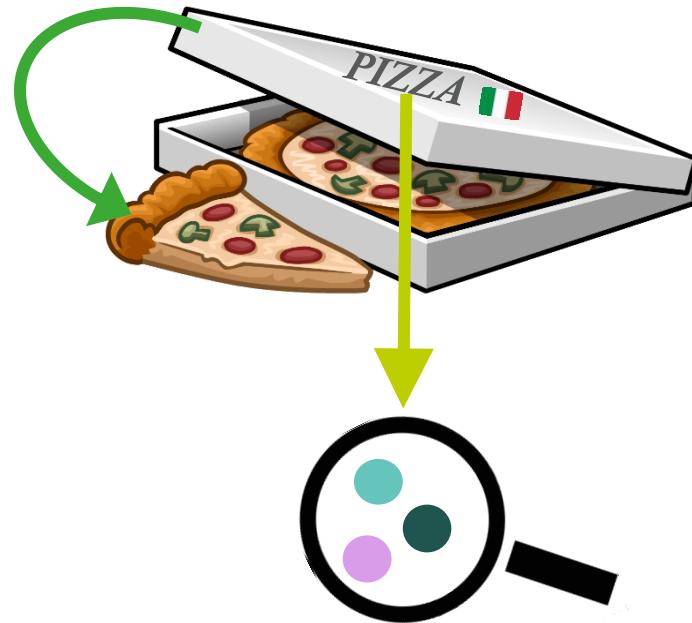


# FCM DATABASES

## Current situation and future developments

# Introduction

## MIGRATION

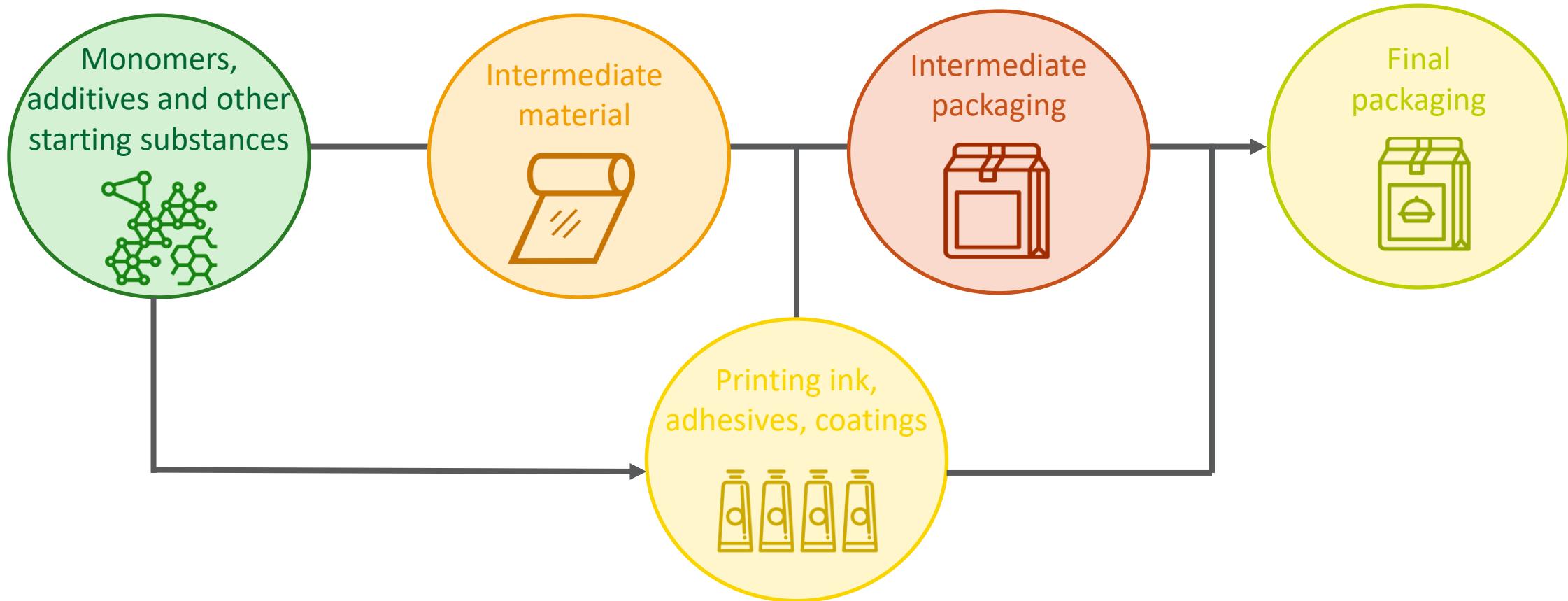


## Exposure

Thousands of substances can migrate from food contact materials

How can these substances be managed?

# Manufacture of food contact materials



Which substances can intentionally be added to a FCM?

# Inventories of intentionally added substances

## Regulation (EU) No 10/2011

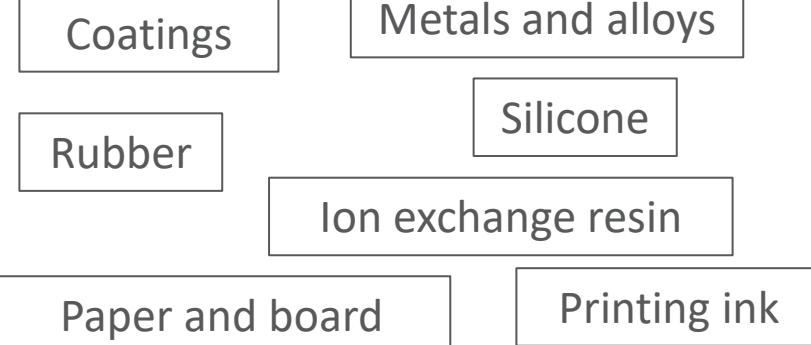


## National legislation



And other European countries

## Council of Europe Resolutions & Technical guides



Databases and inventories were developed

# Inventories of intentionally added substances

## Database of substances known by Member States of the Council of Europe and used in Food Contact Materials



ISP WIV  
WETENSCHAPPELIJK INSTITUUT VOLKSGEZONDHEID  
INSTITUT SCIENTIFIQUE DE SANTE PUBLIQUE

Database of Substances known by Member States of Council of Europe and used in Food Contact Materials

## Welcome

Database of Substances known by Member States of Council of Europe and used in Food Contact Materials.

This database is an initiative of Belgian authorities and is supported by contributions of the Council of Europe (CoE): the Belgian Scientific Institute for Public Health is managing the database of substances known by the member states of the Council of Europe (CoE) and used in Food Contact Materials (FCM).

The database is accessible for the Council of Europe member states delegates and is accessible for public bodies and enterprises on a yearly subscription basis.

You could see a sample of the generated report by [clicking here](#)

Available online until 2021  
but no funding to maintain the database

In 2022  
Updated and used in research projects

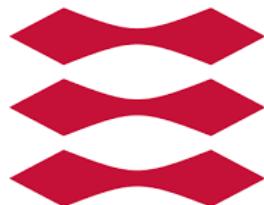
**~ 10 000 substances**

Information available in the database:

- Chemical information (CAS No, SMILES, etc.)
- Source and restrictions
- *In silico* predictions of human toxicity

# Inventories of intentionally added substances

## Database of substances developed in Denmark



In collaboration with

**EB Consult**

***2040 substances***

Origin of the substances:

- EFSA
- FDA (CEDI database)
- Other inventories of FDA
- Chemical analyses

Information available in the database:

- Chemical information (CAS No., molecular mass, chemical formula, SMILES, etc.)
- Source
- *In silico* predictions on human toxicity using VEGA HUB (<https://www.vegahub.eu>)

For more information, please contact Elena Boriani (EB consult)

# Inventories of intentionally added substances

## Council of Europe



Procedure for data submission has been established

Evaluation must be carried out according to internationally recognised scientific principles

Proposed requested information:

- Type(s) of evaluated food contact material
- Chemical name (IUPAC nomenclature, CAS No.)
- Limits, specifications and restrictions
- Applications
- Date of evaluation/approval
- Reference documents
- Short summary/conclusion of the evaluation
- URL of the published opinion (if available)

**CoE member states are strongly encouraged to submit updates on their officially evaluated substances**

# Inventories of intentionally added substances

## Baseline study performed by the JRC



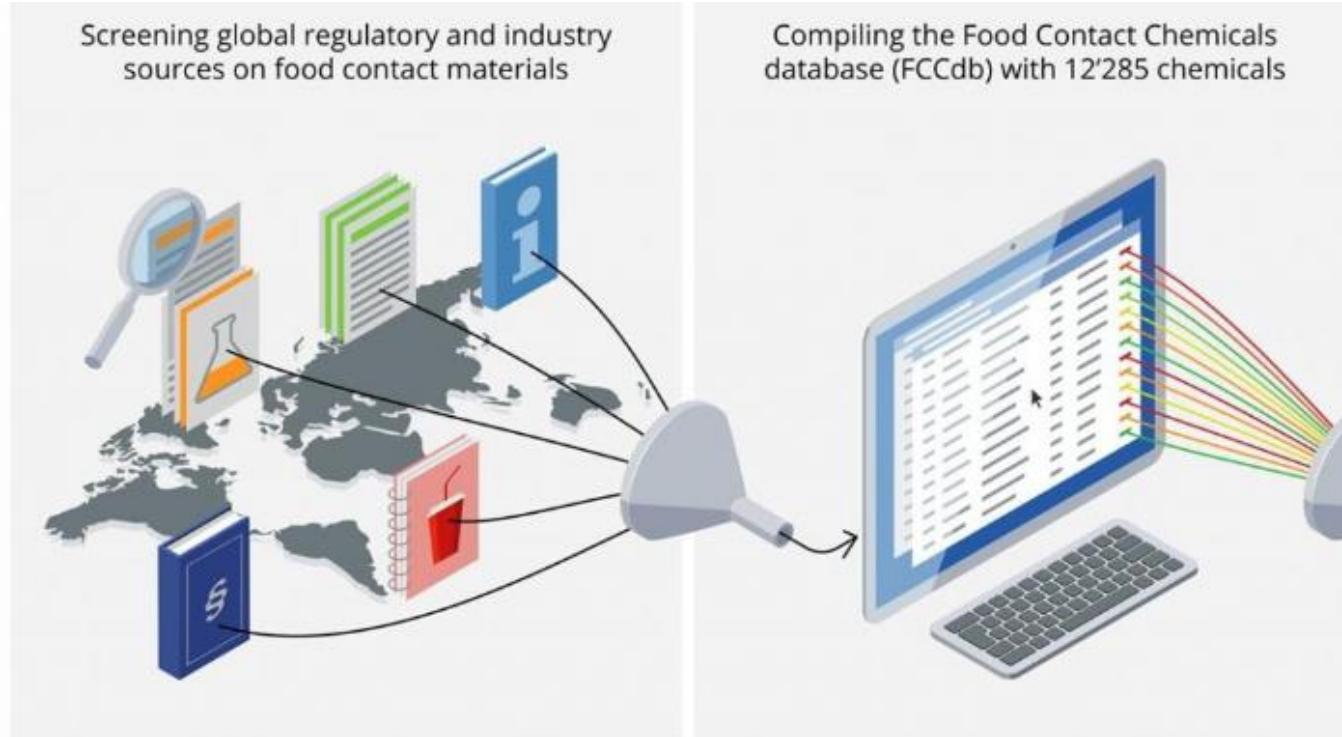
**~ 8 000 substances**

### Origin of the substances:

- Lists of (authorised) substances available in the Member States
- Council of Europe Resolutions and Technical Guides
- Lists of European professional associations
- Other databases (e.g. Decernis, Norden, etc.)
- Questionnaires

# Inventories of intentionally added substances

## Food Contact Chemicals database (FCCdb)



**67 sources**

**12 285 substances**

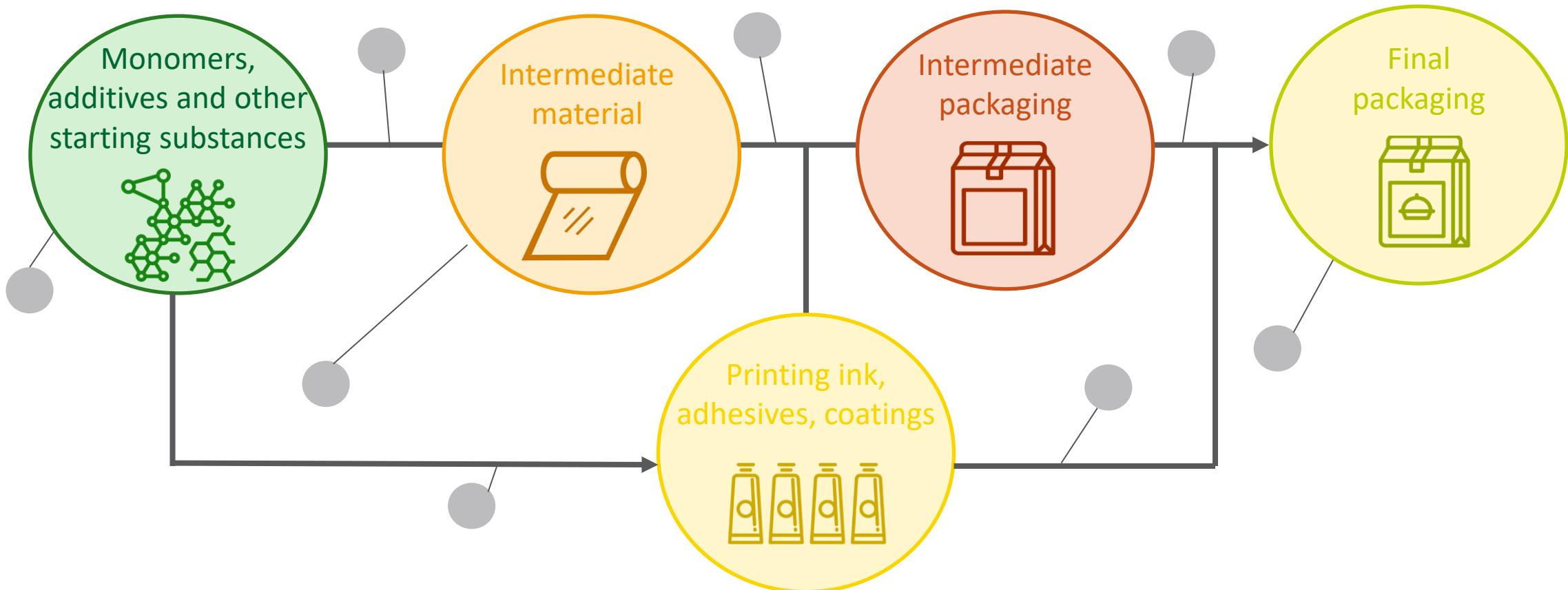
Regulatory & industry inventories



Information available in the database:

- Chemical information (CAS No., synonyms)
- Source
- Hazard information from:
  - a) GHS classification
  - b) Chemicals of concern due to endocrine disruption or persistence-related hazards
  - c) EU/US regulatory lists of hazardous substances

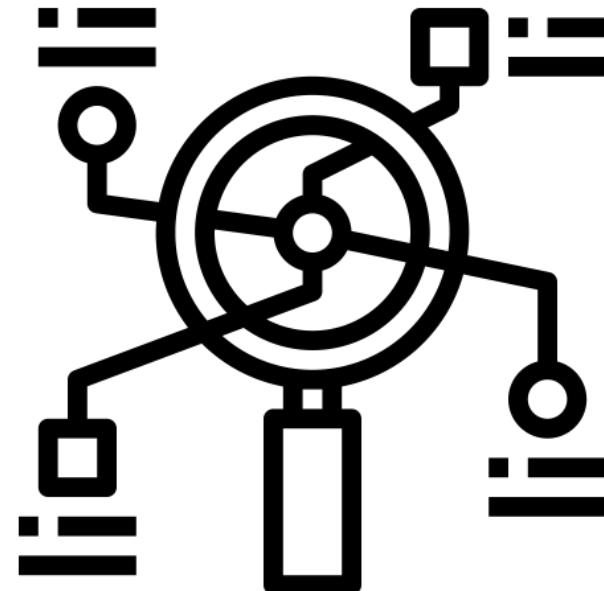
# What about non-intentionally added substances?



At each step of the production process, non-intentionally added substances can be present  
e.g. breakdown products, impurities, reaction products, contaminants, etc.

# Inventories of non-intentionally added substances

## Inventories of identified NIAS not readily available



Many research is performed and many NIAS are identified,  
but the information is not collected and saved in an open-source database

# Prediction of non-intentionally added substances

## Database of predictable oligoesters

Theoretical combination of 17 polyols and 15 polyacids with a cut-off < 1000 Da



NIAS-db 1.0

Search by

Mass Formula

Deviation (mDa) Formula Name Cyclic EG PG BD NPG CHDM TCDDM AA PA HHA NA SeA

Deviation (mDa)	Formula	Name	Cyclic	EG	PG	BD	NPG	CHDM	TCDDM	AA	PA	HHA	NA	SeA
-0.22	C21H26O8	NPG+PA+HHA	0	0	0	1	0	0	0	1	1	0	0	0
-0.22	C21H26O8	c(EG+NPG+AA+PA)	1	1	0	0	1	0	0	1	1	0	0	0
-0.22	C21H26O8	c(PG+BD+AA+PA)	1	0	0	0	0	1	1	0	0	0	0	0
-0.22	C21H26O8	c(2EG+HHA+NA)	0	0	0	0	0	0	1	1	0	1	1	0

monomers

EG, PG, BD, NPG, CHDM, TCDDM

NIAS-db

Open-source software  
(DOI: 10.15454/HHY2Z2)

# Inventories of intentionally added substances

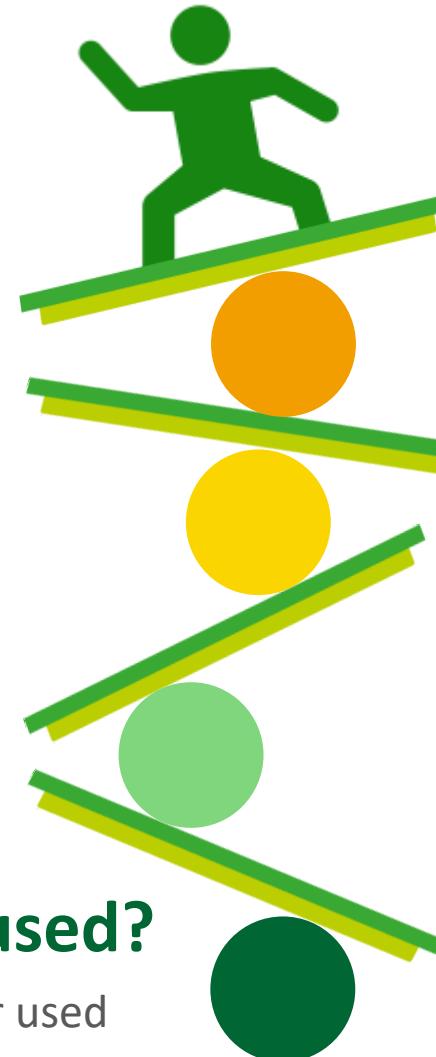
## Issues & Challenges

### Sustainable financing

To ensure the future of the database

### Are the substances being used?

Some historical substances are no longer used



### Keeping lists up-to-date

New or updates of legislation, evaluation status of substances, etc.

### Complete missing information

SMILES, analytical data, (predicted) toxicological data, etc.

# Substances used or present in FCM

## Flavourings, Additives, and food Contact materials Exposure Tool (FACET)



Objective: Estimate the dietary exposure to flavourings, additives and food contact material substances and compare the results with available safety limits (2008-2012)



Publically available inventories



*6 475 substances*

### FACET Industry Group

collected data  
on occurrence and concentration range  
of substances in inks, adhesives, plastics,  
metal, paper and board

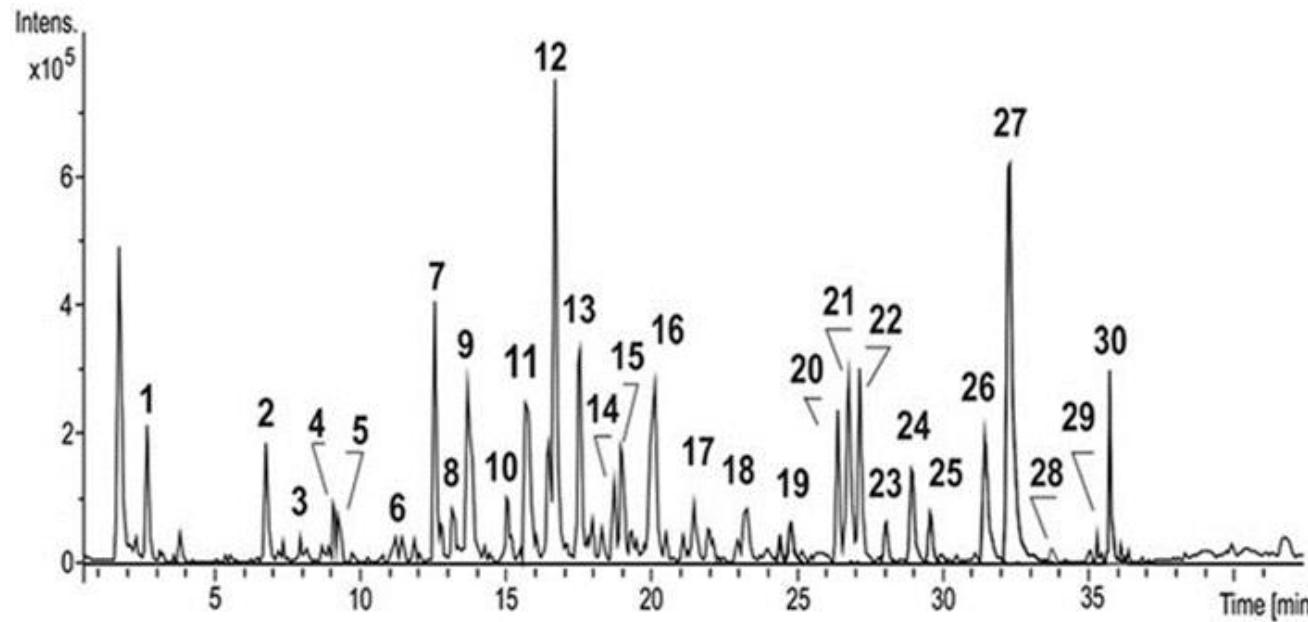


Data embedded in  
the FACET software

*??? substances*

# Substances used or present in FCM

## Analysis of the actual migration



Identification of all migrating substances is very challenging



Use of  
**Mass Spectra Libraries**

# Substances used or present in FCM

## Analysis of the actual migration

### (Commercial) libraries

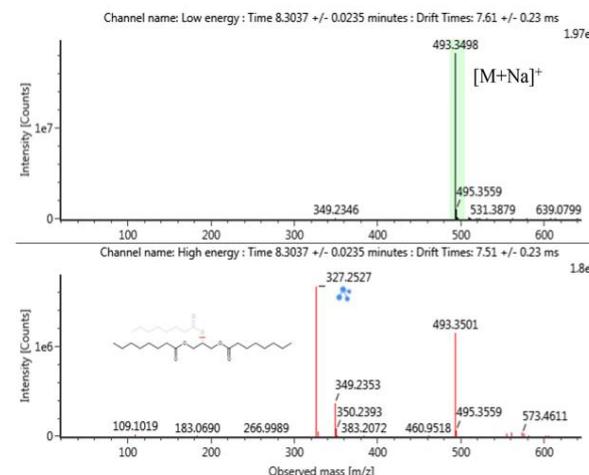


### In-house MS/MS libraries

Most libraries are not publically available

Dedicated libraries linked to vendor software (e.g.  $m/z$  Cloud)

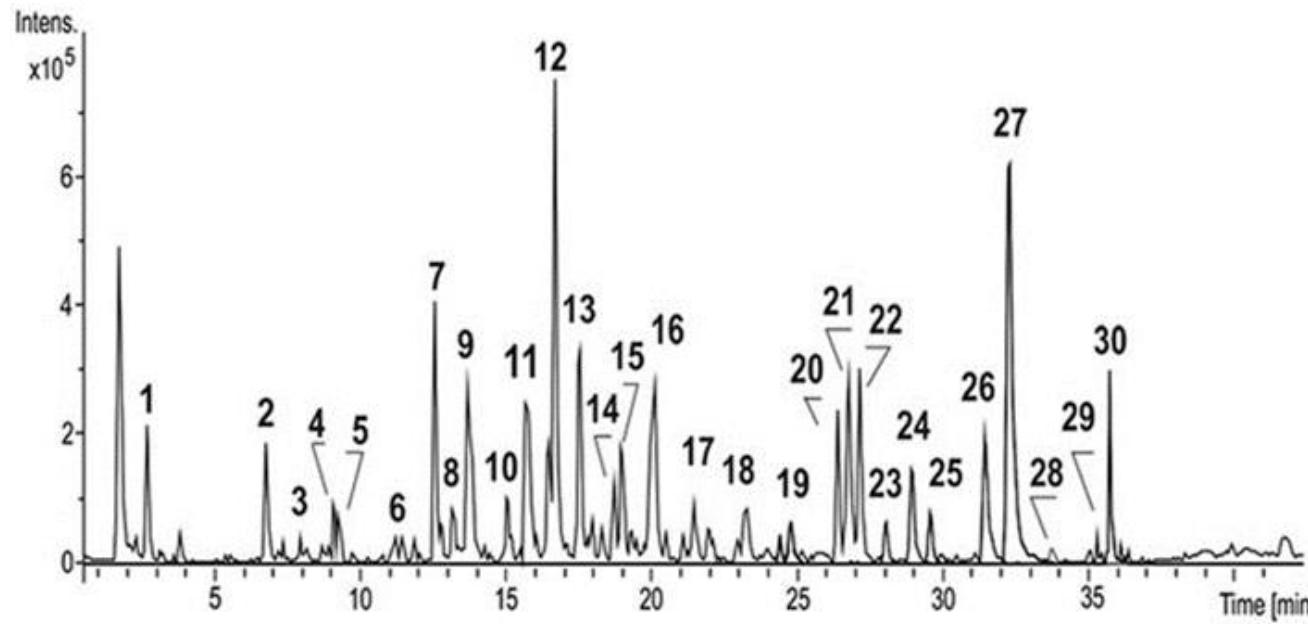
Open-source database created by C. Nerin et al.



$> 500$   
*plastic-related substances*  
(<https://zenodo.org/record/4454645>)

# Substances used or present in FCM

## Analysis of the actual migration



Identification of all migrating substances is very challenging



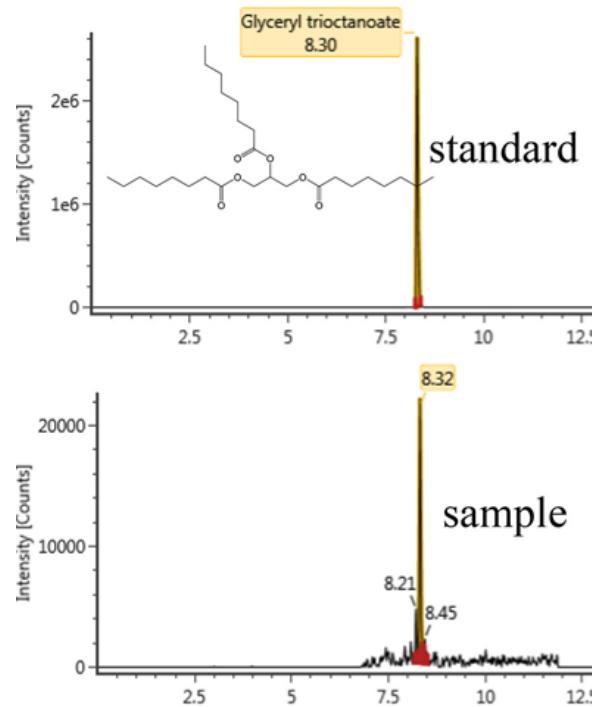
Development of  
**Prediction models**

# Substances used or present in FCM

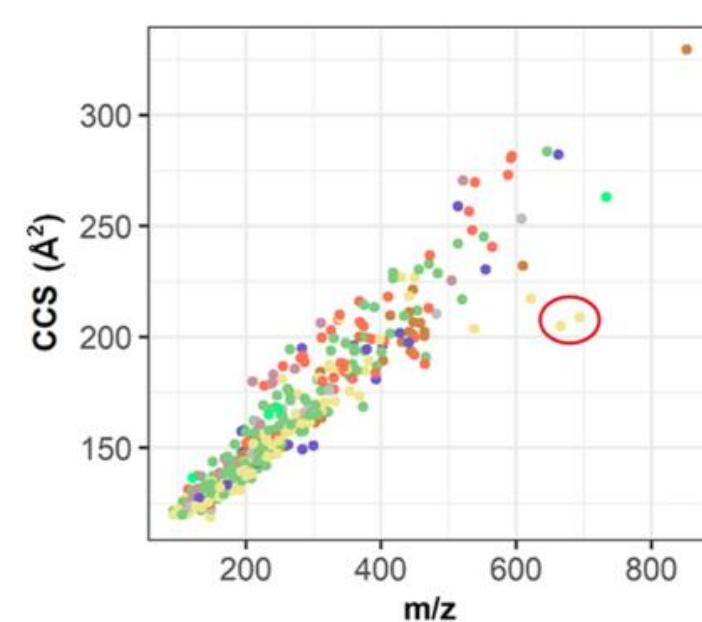
## Analysis of the actual migration

### Prediction tools developed by C. Nerin et al.

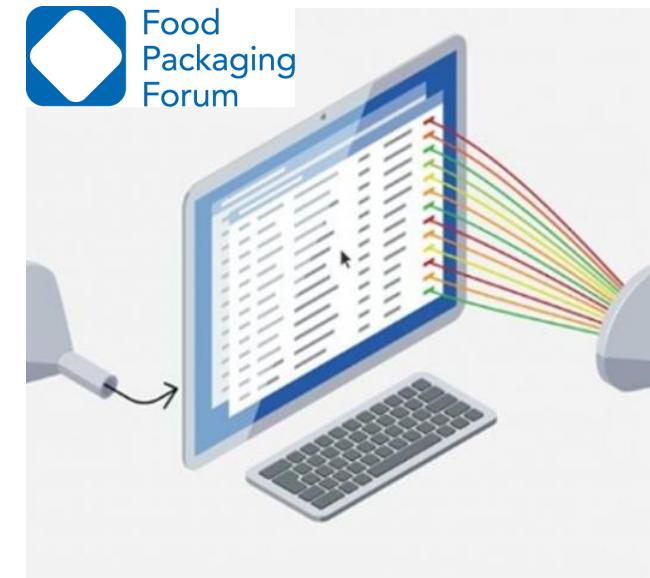
#### Retention time



#### Ion Mobility (CCS)



### Applied to FFCdb



> 10 000 substances

*Open-source in the future*

# Substances used or present in FCM

## Analysis of the actual migration

Database on migrating and extractable food contact chemicals

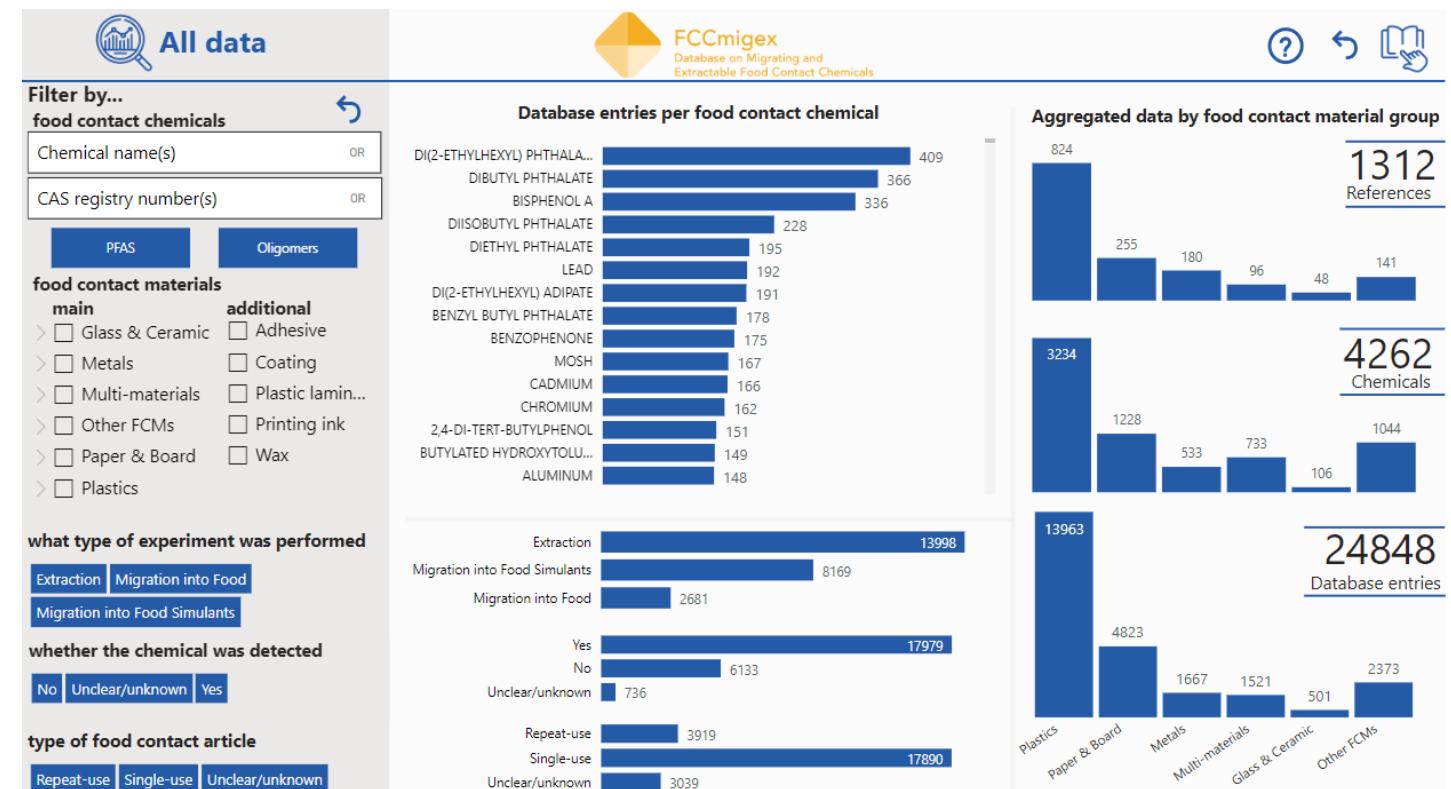


### FCCMigex Database

1 312  
studies and reports

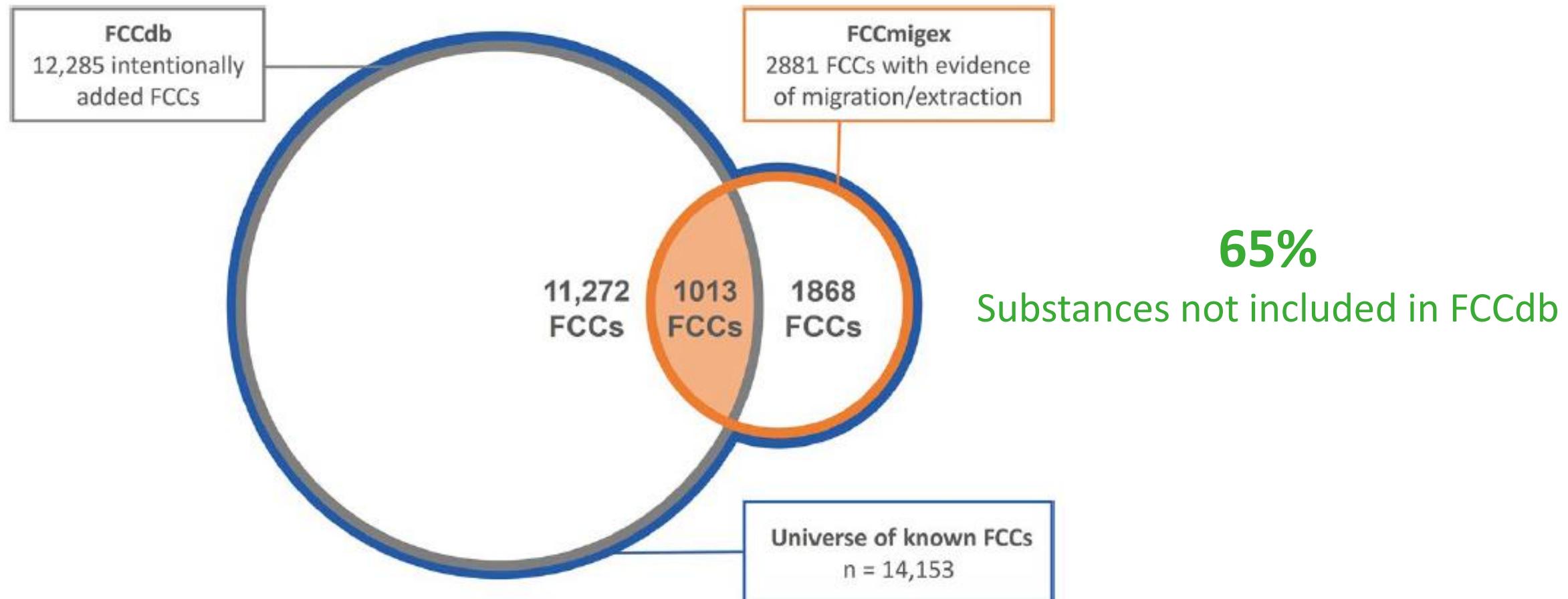
24 848  
Database entries

4 262  
Chemicals were found  
(mostly in plastic FCM)



# Substances used or present in FCM

## FCCMigex Database



# Join forces to obtain the ultimate FCM database

