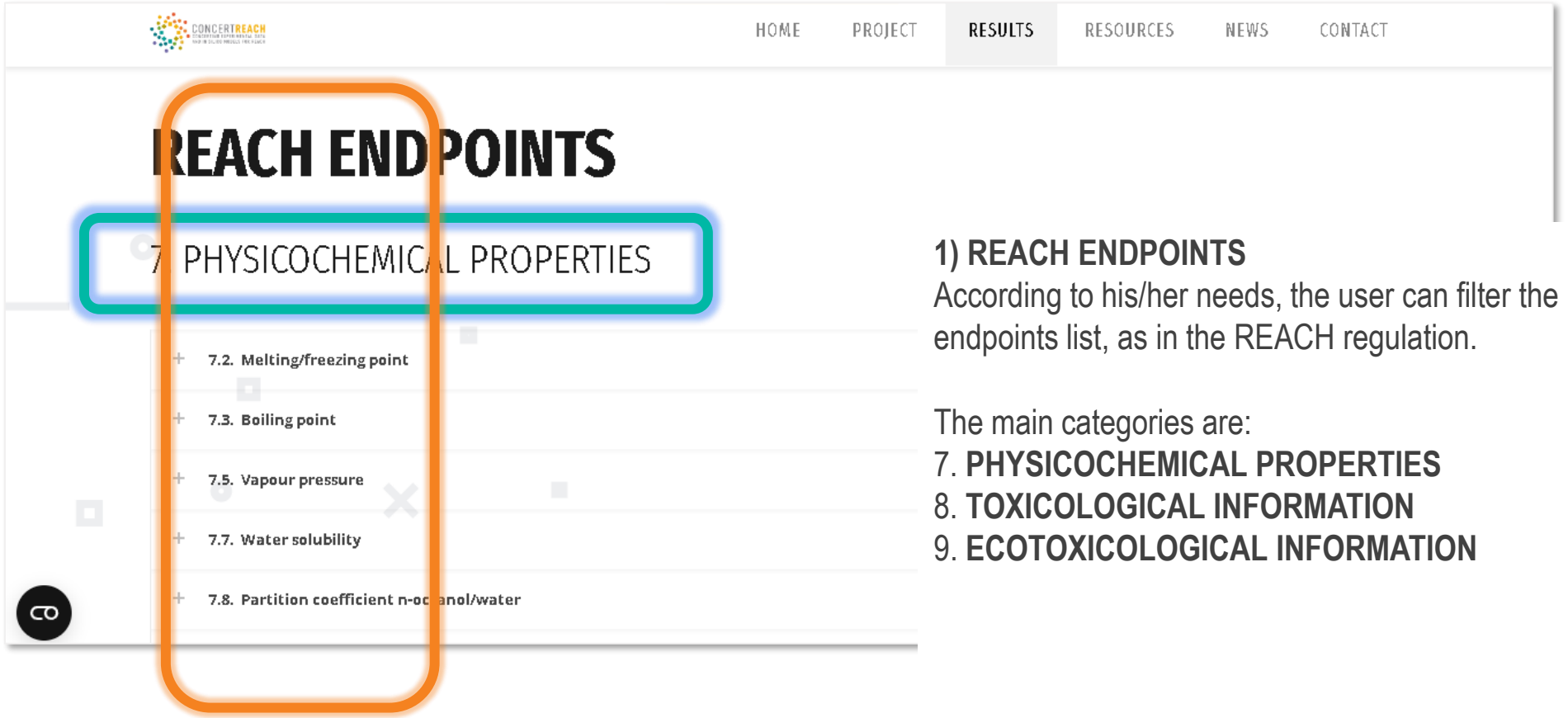

1) REACH ENDPOINTS

According to his/her 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

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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

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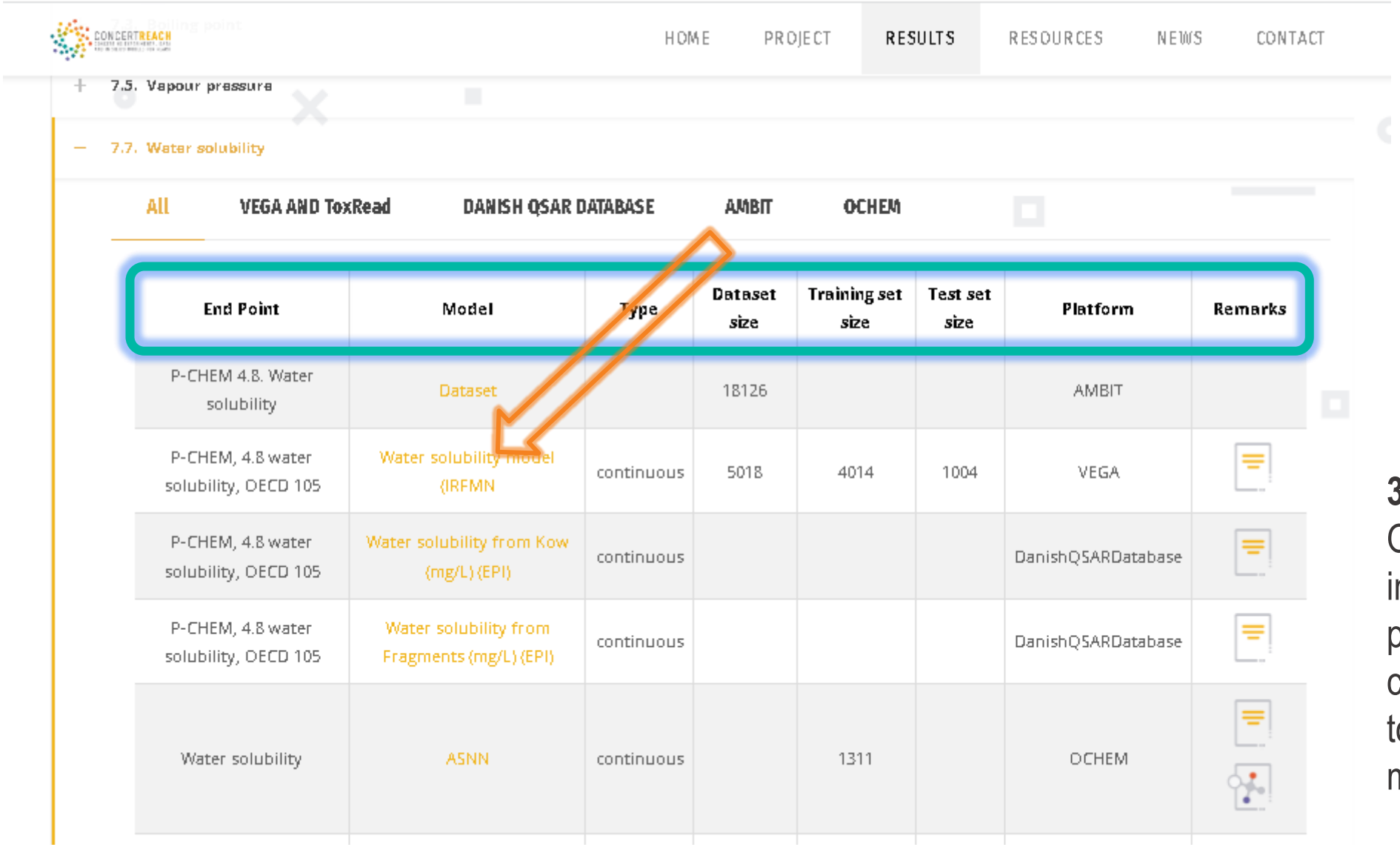

3) PREDICTING

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.

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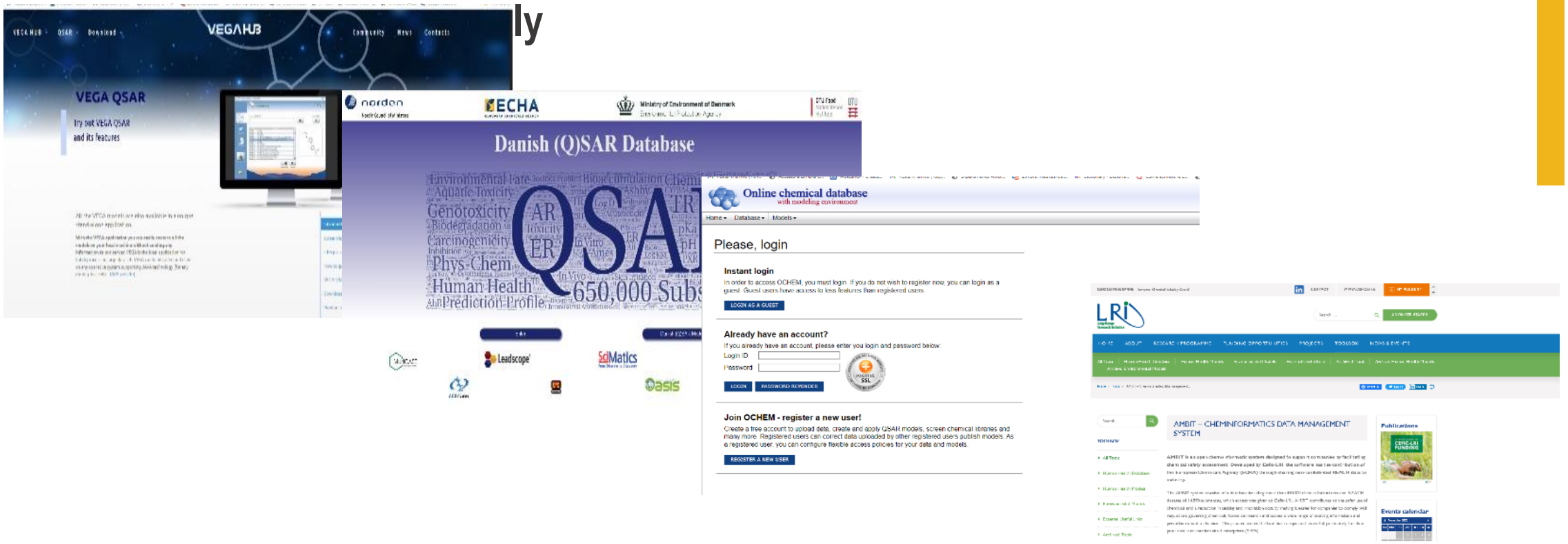


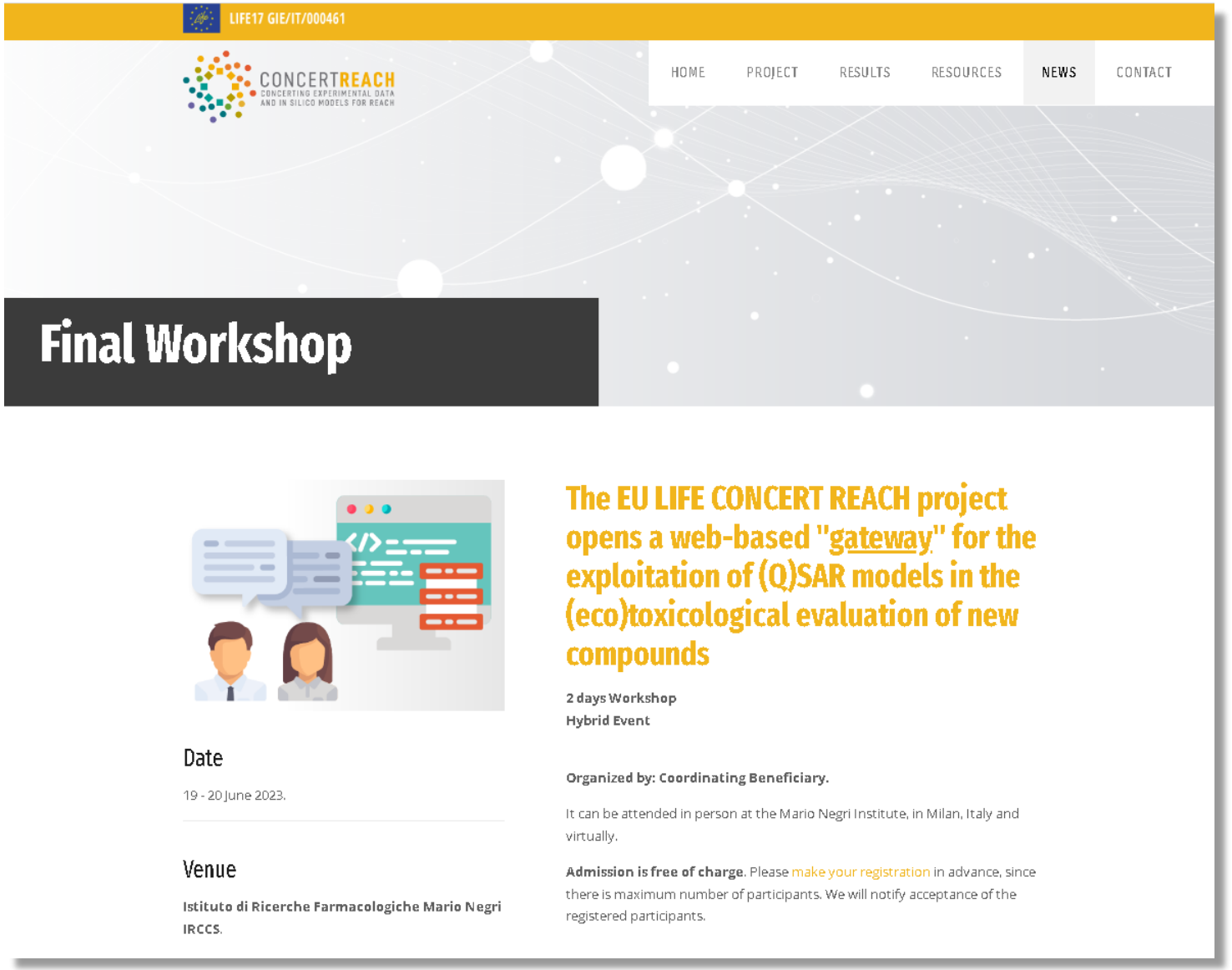
2-day workshop

Monday 19/06, full day

Workshop presentations

Tuesday 20/06, morning

Training sessions



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

THANKS

Does anyone have any questions?
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