



OpenFoodTox: Chemical Hazards Database @ EFSA

Anastasia Livaniou
Evidence Management Unit

Jean-Lou Dorne
Scientific Committee and
Emerging Risks Unit

EFSA Stakeholder Forum 2018
November 20, 2018

Outline

- Background
- Purpose of the OpenFoodTox DB
- Content
- Ways to explore data
- Data sharing activities and Harmonised Templates
- Live Demo
- CEFIC Use case: AMBIT, by Dr Bruno Hubesch
- Part 2: The future of OpenFoodTox and TK modelling platform, by JL Dorne

From Question to Answer



Four pillars of Chemical Risk Assessment

Step 1

Hazard Identification

Identify toxic effects

Step 2

Hazard Characterisation

Quantify toxic effects:

- Dose response
- Reference Point
- Reference value

Step 3

Exposure Assessment

**Occurrence
x Consumption**

Step 4

Risk Characterisation

**Hazard vs
Exposure: Risk**

OpenFoodTox:

History of OpenFoodTox

EFSA Strategy 2012

Database of EFSA's chemical risk assessments in food and feed

- Open-source
- Structured
- Common standards

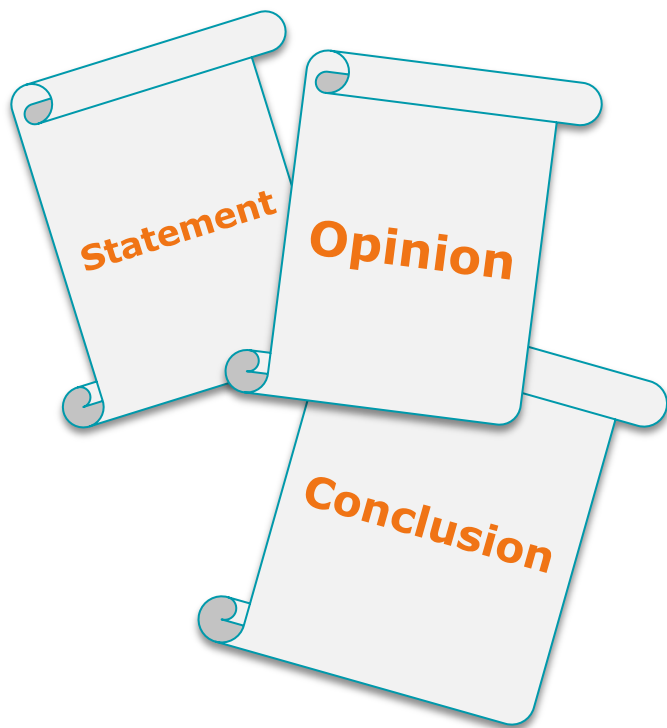
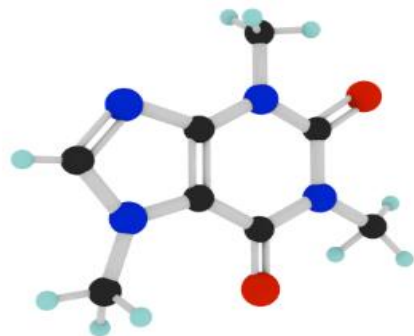
EFSA Strategy 2020

Widen EFSA's evidence base and optimise access to its data

- Open Data approach
- Improve data interoperability
- Structured scientific data



OpenFoodTox: Purpose



Inventory of EFSA's chemical RA since its creation in 2002

Easy Reference and Crisis

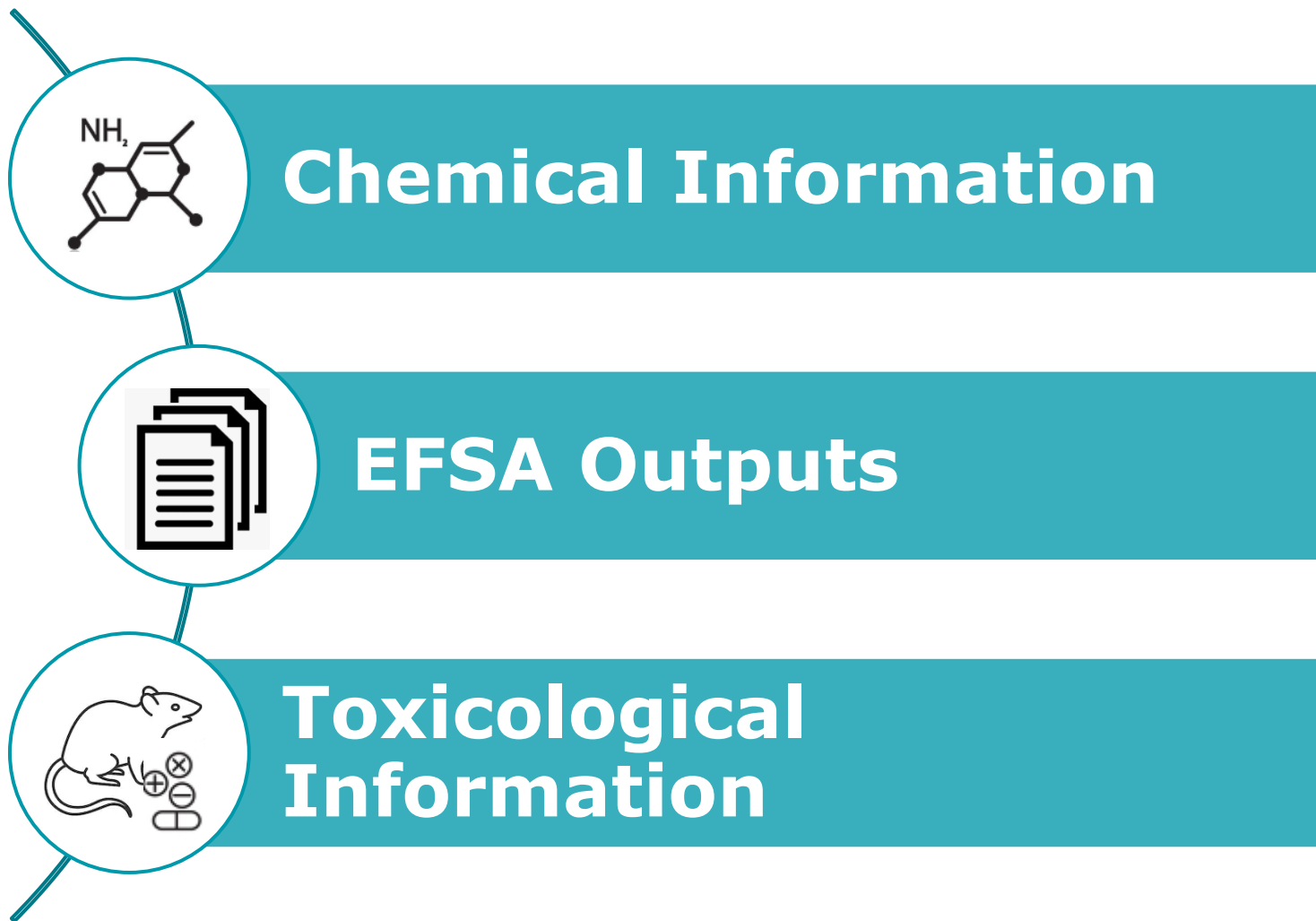
- Crisis: Free, Quick, Easy access to EFSA's Chemical Hazards Data
- Tool for stakeholders

Avoid duplication of efforts

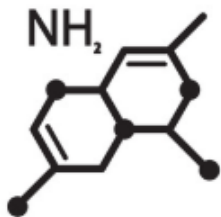
International Harmonisation and Data Sharing

- OECD Harmonised Templates
- Data sharing

OpenFoodTox: Content



OpenFoodTox: Content



Chemical Information

Substance Identity

CAS, IUPAC, SMILES etc.

- Single Substances (e.g. flavourings)
- Group of Substances (e.g. mixture or formulation)

OpenFoodTox: Content

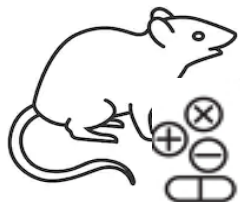


EFSA Outputs

Title, Publication date, link etc.

- Opinions
- Conclusions on Pesticides
- Statements

OpenFoodTox: Content



Toxicological Information

Genotoxicity

Reference Points

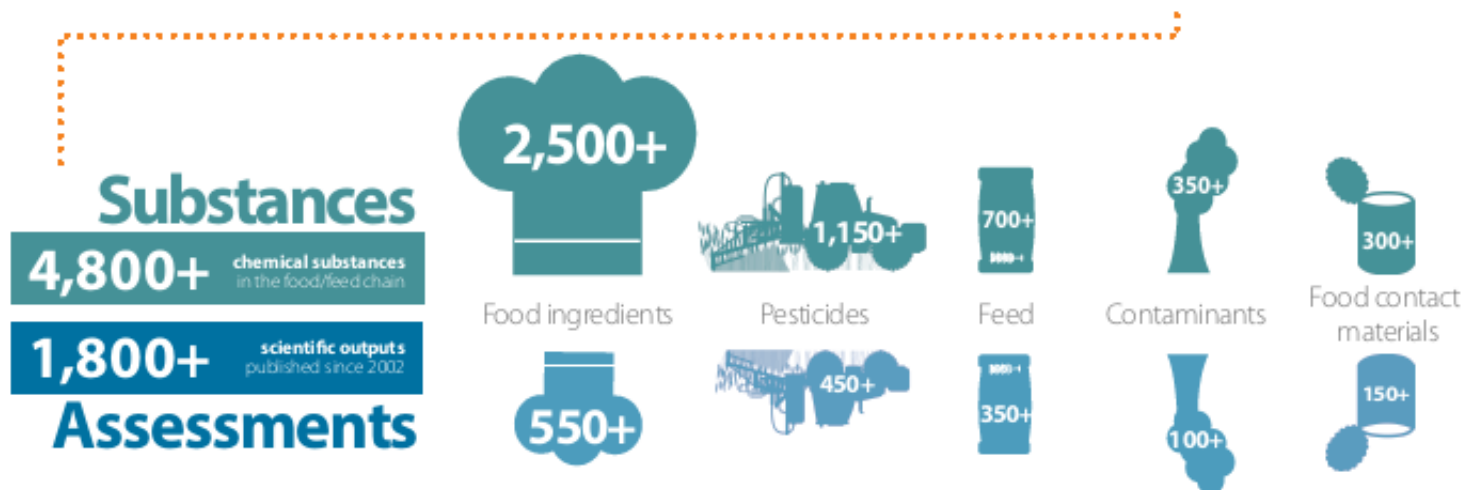
- Human and Animal health
- Ecological RA

Reference Values

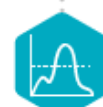
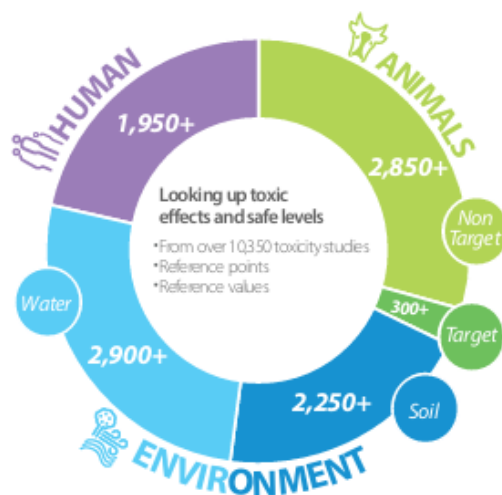
- Regulated products: e.g. ADI for pesticides
- Nutrients: e.g. DRV for vitamins and minerals
- Contaminants: TDI for acrylamide

OpenFoodTox in numbers

OpenFoodTox provides **chemical hazards data**:



Use OpenFoodTox for



information on chemical characterisation, regulations, EFSA outputs, toxicity, reference points (NOAEL, BMD, LD50, etc.) and reference values (ADI, TDI, PNEC, etc)*, uncertainty factors, EFSA scientific outputs.



developing future **methods and tools** as alternatives to animal testing.

Associated Publications

EDITORIAL



APPROVED: 8 December 2016

doi: 10.2903/j.efsa.2017.e15011

Editorial: OpenFoodTox: EFSA's open source toxicological database on chemical hazards in food and feed

Jean Lou Dorne^a, Jane Richardson^b, Georges Kass^a, Nikolaos Georgiadis^c,
Mario Monguidi^d, Luca Pasinato^d, Stefano Cappe^e, Hans Verhagen^f,
Tobin Robinson^g

Since its inception in 2002, the European Food safety Authority (EFSA) has produced more than 4,400 substances in over 1,650 Scientific Opinions, Statements and Conclusions. The work of its Scientific Panels, Units and Scientific Committee. For each individual substance, a summary of human health, animal health and ecological hazard assessments has been structured into EFSA's Chemical Hazards Database: OpenFoodTox. OpenFoodTox provides data for substance characterisation, links to the relevant EFSA output, background information and summaries of critical toxicological endpoints. An online MicroStrategy¹ tool enables the summarisation of data sheets for each individual substance in PDF or Excel format. OpenFoodTox is a tool and source of information for scientific advisory bodies and stakeholders with an interest in risk assessment. This editorial provides a snapshot description of OpenFoodTox as a

EXTERNAL SCIENTIFIC REPORT



APPROVED: 25 May 2018

doi:10.2903/sp.efsa.2018.EN-1438

Final report on the update and maintenance of OpenFoodTox: EFSA's Chemical Hazards Database

S-IN Soluzioni Informatiche

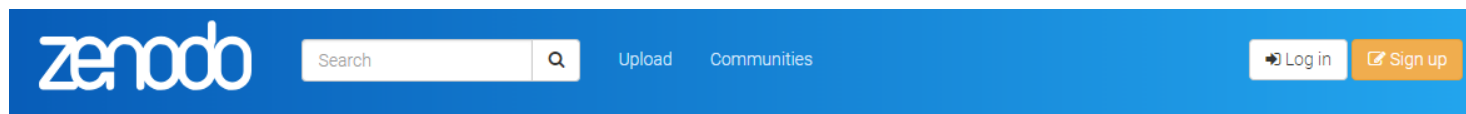
Lidia Ceriani, Andrea Ciacci, Rossella Baldin, Simona Kovarich, Manuela Pavan, Elena Fioravanzo, Arianna Bassan

Abstract

The present document is a summary of the update and maintenance of the EFSA's Chemical Hazards Database 'OpenFoodTox' that has been developed over the last 6 years to map hazards data as published in the EFSA opinions, statements and conclusions. More specifically, the repository holds summary data on identification of chemicals, document descriptors, hazard identification, and hazard characterisation. The repository includes data extracted from opinions and statements adopted by a number of EFSA panels including NDA (vitamins and minerals, novel foods, dietetic products), CONTAM (contaminants in the food chain, contaminants in the feed chain), FEEDAP (feed additives-application linked to 1381/2003, feed additives-application under to 1381/2003, feed additives-other), AFC (food additives, food contact materials, nutrient sources, processing aids, flavourings), CEF (food contact materials, food manufacturing processes, processing aids, flavourings), ANS (food additives, nutrient sources) and the Pesticides unit. Substances which do not fall within the category of

OpenFoodTox: How to get the data ?

<https://doi.org/10.5281/zenodo.780543>



July 13, 2018

OpenFoodTox: EFSA's chemical hazards database

Bassan, Arianna; Ceriani, Lidia; Richardson, Jane; Livaniou, Anastasia; Ciacci, Andrea; Baldin, Rossella; Kovarich, S; Fioravanzo, Elena; Pavan, Manuela; Gibin, Davide; Di Piazza, Giulio; Pasinato, Luca; Cappé, Stefano; Verhagen, Hans; Robinson, Tobin; Dorne, Jean Lou

Background: EFSA's remit and chemical risk assessment of regulated products and contaminants

The European Food Safety Authority (EFSA) has the remit to provide scientific advice to risk managers and decision makers through risk assessment and risk communication on issues related to "food and feed safety, animal health and welfare, plant health, nutrition, and environmental issues". Risk assessment has been defined as "a scientifically based

sure assessment and risk

n to determine safe levels of ex
th, animal health, environmental
re most often derived by
n uncertainty factor³ is applied.

risk assessments for **more than**
through the work of its scientifi

c panels and four supporting units.

ation and characterisation for the
tives, pesticides and contaminants)

ground European legislation, and a

sing OECD Harmonised Template
dTox provides open source data for

1,346

views

863

downloads

[See more details...](#)

	All versions	This version
Views ?	1,346	1,058
Downloads ?	863	763
Data volume ?	2.6 GB	2.4 GB
Unique views ?	1,182	936
Unique downloads ?	333	296

Publication date:

July 13, 2018

DOI:

DOI [10.5281/zenodo.1252752](https://doi.org/10.5281/zenodo.1252752)

Keyword(s):

contaminants critical study data collection data model
feed additives food additives food contact materials
nutrient sources pesticides processing aids
safety assessment substance toxicology
hazard characterisation human health animal health
acute toxicity sub-chronic toxicity chronic toxicity
reference point reference value acute toxicity

Files (12.1 MB)

Name	Size	Download
EFSAOuputs_KJ_2018.xlsx	232.3 kB	Download
md5:8536450d780499b1144dc94eabfc5a58 ?		
Genotoxicity_KJ_2018.xlsx	104.8 kB	Download
md5:142e7ea48c47c0ec34e78dda9912e64 ?		
OpenFoodToxTX22291_2018.xlsx	11.2 MB	Download
md5:13398d3c33717a077135c2e007458160 ?		
ReferencePoints_KJ_2018.xlsx	159.5 kB	Download
md5:f557fe33d5e6eb627e75db1807919a ?		
ReferenceValues_KJ_2018.xlsx	99.6 kB	Download
md5:e4474f69e35cb022370c923dd452c16f ?		
SubstanceCharacterisation_KJ_2018.xlsx	258.7 kB	Download
md5:1ce0921f350f0c405f8ced2b04b89abc ?		

OpenFoodTox: How to explore the data ?

<https://www.efsa.europa.eu/en/microstrategy/openfoodtox>

FILE

Y FILTER

Substance Browser

Apply

▼ Substance name (1 S...

Boron co... x

▼ Compound CAS number

Search Compound CAS number

Please, use one search field at a time and click on "Apply". If more than one filter is used, the tool will intersect all searched data. If you wish to see the alternative names (synonyms) of a substance please, select the substance name in the Substance characterisation table.

Substance Characterisation

Substance	has	Component	CAS number	EC Ref No	Molecular formula	Smiles	Synonym
Boron compounds	not part of group assessment	Borate			(BO3)3-	B([O-])([O-])[O-]	Boron compounds
Boron compounds	not part of group assessment	Boric acid	11113-50-1		BH3O3	B(O)(O)O	E 284

EFSA outputs

Substance	Author	Published	Output Id	Title	Output Type	Legal Basis	Url
Boron compounds	EFSA CONTAM	07/13/2005	43	Opinion of the Scientific Panel on Contaminants in the Food Chain on a request of the Commission related to concentration limits for boron and fluoride in natural mineral waters	EFSA opinion	Regulation (EC) No 178/2002	http://dx.doi.org/10.2903/j.efsa.2005.237

Hazard Characterisation: Reference points

Substance	Author	Year	Output Id	Study	Test Type	Species	Route	Duration (days)	Endpoint	Qualifier	Value	Unit	Effect	Toxicity
Boron compounds	EFSA NDA	2004	2	Human health	reproduction toxicity	Rat	oral; feed	21	NOAEL	=	9.6	mg/kg bw/day	body weight	teratogenic
Boron compounds	EFSA CONTAM	2005	43	Human health	reproduction toxicity	Rat	oral; feed	21	NOAEL	=	9.6	mg/kg bw/day	body weight	teratogenic

Hazard Characterisation: Reference values

Substance	Author	Year	Output Id	Assessment	Qualifier	Value	Unit	Population
Boron compounds	EFSA NDA	2004	2	UL	=	0.16	mg/kg bw/day	Consumers - Adult women, lactating
Boron compounds	EFSA NDA	2004	2	UL	=	0.16	mg/kg bw/day	Consumers - Adult women, pregnant

Genotoxicity

Substance	Author	Year	Output Id	Genotoxicity
Boron compounds	EFSA NDA	2004	2	Negative
Boron compounds	EFSA CONTAM	2005	43	No data
Boron compounds	EFSA AFC	2006	377	No data
Boron compounds	EFSA CEF	2012	472	No data
Boron compounds	EFSA CEF	2013	2392	No data

Substance Browser

Reference Values

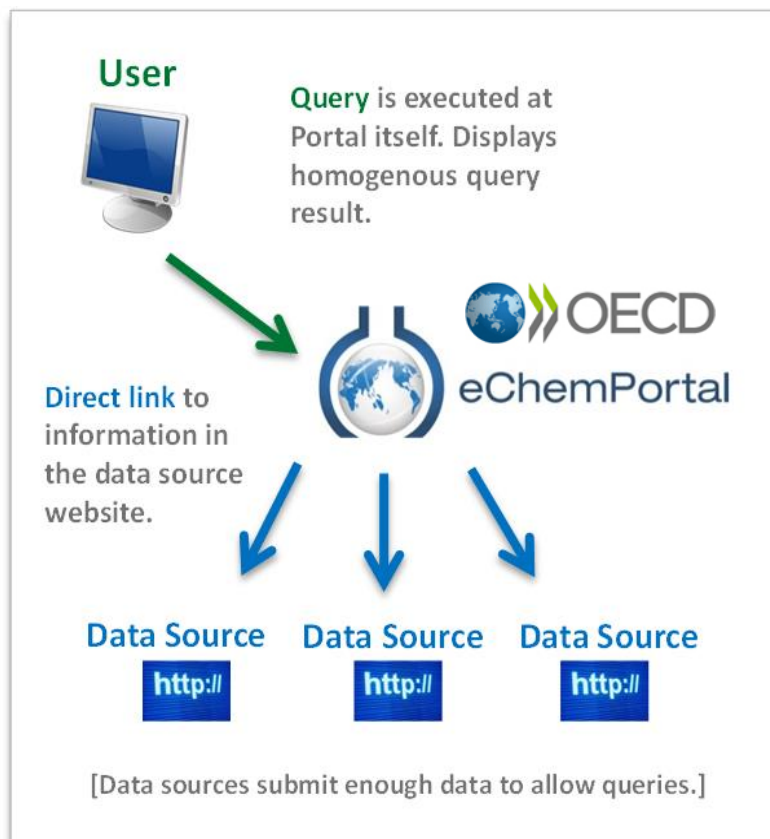
Reference Point

Background Documents

14

Cooperation and Data sharing

OpenFoodTox is integrated with:



■ eChemPortal

Free access to chemical information of regulatory relevance

- **Properties & Effects**
- Exposure and use
- **GHS** classification results

■ Predictive modelling tools

USEtox[®]
Joint Research Centre

Aquatic toxicity model

VEGAHUB

ambit

■ OpenFoodFacts

Structured Data as a cooperation tool

OECD Harmonised Templates

[Physico-chemical properties \(incl. nanomaterials\)](#)

[Degradation and accumulation](#)

[Effects on biotic systems](#)

[Health effects](#)

[Pesticide residue chemistry](#)

[Analytical methods](#)

[Efficacy](#)

[Emissions from treated articles](#)

[Intermediate effects](#)

[Use and exposure information](#)

[Generic elements for all OHTs](#)

- OHTs 1 to 23-5 & 101 to 113

- OHTs 24 to 40

- OHTs 41 to 57

- OHTs 58 to 84 & 86

- OHTs 85-1 to 85-10

- OHT 87

- OHTs 88 & 89

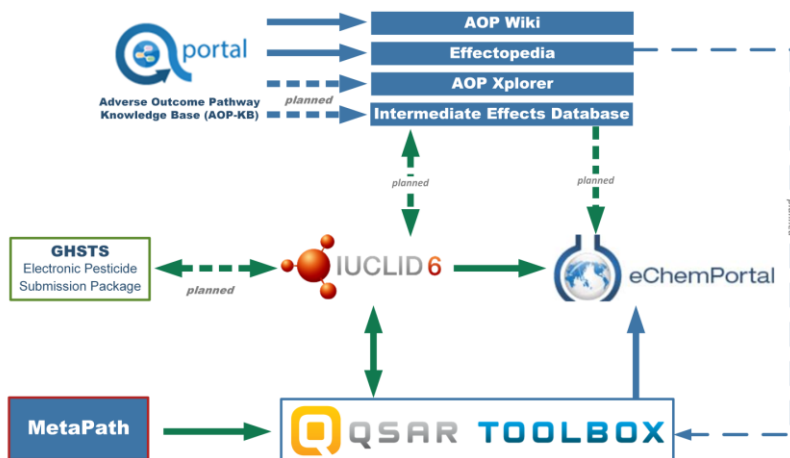
- OHT 90

- OHT 201

- OHTs 301 to 306

- Literature reference - Test material information
Reference substance - Chemical inventory

- International Standard and electronic data format
- OECD Test Guidelines or others
- Summarises properties & effects (human health and environment)
- Harmonised tools for DB managers: models for chemicals reporting



www.oecd.org/ehs/templates

Using OpenFoodTox in the EU-Datathon



Open Food Facts gathers information and data on food products from around the world.

Add a product

Picture with barcode

or Barcode

Add

Product without barcode

Sign in

Sign-in to add or edit

Username or e-mail address

Open Food Facts - World

Discover

Open Food Facts is a food products database made by everyone, for everyone.

You can use it to make better food choices, and as it is open data, anyone can re-use it for

→ [Learn more about Open Food Facts](#)

Last products added:

→ [products from the mobile app that need to be completed](#)

689922 products

Drilldown into products by... ▼



Ingredients

→ Ingredients are listed in order of importance (quantity).

Ingredients list:

Sirop de glucose, sucre de canne, gélatine de porc, amidon de maïs, acidifiant, caramelisé, amidon de blé.

Substances or products causing allergies or intolerances: [Gluten](#)

Additives:

- [E428 - Gelatine](#)
- [E330 - Citric acid](#)
- [E270 - Lactic acid](#)



Open Food Facts is made by a non-profit association, independent from the industry. It is made for all, by all, and it is funded by all. You can support our work by [donating to Open Food Facts](#) and also by [using the Lilo search engine](#).

E330 - Citric acid

Additives: E330 - Citric acid

Functions: Antioxidant, Sequestrant

Citric acid is a weak organic acid that has the chemical formula $C_6H_8O_7$. It occurs naturally in citrus fruits. More than a million tons of citric acid are manufactured every year. It is used widely as an acidulant in soft drinks. A polyatomic anion found in solution. An example of the former, a salt is trisodium citrate; an ester is triethyl citrate.

Risk of overexposure

EFSA evaluation: [Scientific Opinion on the safety evaluation of the active substances citric acid -E330, cellulose and polyacrylic acid sodium salt crosslinked, in active food contact materials.](#) (2013-04-09)

Names: Acide citrique, $C_6H_8O_7$, CAS 77-92-9, $C_6H_8O_7 \cdot H_2O$, Citric acid

Summary

- OpenFoodTox in line with EFSA **Strategy** for open data
- Contains information on:
chemical, EFSA's output, Hazard Assessments summaries
- **Structured data** based on OHTs: increased ability to share data
- Integrated in eChemPortal and predictive tools

Acknowledgments & References

S-IN Soluzioni Informatiche Srl: Arianna Bassan, Lidia Ceriani
Jane Richardson and Luca Pasinato (EFSA)

References

- Dorne JL, Richardson J, Kass G, et al. (2017) Editorial: OpenFoodTox: EFSA's open source toxicological database on chemical hazards in food and feed. EFSA Journal 2017;15(1):e15011, 3 pp. <https://doi.org/10.2903/j.efsa.2017.e15011>
- S-IN Soluzioni-Informatiche (2013) Report on "Data collection and data entry for EFSA's chemical hazards database NP/EFSA/EMRISK/2011/01". Supporting Publications 2013:EN-458, 140pp. <https://doi.org/10.2903/sp.efsa.2013.EN-458>
- S-IN Soluzioni Informatiche (2018) Update and maintenance of the EFSA's Chemical Hazards Database. EFSA supporting publication 2018:EN-1438, 60 pp. <https://doi.org/10.2903/sp.efsa.2018.EN-1438>
- Benfenati E, et al. (2017) Developing innovative in silico models with EFSA's OpenFoodTox database. EFSA supporting publication 2017:EN-1206, 19pp. <https://doi.org/10.2903/sp.efsa.2017.EN-1206>

Explore/Download the dataset

- Bassan A, Ceriani L, Richardson J, Livaniou A, Ciacci A, et al. (2018). OpenFoodTox: EFSA's chemical hazards database [Data set]. Zenodo. <https://doi.org/10.5281/zenodo.780543>
- <https://www.efsa.europa.eu/en/microstrategy/openfoodtox>

Other sources:

- <https://www.efsa.europa.eu/en/press/news/170118-0>
- [Infographic : OpenFoodTox – chemical hazards database](#)
- [eChemPortal](#)
- [OpenFoodFacts](#)

THANK YOU!



Subscribe to

www.efsa.europa.eu/en/news/newsletters

www.efsa.europa.eu/en/rss



Engage with careers

www.efsa.europa.eu/en/engage/careers



Follow us on Twitter

[@efsa_eu](https://twitter.com/efsa_eu)

[@plants_efsa](https://twitter.com/plants_efsa)

[@methods_efsa](https://twitter.com/methods_efsa)

Do you have questions?

Anastasia.LIVANIOU@efsa.europa.eu

Jean-Lou.DORNE@efsa.europa.eu

Jane.RICHARDSON@efsa.europa.eu

Exercise

<https://www.efsa.europa.eu/en/microstrategy/openfoodtox>

Exercise:

- Find the substances:
Chlorpyrifos, E210, melamine, lycopene
- Find the substance with CAS number:
210880-92-5 (Clothianidin) & 65195-55-3 (abamectin)
- Find all ADIs for all consumers' groups and export to Excel
- Find all endpoints (NOEC, LC50) for rainbow trout in Ecotox studies