In-silico predictions
a practical case of Reach Registration

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CONCERTREACH
CONCERTING EXPERIMENTAL DATA AND IN SILICO MODELS FOR REACH

LIFE17 GIE/IT/000461

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Dyestaff Cooperation (1)

In 2012 a Group of 10 – 12 Italian SMEs, delivering dyes to textile, leather and paper industries, set up a Reach Consortium coordinated by Centro Reach Srl with the aim to find an economically sustainable way to register the most number of substances they had on the market at that time

- over 600 mainly below 10 t/y –

In a 2. stage also a Dutch company joined while some of the founding members left the Cooperation

Dyestaff Cooperation (2)

The cost proposed at that time by the LR/Data Owners to purchase all the LoAs (several million €) went much beyond the financial capacity of these SMEs even reducing significantly the number of substances to register.

Key market point to consider here – dyes destinated to fashion sector has continuous fluctuations!

Particular colour effects depend on different combination of primary colours and other tones; need to have available a significant range of tones/colours and manage an important number of dyeing techniques

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Dyestaff Cooperation (3)

Negotiations for LoAs with LR/Data Owners organized in 3 big EU Consortia failed.
Dyestaff Cooperation decided to try exploit available NTM, in particular in-silico testing solutions like (Q)SAR and Read-Across, to cover most of the safety data needed for endpoints (mainly for lowest tonnage-band) required by Registration dossiers and Risk Assessment in REACH, trying to avoid as much as possible “need for citation of LR data”
Strong and long-lasting cooperation with M Negri Institute in support of these SMEs was a crucial basis for this strategy.

Dyestaff Cooperation (4)

Under REACH the joint submission of registration dossier is compulsory for registrants of the same substance.

Dyestaff Companies had to go for Opt-Out procedure in order to submit separately substance information in compliance with article 11(3) of Reach and to produce independently technical and scientific acceptable information being cheaper than other information made available with LoAs.

Dyestaff Cooperation (5)

Finally in 2018 Dyestaff Cooperation members submitted over 100 registrations thanks to significant support of NTM methods but were obliged to cite also certain number of data coming from animal testing data from the LRs.

How did the companies compile the registration dossiers with the technical support of C. Maculan?

REACH registration dossier (1)

Regulation EC 1907/2006, REACH, defines that a producer or importer of a chemical substance in a quantity higher than 1 t/y, has the obligation to register the substance with the European Chemicals Agency ECHA. The registration contains scientific information of the chemical-physical, toxicological and ecotoxicological type of substance.

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REACH registration dossier (2)

Dyestaff Companies had mainly the need to obtain the registration of their substances in the tonnage-band 1-10 tpa delivering the technical and scientific data required by Annex VII of the Regulation

REACH registration dossier (3)

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Information required for standard registration of 1-10 tonnes a year (Annex VII of REACH)	
Non-vertebrate animal endpoints	**Vertebrate animal endpoints**
Description of the state of the substance at 20°C / 101.3 kPa	Acute toxicity: oral
Melting/freezing point	
Boiling point (if applicable)	
Relative density	
Vapour pressure (if applicable)	
Surface tension (if applicable)	
Water solubility	
Partition coefficient	
Flash-point	
Flammability	
Explosive properties	
Self-ignition temperature	
Oxidising properties	
Granulometry (if applicable)	
In vitro skin irritation/corrosion	
In vitro eye irritation	
Skin sensitisation	
In vitro gene mutation in bacteria	
Short-term toxicity on invertebrates	
Growth inhibition study aquatic plants	
Ready biodegradability (if applicable)	

REACH registration dossier (4)

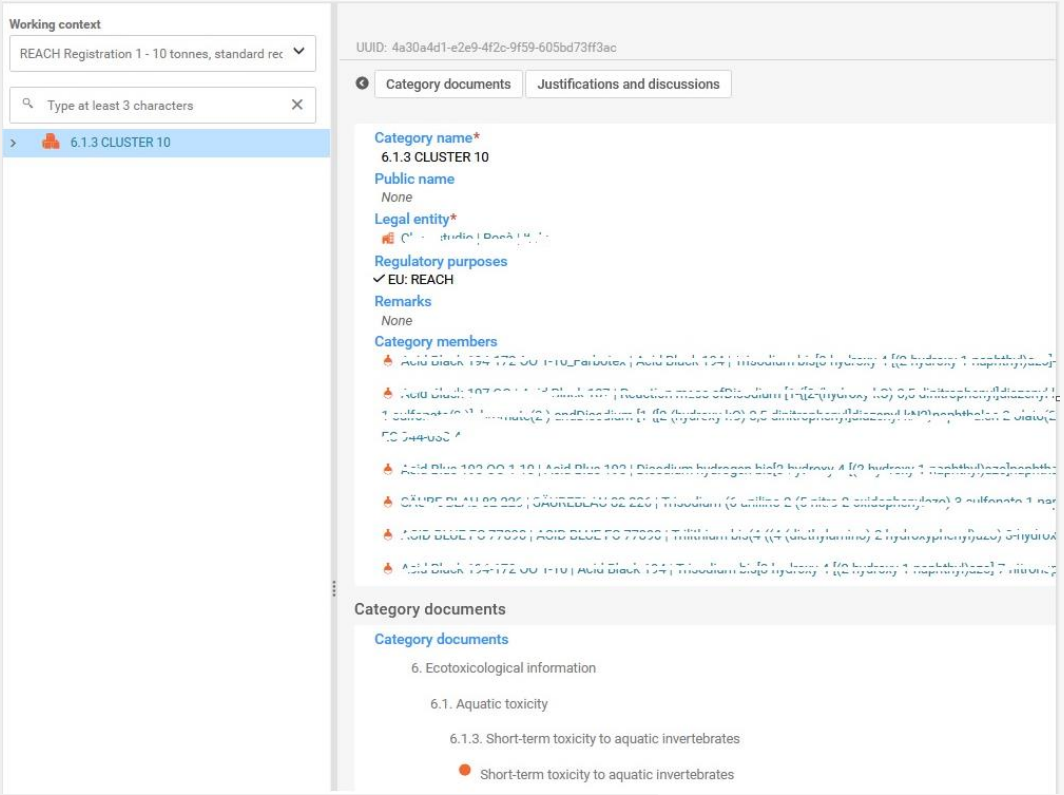
The cooperation with M Negri Institute allowed Dyestaff Companies to develop data regarding the endpoints:

- Ready biodegradability
- In vitro skin irritation/corrosion
- In vitro eye irritation
- Skin sensitisation
- In vitro gene mutation in bacteria
- Short-term toxicity on invertebrates
- Growth inhibition study aquatic plants
- Acute toxicity: oral

REACH registration dossier (5)

Depending on the chemical structure of each substance subject to registration and to the availability of experimental data from substances with similar chemical structures, M Negri Institute delivered us in-silico elaborations considering the scientifically best solutions ((Q)SAR and/or Read-Across) on a case-by-case basis to produce the technical-scientific data required by the Reach Regulation for the previously mentioned endpoints in the registration dossiers.

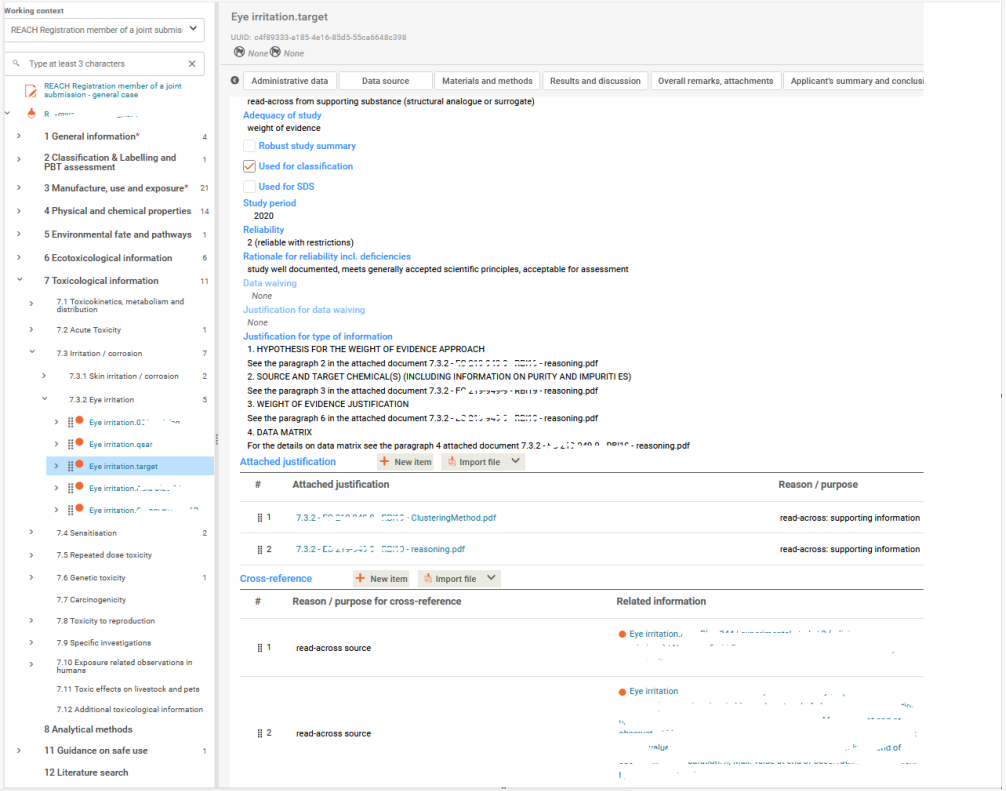
REACH registration dossier (6)



Example:

read-across based on grouping of substances (category approach)

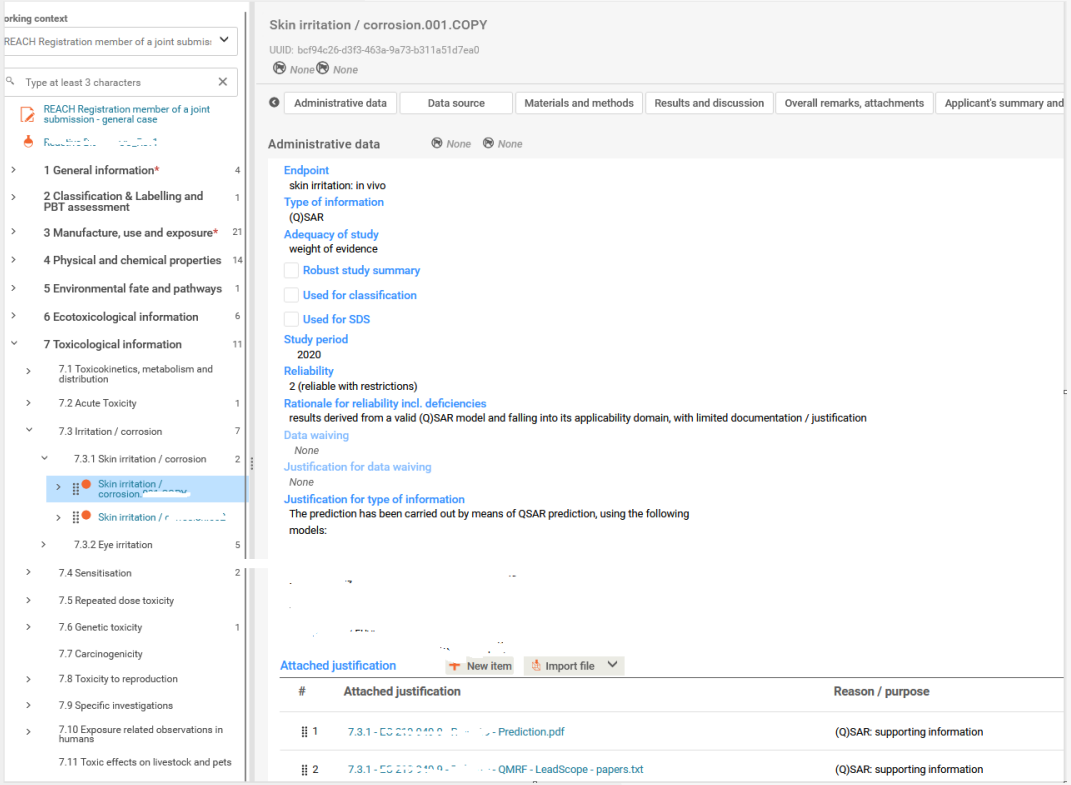
REACH registration dossier (7)



Example:

read-across from supporting substance (structural analogue or surrogate)

REACH registration dossier (8)



Example:

(Q)SAR

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Thank You For Your Attention