



# IPChem

The information Platform for Chemical  
Monitoring

European Commission, Joint Research Centre

February 2017

# OVERVIEW OF IPChEM

- Policy questions behind IPChEM
- IPChEM approach and salient elements
- IPChEM specific objectives
- The specific objectives in practice

<https://ipchem.jrc.ec.europa.eu>

## ***EC Communication “The combination effects of chemicals Chemical mixtures”***

promoting a more coherent approach to the generation, collection, storage and use of chemical monitoring data in relation to humans and the environment

### ***7th Environment Action Programme (2014-2020)***

Improve the knowledge and evidence base for Union environment policy “*developing a comprehensive chemical exposure and toxicity knowledge base...(by 2020)*”

#### ***DGs requests to assess:***

- Effectiveness and efficiency of the EU regulatory framework implementation
- Revision of integration of the current EU Regulatory framework

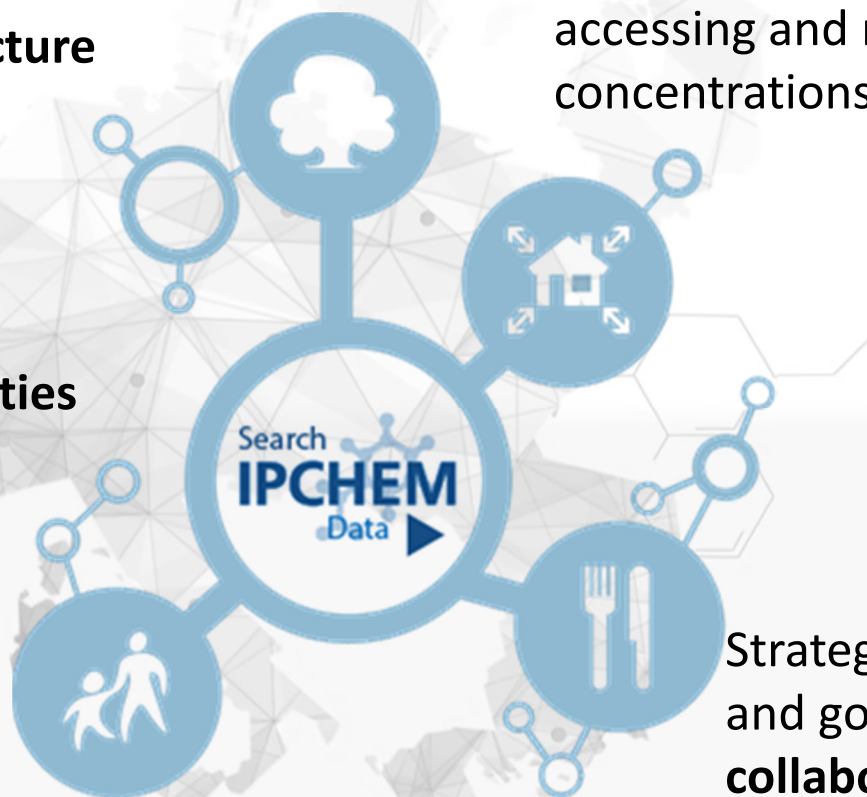
# IPChEM

one access point, all the information

Developed as  
**distributed infrastructure**

**It is a unique access point** for searching,  
accessing and retrieving data on chemical  
concentrations in different media

**It offers hosting facilities**  
for orphan data and  
research results.



Strategy, user requirements, Data Policy  
and governance **defined in  
collaboration** with IPChEM partners

*IPChEM approach and salient elements*





# IPCheM is based on collaborations



*IPCheM approach and salient elements*

# IPChEM as improver

## **Comparability**

i.e. the spatial and temporal comparative analysis across chemicals/media

## **interoperability**

with relevant (international) Information systems/web services for establishing a more comprehensive knowledge framework on chemical exposure

## **Data quality**

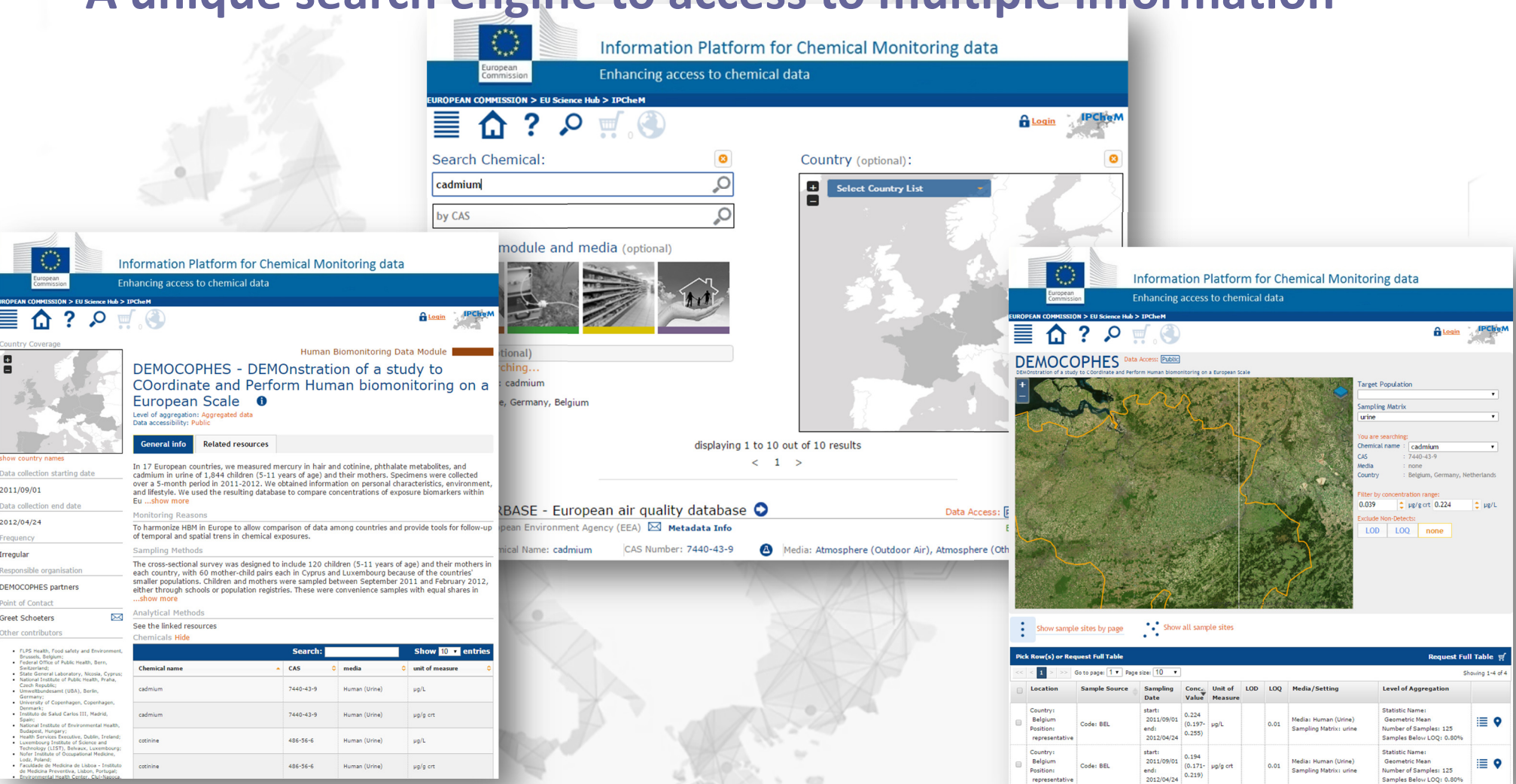
to properly understand and use the data accessible and retrievable through IPChEM



**IPChEM  
OBJECTIVES**

*IPChEM approach and salient elements*

# A unique search engine to access to multiple information



The screenshot displays the IPChem (Information Platform for Chemical Monitoring data) search engine interface. The main search results for "cadmium" are shown, including a map of Europe with a red dot indicating the location of the study. The search results are filtered by "Country (optional)" and "module and media (optional)". The results table shows the following data:

Chemical name	CAS	media	unit of measure
cadmium	7440-43-9	Human (Urine)	µg/L
cadmium	7440-43-9	Human (Urine)	µg/g crt
cotinine	486-56-6	Human (Urine)	µg/L
cotinine	486-56-6	Human (Urine)	µg/g crt

The interface also includes a sidebar with navigation options, a search bar, and a map of Europe. The search results are displayed in a table format, and the interface is designed to be user-friendly and accessible.

*The IPChem specific objectives in practice*

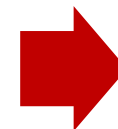
## DATA COMPARABILITY

### IPChem metadata and internal DATA MODEL

From the “Chemical Monitoring data” definition



Design of the IPChem metadata and internal data model



ETL mechanism for data mapping, transformation and integration

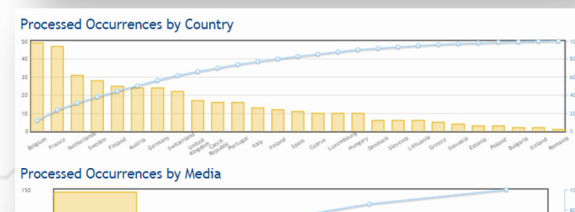
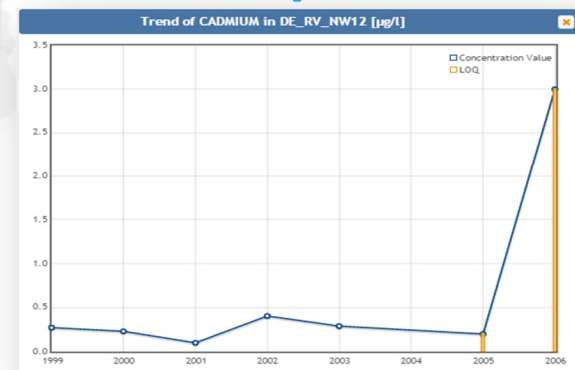
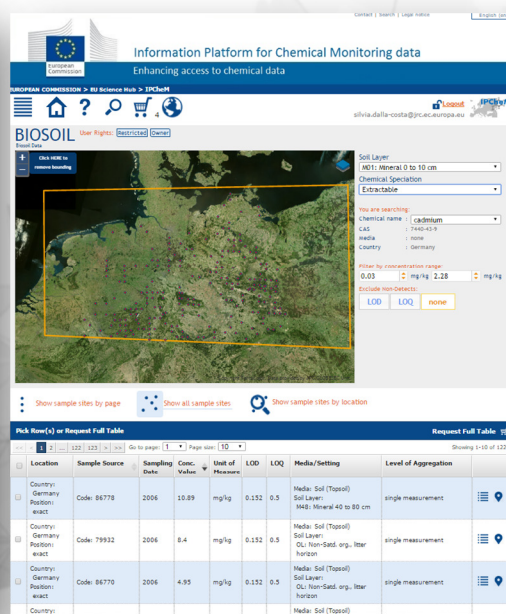
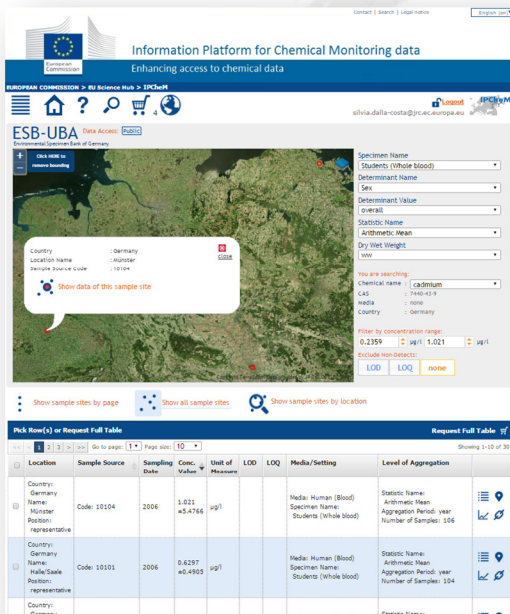
- Step towards harmonisation of data and vocabularies
- “light” approach: all mapping/transformation and integration tasks of the data source are managed by the IPChem Team via the IPChem ETL mechanism

*The IPChem specific objectives in practice*

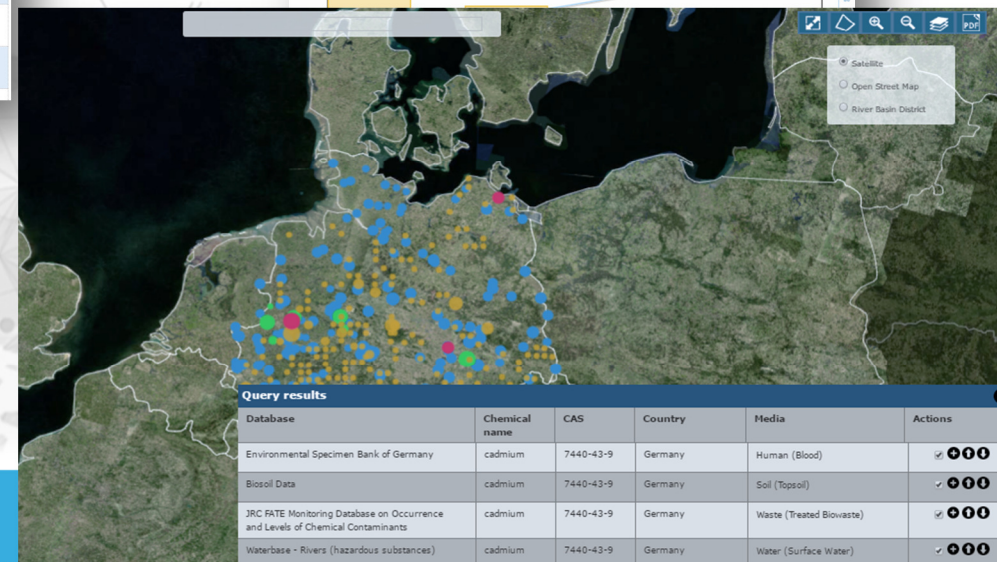


# different data visualisation options

## DATA COMPARABILITY



- Comparison of concentration measurement for:
  - 1 chemical in ≠ area and/or ≠ media
  - ≠ chemicals for the same area and/or the same media



*The IPChemM specific objectives in practice*



# INTEROPERABILITY

Direct access (from the “structural information and properties” window) to:

- The OECD eChemPortal
- The REACH Substance Registry
- Various web sites via ChemAgora service

## STRUCTURAL INFORMATION AND PROPERTIES

Chemical Name: **pcb118**  
CAS Number: **31508-00-6**  
InChIKey: **IUTPYMGCWINGEY-UHFFFAOYSA-N**

Links provided by ECHA  
> [eChemPortal](#)

Links provided by ChemAgora  
> [ChEBI](#)  
> [PubChem](#)  
> [CheLIST](#)

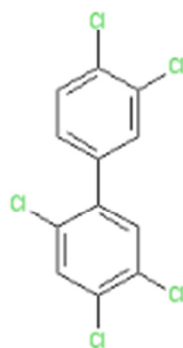


Image Source: NCI/CADD CIR



## The Global Portal to Information on Chemical Substances

eChemPortal

- Home
- Substance Search
- Property Search
- GHS Search
- What's new?
- General Information
- Participating Databases
- Roles & Responsibilities
- Linking to eChemPortal
- Schedules of Assessments
- Source Search
- GHS Classifications
- Useful links
- FAQ
- How to search for information
- Contact us
- Disclaimer

## Substance Search

Substance Search Search Result Step 1

## Search history & Ways to proceed

- You searched for Number: 31508-00-6  
Participants: ACTOR, AGRITOX, APVMA-CR, inventory, ECHA CHEM, EFSA, GDL, GHS-3, GOSL, HPV15, HS, JECDB, NICNAS Other, NICNAS, SPIN, UK, CLKMP Outputs, US
- Click any of the links below to see details

## Search information

For more details on the substance search mechanism, please go to [the help menu](#).

## Overall query results


Click the following link to see details for all query results.

- 4 Line(s) with 6 Hit(s) found as overall query results (including indirect query results)

## Query results, level 1

Your search criteria retrieved the substance(s) below or the same substance(s) identified by another identifier. Click on the column headers to sort the results in the table.

Hit(s)	Number	Name
3	31508-00-6 (CAS Number)	PCB-118 (Unknown)
1	31508-00-6 (CAS Number)	1,1'-Biphenyl, 2,3,4,4',5-pentachloro- (Unknown)
1	31508-00-6 (CAS Number)	PCB 118 (2',3,4,4',5'-PCB) (Unknown)
1	31508-00-6 (CAS Number)	1,1'-BIPHENYL, 2,3,4,4',5-PENTACHLORO- (Unknown)
4 Line(s) with 6 Hit(s).		



NIH NLM National Center for Biotechnology Information

PubChem OPEN CHEMISTRY DATABASE

Search Compounds

Compound Summary for CID 35823

Download Share Help

Cite this Record

PCB 118

STRUCTURE VENDORS LITERATURE PATENTS BIOACTIVITIES

PubChem CID: 35823

PCB 118: 31508-00-6; 2,3,4,4',5-PENTACHLOROBIIPHENYL; PCB No 118; 1,1'-Biphenyl, 2,3,4,4',5-pentachloro-;

Chemical Names: Biphenyl, 2,3,4,4',5-pentachloro- More...

Molecular Formula: C<sub>12</sub>H<sub>5</sub>Cl<sub>5</sub>

Molecular Weight: 326.422 g/mol

InChI Key: IUTPYMGCWINGEY-UHFFFAOYSA-N

Substance Registry: FDA UNII

Safety Summary: Laboratory Chemical Safety Summary (LCSS)

PUBCHEM > COMPOUND > PCB 118 Modify Date: 2017-01-23; Create Date: 2005-03-27

Contents

1 2D Structure

2 3D Conformer

3 Names and Identifiers

4 Chemical and Physical Properties

Search Download Get Image

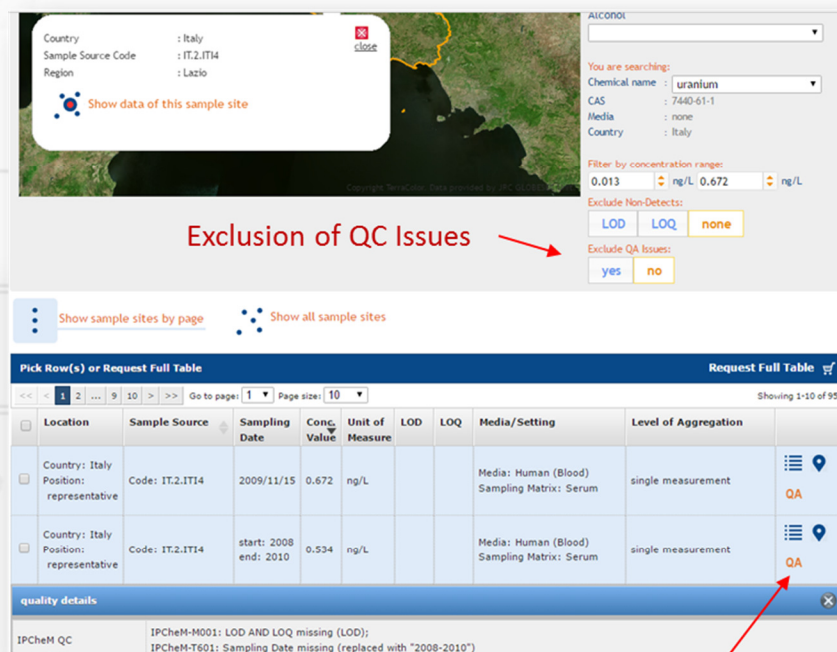
*The IPChem specific objectives in practice*

## DATA QUALITY

IPChem team with partners worked on:

- Definition of Central IPChem Quality Control Rules
- Rules are ingested into IPChem ETL and launched
- IPChem ETL creates the QC Report for data providers
- Any remaining quality issues are flagged and displayed into the IPChem DB console

Quality Control category	Examples of rules
Quality control of measurement values	Concentration Value missing [<details>]
	Concentration Value < 0 [<details>]
Violation of logical rules	Mean < Minimum
	(Number Of Samples) AND (Standard Deviation <> 0)
Quality control of spatial information	point coordinates outside country boundary
	point coordinates missing OR 0
Quality control of temporal information	Sampling date missing
	Sampling date out of the temporal coverage declared into the metadata
Quality control of Unique Identifiers	Unique Identifier for Record is missing
	Unique Identifier for Record is duplicated



Country : Italy  
Sample Source Code : IT.2.IT14  
Region : Lazio

Show data of this sample site

Exclusion of QC Issues

Filter by concentration range: 0.013 ng/L 0.672 ng/L

Exclude Non-Detects: LOD LOQ none

Exclude QA Issues: yes no

Show sample sites by page Show all sample sites

Location	Sample Source	Sampling Date	Conc. Value	Unit of Measure	LOD	LOQ	Media/Setting	Level of Aggregation	Quality Issue Flag
Country: Italy Position: representative	Code: IT.2.IT14	2009/11/15	0.672	ng/L			Media: Human (Blood) Sampling Matrix: Serum	single measurement	QA
Country: Italy Position: representative	Code: IT.2.IT14	start: 2008 end: 2010	0.534	ng/L			Media: Human (Blood) Sampling Matrix: Serum	single measurement	QA

quality details

IPChem QC

IPChem-M001: LOD AND LOQ missing (LOD);  
IPChem-T601: Sampling Date missing (replaced with "2008-2010")

Quality Control Issue, Code and description

Quality issue flag

*The IPChem specific objectives in practice*

# STATUS OF THE ACTIVITIES

- Data Integration
- Implementation of the IPCheM Data Policy
- Collaboration and relations with research consortia and international organisations

<https://ipchem.jrc.ec.europa.eu>



22.537.315

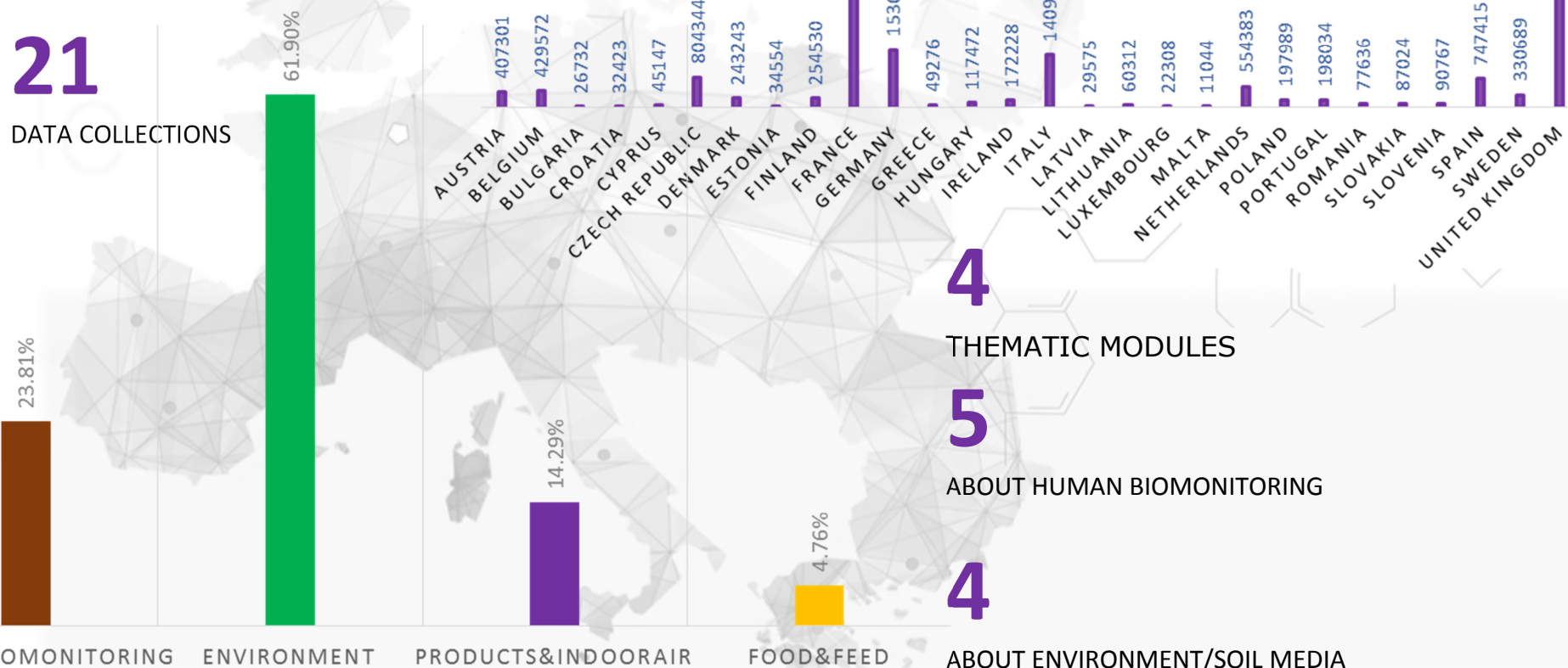
CONCENTRATION MEASUREMENTS

1.600

SUBSTANCES AND COMPOUNDS

21

DATA COLLECTIONS



Data integration- current status





CONTRIBUTORS

USER GROUPS

COMMISSION SERVICES

European Commission Services and EU Agencies

DATA OWNERS/PROVIDERS

# IPChem DATA POLICY

promotes

OPEN DATA PRINCIPLES

respects

DATA PROTECTION REGULATION

EU National Bodies

EU Member States Competent Authorities, including Competent Authorities in Countries from the European Free Trade Area and EU Candidate Countries.

General Public

Including Industry, Scientific Communities, International and Non-Governmental Organisations

*Implementation of the IPChem Data Policy*





# DIFFERENT LEVEL OF DATA GRANULARITY

Information Platform for Chemical Monitoring data  
Enhancing access to chemical data

EUROPEAN COMMISSION > EU Science Hub > IPCheM

FLEHS Data Access: Public  
Flemish Environment and Health Study



Show sample sites by page Show all sample sites

Pick Row(s) or Request Full Table  
Go to page: 1 Page size: 10

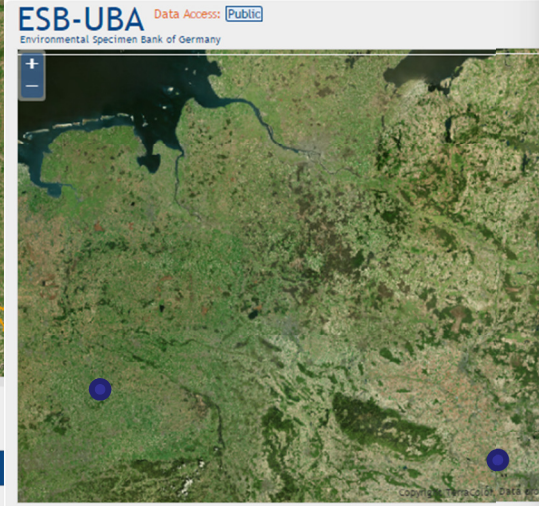
Location	Sample Source	Sampling Date	Conc. Value	Unit of Measure	LOD	LOQ
Country: Belgium Position: representative	Code: Rural area	start: 2002/01 end: 2004/01	0.499 ±0.589	µg/L	0.09	

Non-Detects representation:  
<LOD indicates a Conc.Value lower than the limit of detection, also used when 'zero' or 'n.d'.

Information Platform for Chemical Monitoring data  
Enhancing access to chemical data

EUROPEAN COMMISSION > EU Science Hub > IPCheM

ESB-UBA Data Access: Public  
Environmental Specimen Bank of Germany



Show sample sites by page Show all sample sites

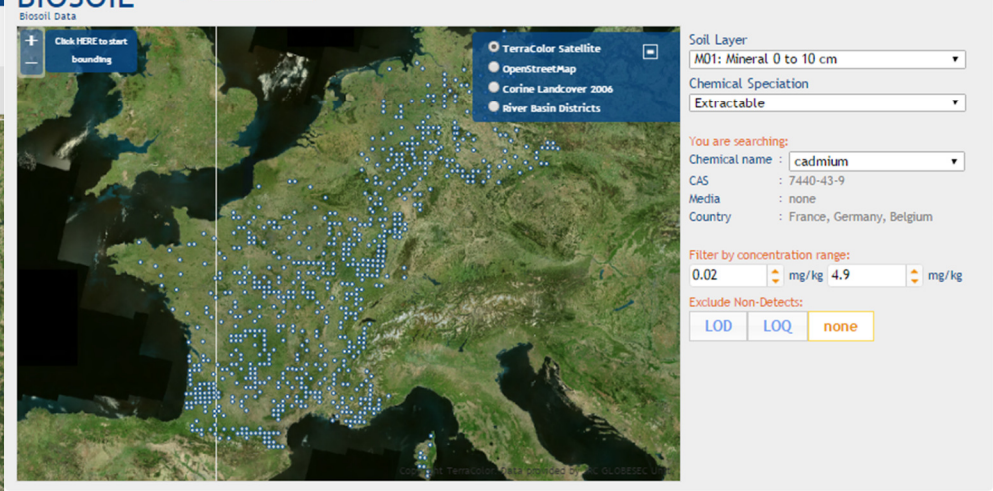
Pick Row(s) or Request Full Table  
Go to page: 1 Page size: 10

Location	Sample Source	Sampling Date	Conc. Value	Unit of Measure	LOD	LOQ
Country: Germany Name: Münster Position: representative	Code: 10104	2006	1.021 ±5.4766	µg/l		

Information Platform for Chemical Monitoring data  
Enhancing access to chemical data

EUROPEAN COMMISSION > EU Science Hub > IPCheM

BIOSOIL User Rights: Restricted Owner



Show sample sites by page Show all sample sites Show sample sites by location

Pick Row(s) or Request Full Table Request Full Table  
Go to page: 1 Page size: 10 Showing 1-10 of 756

Location	Sample Source	Sampling Date	Conc. Value	Unit of Measure	LOD	LOQ	Media/Setting	Level of Aggregation
Country: France Position: exact	Code: 96895	2006	4.9	mg/kg	0.152	0.5	Media: Soil (Topsoil) Soil Layer: M01: Mineral 0 to 10 cm	single measurement
Country: France Position: representative	Code: 97012	2006	3.2	mg/kg	0.152	0.5	Media: Soil (Topsoil) Soil Layer:	single measurement

Students (Whole blood) Aggregation Period: year Number of Samples: 106  
Statistic Name:

## Implementation of the IPCheM Data Policy

# IPChemM as a platform for data collection and exchange within research projects



European Human Biomonitoring Initiative

**solutions**

For present and future emerging pollutants in land and water resources management



**HEALS**

Health and Environment-wide Associations based on Large population Surveys



**EDC-MixRisk**

safe chemicals for future generations

Effects of mixtures of endocrine disruptive chemicals on children



Collaborative design and implementation of IPChemM tools

Project Community space in IPChemM

Contribution to the IPChemM Data Policy implementation

Collection of user/community requirements and feedback

Research outcomes storage and publication

*Collaboration with research consortia and international organisation*

# IPChEM and HBM4EU

- New HBM data
- Existing HBM data
- Enhanced data and metadata model and functionalities



- Dissemination of results
- Long-term repository
- Tool for data sharing
- Tool for data analysis
- Cross-media analysis

*Collaboration with research consortia and international organisation*



# IPChem<sub>and</sub> HBM-OECD database



## OECD HBM database

OECD high priority for: Provision of Knowledge and Information included “Methodologies for Exposure assessment - one inventory or database compiling exposure data or methodologies”

PILOT designed and developed by Health Canada (2015-2016)



Ongoing feasibility study on synergistic development and integration of HBM-OECD in IPChem

*Collaboration with research consortia and international organisation*

Please contact us:

[ipchem-support@jrc.ec.europa.eu](mailto:ipchem-support@jrc.ec.europa.eu)

## The IPChem team



### Scientific coordinator:

- Stylianos Kephelopoulos

### Technical coordinator:

- Silvia Dalla Costa

### Developing and support team:

- Alberto Cusinato
- Vittorio Reina
- Otmar Geiss
- Alexandre Zenié
- Anita Radovnikovic
- Salvatore Tirendi
- Paolo Leva

