sOFT-ERA

Further development and update of the OpenFoodTox database: OFT 3.0

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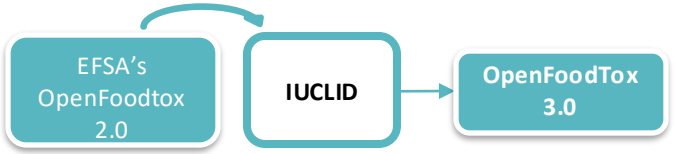
Introduction

The **OpenFoodTox database** aims at mapping hazards data published in outputs EFSA (opinions, statements, conclusions) with regards to risk assessments of chemicals in food and feed.

The **aims** of this contract are: to further improve the interoperability of the EFSA's OFT 3.0 database with IUCLID 6 and the EU Common Data Platform on Chemicals in line with the One Substance-One Assessment approach as part of the Chemical Strategy for Sustainability;

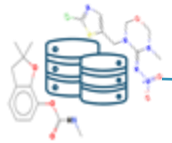


Objectives

- Objective 1: Update of OFT database
- Objective 2: Further development of OFT 3.0
- **Objective 3: Development of in silico models and implementation within EFSA tools**
- Objective 4: Establishment of process workflow for the integration of hazard data into IUCLID/OFT 3.0 as a part of the EFSA outputs publication

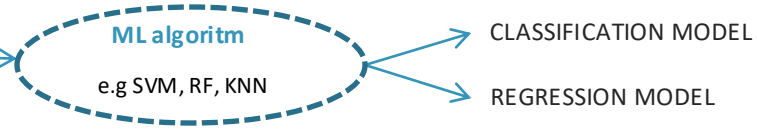
Methodologies

DATA COLLECTION



DATASET

IN SILICO APPROACHES



VERA Alerts and VERA Entities

1. Unsupervised

Selecting similar compounds regardless of the endpoint of interest

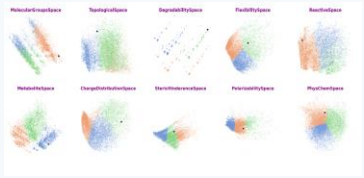
How? Using clustering of subspaces

2. Supervised

Using selected similar to perform the assessment

How? With ***two different approach***

2a. VERA Entities



How?

1. *Selecting similar for each subspaces*
2. *Selecting similar with experimental value*
3. *Weight results according to logistic regression and similarity indices*

2b. VERA Alerts

How? *Using a* ***Subspace Fingerprint*** *– defined by the Target*

Similars are those with the same subspace fingerprint of the target

Then searching for…

Structural Similarity 

Structural Alerts 

Molecular Groups 

Results

MODEL NAME	ENDPOINT	SPECIES
Henry's law constant models	Henry's law constants	na
Model for the minimal inhibitory concentration (pMIC) of polypeptides	minimal inhibitory concentrations (pMIC)	na
Model on blood-barrier permeation of organics compounds	blood-barrier permeation	na
Model for the retention time of pesticide	retention time (Rt)	na

MODEL NAME	ENDPOINT	SPECIES
Model for toxicity towards Tadpole	pLC50	Rana japonica and Rana chensinensis
EC50 acute toxicity towards S. duckweed	EC50	Swollen duckweed
NOEC chronic toxicity towards Harlequin fly	NOEC	Harlequin fly
Avian reproduction toxicity	NOEC	Colinus virginianus
Model for Assess Aquatic Toxicity Profiles of Fullerene Derivatives (FD)	effects of FDs on TcAChE (acetylcholinesterase)	Torpedo californica