

News on EURL DataPool Service

Outline

- **Accurate Mass Data DB**
- **PestiPedia**
- **Analytical Capabilities on Pesticides** (WD
SANCO/12745/2013 rev. 9(1))
- **Update of official sample scope**
- **CS2 Data Collection Project**
- **Outlier-Test in Method Validation DB**

EUPT Archive

Lab Network

Analytical Methods

Compound Stability

**EURL
DataPool
Service**

**Method Validation
Data**

Accurate Mass Data

NEW!

Compounds

Commodities

**MRL Residue
Definitions**

EUPT Archive

Lab Network

Analytical Methods

**EURL DataPool
Service**

Compound Stability

**Method Validation
Data**

**heavily relying on
contributions by
experts
from network!**

NEW!
Accurate Mass Data

Compounds

Commodities

**MRL Residue
Definitions**

Tools offered

Lab
Networking

Surveys

Search Tool for
Accurate Mass
Data

PestiPedia

Check
myScope

EUPT
Registration

MU Estimation
(based on PT-results &
validation data)

Calculation of
MRL Residue
Definition's Sum



EURL DataPool
Service

1. Go to „https://www.eurl-pesticides-datapool.eu“

1

http://www.eurl-datapool.eu/

2



Login

Create an Account About

EURL-DataPool

EU Reference Laboratories Residues of Pesticides

Home Reference Labs Tutorials

2. Click on „Login“

Welcome to EURL DataPool!

The **EURL DataPool website** has been created by the **EU Reference Laboratories (EURLs) for Residues of Pesticides** with the aim to provide information needed for proper decision-making in pesticide residue analysis.

The EURL DataPool website currently offers the following databases/views allowing systematic collection and online retrieval of pesticide-related data:

- Pesticide Compound DB
- Method Validation DB
- Lab Network DB (only accessible to members of the official EU-lab network)
- MRL Residue Definitions (issued by EU and Codex Alimentarius)
- Stability of Compounds in Solution
- List of Physicochemical Data
- My EUPT Results (EUPT data extracted from the EUPT Archive DB)
- Online-Tool for Estimation of Measurement Uncertainty based EUPT-results and method validation data (only accessible to NRL members)

Call for data submission: Numerous validation/pesticide stability experiments are being performed by various laboratories around the world. Nevertheless, there has traditionally been a lack of coordination in bringing this data together to allow overall data processing and assessment. This project aims to close this gap. **We thus greatly welcome and encourage any contributions.**

- If you would like to submit your method validation results, please take a look under [Submission of Method Validation Results](#).
- If you would like to submit your results of pesticide stability experiments, please download our template for data submission: [Submission of Compound Stability Data](#).

Accurate Mass DB | Search Tool



EURL-DataPool

1

[Home](#) [Compound Data](#) [Regulatory](#) [myLab](#) [EURL Network](#) [Administration](#) [Reference Labs](#)

[Compounds](#) [Accurate Mass Data](#) [Method Validation Data](#) [Stability of Compounds](#)

GC-High Reso

GC-High Resolution MS Data

LC-High Resolution MS Data

2

Experimental m/z in range from: to:

Compound

Compound Group

GC Amenable

Accurate Mass DB (GC) | Query

[Home](#) [Compound Data](#) [Regulatory](#) [myLab](#) [EURL Network](#) [Administration](#) [Reference Labs](#) [Tutorials](#)

Compounds ▾ Accurate Mass Data ▾ Method Validation Data ▾ Stability of Compounds ▾

GC-High Resolution MS Data

Experimental m/z in range from: to:

Select GC Ionization Mode ▾

Filter

Select GC Ionization Mode

EI (TOF)

EI (Orbitrap)

Compound	Compound Group	Matrix Eff
----------	----------------	------------

HRMS Data

Ametryn

Ametryn

Yes

No Data

HRMS Data

Disulfoton

Disulfoton

Yes

No Data

HRMS Data

EPN

EPN

Yes

No Data

HRMS Data

Fenoxycarb

Fenoxycarb

Difficult

No Data

HRMS Data

Flubenzimine

Flubenzimine

Yes

No Data

HRMS Data

Mefenpyr-Diethyl

Mefenpyr

Yes

No Data

HRMS Data

Mefentrifluconazole

Mefentrifluconazole

No Data

HRMS Data

Metamitron

Metamitron

Difficult

No Data

Accurate Mass DB (GC) | Query

Home Compound Data Regulatory myLab EURL Network Administration Reference Labs Tutorials

Compounds Accurate Mass Data Validation Data Stability of Compounds

GC-High Resolution MS Data

Experimental m/z in range from: 200.00000 to: 201.05000

Select GC Ionization Mode
EI (TOF)
EI (Orbitrap)

Filter

	Compound	Compound Group		Matrix Eff
HRMS Data	Atrazine	Atrazine	Yes	No Data
HRMS Data	Butamifos	Butamifos	Yes	
HRMS Data	DDD, o,p-	DDT	Yes	
HRMS Data	DDD, p,p-	DDT	Yes	
HRMS Data	DDT, o,p-	DDT	Yes	
HRMS Data	Diclobutrazol	Diclobutrazol	Yes	
HRMS Data	Edifenphos	Edifenphos	Yes	No Data
HRMS Data	Ethoprophos	Ethoprophos	Yes	No Data
HRMS Data	Fenpiclonil	Fenpiclonil	Yes	No Data

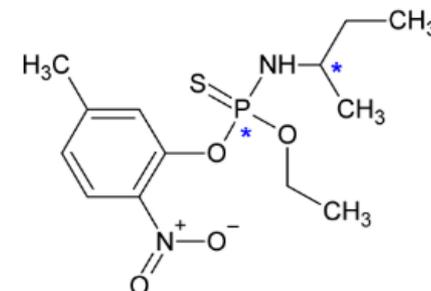


Accurate Mass DB (GC-HRMS) | Result of Query

Butamifos

GC-High Resolution MS

Molecular Formula	C13H21N2O4PS
Monoisotopic Mass [g/mol]	332.09596
GC-Amenable	Yes
Matrix Effects	
Tailing	
GC Decomposition	



Theoretical Ion Mass	Fragment Ion	Ionization Mode	Ion Formula	Remark	Reference
286.102513	Fragment 1	EI (TOF)	C13H21NO2PS		EURL-CF
258.071212	Fragment 2	EI (TOF)	C11H17NO2PS		EURL-CF
231.982791	Fragment 3	EI (TOF)	C7H7NO4PS		EURL-CF
200.010721	Fragment 4	EI (TOF)	C7H7NO4P		EURL-CF
286.102514	Target	EI (Orbitrap)	[C13H21NO2PS]+	Is NOT a molecular ion	EURL-SRM; RIKILT
258.071214	Fragment 1	EI (Orbitrap)	[C11H17NO2PS]		EURL-SRM; RIKILT
231.982794	Fragment 2	EI (Orbitrap)	[C7H7NO4PS]		EURL-SRM; RIKILT
200.010722	Fragment 3	EI (Orbitrap)	[C7H7NO4P]		EURL-SRM; RIKILT

Reference

Title: Compilation of GC-Orbitrap MS Data (2018)

Data Type: Submitted Lab Data

Author: EURL-SRM

Email Address: eurl-srm@cvuas.bwl.de

Website: <http://www.eurl-pesticides.eu>

Author: Dr. J.G.J (Hans) Mol

Institute: RIKILT Wageningen University & Research

Website: <http://www.wur.nl/rikilt>

Accurate Mass DB (LC-HRMS) | Result of Query

Home Compound Data Regulatory myLab EURL Network Administration Reference Labs Tutorials

Compounds Accurate Mass Data Method Validation Data Stability of Compounds

LC-High Res **LC-High Resolution MS Data**

Experimental m/z in range from: 56.00000 to 1000.00000 Select LC Ionization Mode Filter

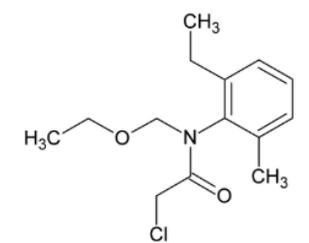
Compound	Compound Group	LC/MS Amenable
Acephate	Acephate	Yes
Acequinocyl	Acequinocyl	Yes
Acetamiprid	Acetamiprid	Yes
Acetamiprid, N-de	Acetamiprid, N-de	Yes
Acetochlor	Acetochlor	Yes
Fluthiacet	Fluthiacet	Yes
Fluthiacet, nyl	Fluthiacet, nyl	Yes
Mefenacet	Mefenacet	Yes

HRMS Data

Acetochlor

LC-High Resolution MS

Molecular Formula	C14H20ClNO2
LC/MS-Amenable	Yes
Remark	



Theoretical Ion Mass Ion Type Ionization Mode Ion Formula Remark Reference

270.1255	Molecular Ion, [M+H] ⁺	ESI(+)	C14H21ClNO2	fragment 224 > molecular ion; same RT and m/z as Alachlor	
148.1121	Fragment 1	ESI(+)	C10H14N		
133.0886	Fragment 2	ESI(+)	C9H11N		
224.0837	Fragment 3	ESI(+)	C12H15ClNO	fragment 224 > molecular ion	

(Cooperation with Swedish NRL (National Food Agency, Sweden) is ongoing.)

Take Home Message

**Online-Search for HR-MS data
is available.
Submission of HR-MS data is
highly welcome!**



PestiPedia

Home

Observations on Properties of Pesticides ▾

Compilation of CS2 Data ▾

Additional Info ▾

Welcome to PestiPedia!

PestiPedia was designed to make compilation of data relevant to pesticide residue analysts straightforward.
Find below information about ongoing projects:

- Cooperation with **WG on Pesticides of the German Chemical Society (“AG Pestizide”)**
- **pesticide-residue-experts** can make **contributions** to aspects that are relevant in pesticide residue analysis.
- individual contributions will be discussed by registered experts and the outcome will be imported into the EURL DataPool

1

List of Compounds

To search for a specific compound, click on the "Advanced Search"-feature (see below), choose the column that should be searched through, add the filter text and click on the „Add" button.

Click on the link "Open" in the column "Datasheet" in order to make your contributions to this compound.

2

Showing 1-100 of 1423 [Advanced Search](#)

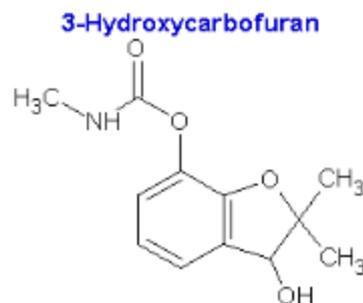
100 per page

Page 1 of 15



Datasheet	Compound	Compound Group	Pesticide Property	Status
Open	1,2-Benzisothiazol-3(2H)-one	1,2-Benzisothiazol-3(2H)-one	No Data	
Open	1-MCP	1-MCP	Neutral interm. polar (pKow 0.5-4.5)	
Open	2,4,5-T	2,4,5-T	Potentially anionic	
Open	2,4,5-T-Methylester	2,4,5-T	Neutral interm. polar (pKow 0.5-4.5)	
Open	2,4,5-TP	2,4,5-TP	Potentially anionic	
Open	2,4-D-Methylester	2,4-D	No Data	Prio I
Open	2,4-D	2,4-D	Potentially anionic	Prio I

3-Hydroxycarbofuran



Choose one of the buttons below to make your contribution to a specific topic:

[Stability of Pure/Neat Standards](#)[Stability of Standard Solutions](#)[Stability in Matrix-Extracts](#)[LC-MS Behaviour](#)[GC Behaviour](#)[Losses during Extraction/Cleanup](#)[Practical/Legal Aspects](#)

Stability of Pure/Neat Standards

Stability of Standard Solutions

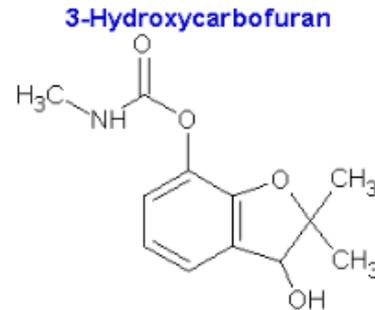
Stability in Matrix-Extracts

LC-MS Behaviour

1

3-Hydroxycarbofuran

[More Details from DataPool](#)



Existing Data

LC-MS Ame

Remark

To add NEW or ADDITIONAL data sets on LC-MS Behaviour, click on the buttons below:

General Info

Ionization, Fragmentation & Identification

Compromized Identification and Interferences

Sensitivity

To see Your Contribution(s) or the Compilation of all contributions collected on "LC-MS Behaviour"

Tab UR contributions show the prefix "Yours". Your contributions have

Open here the form to make comments on e.g. "Sensitivity".

2

PestiPedia | Form to Enter Observations

Observations on LC-MS Behaviour - Sensitivity close

When submitting data on SENSITIVITY, please always provide relevant info on commodity group, extraction method and detection system. In the case of MS or MS/MS please also indicate the mass, accurate mass, or mass transition to which each sensitivity statement applies.

Commodity Group(s)

- PO - High Water Content
- PO - High Acid Content
- PO - High Oil Content, wet, (e.g. avocado, olives)
- PO - High Oil Content, dry, (e.g. oily seeds, nuts)
- PO - Specific Commodities (e.g. dry herbs, spices, tea)
- AO - Muscle
- AO - Fat
- AO - Kidney
- AO - Liver
- AO - Eggs
- AO - Honey
- AO - milk
- all
-

Choose the commodity groups to which the sensitivity statement applies. (PO: Plant Origin; AO: Animal Origin)

Example Commodities
(If the sensitivity statement applies to individual commodities rather than commodity groups, please name them here.)

Ionization Mode *

Detector *

Remark
(e.g. method applied, model of instrument used)

Sensitivity
For the selected commodity/ies this compound typically gives well quantifiable signals for the mass(es) at the following concentration (C):

Ions / MS/MS-Transition(s) / Accurate Mass(es) Used (1)	Sensitivity (1)
<input type="text" value="252,1365"/>	<input type="text" value="+++ (0.002 < C ≤ 0.005 mg/kg)"/>
... (2)	Sensitivity (2)
<input type="text" value="192,1654"/>	<input type="text" value="+++ (0.005 < C ≤ 0.01 mg/kg)"/>
... (3)	Sensitivity (3)

PestiPedia | Contributions to Specific Topics

Stability of Pure/Neat Standards

Stability of Standard Solutions

Stability in Matrix-Extracts

LC-MS Behaviour

1

Losses during Extraction/Cleanup

Practical/Legal Aspects

3-Hydroxycarbofuran

[More Details from DataPool](#)



Existing Data from EURL DataPool:

LC-MS Amenable Yes

Remark

To add NEW or ADDITIONAL data sets on LC-MS Behaviour, click on the buttons below:

+ General Info

+ Ionization, Fragmentation & Identification

+ Compromized Identification and Interferences

+ Sensitivity

To see Your Contribution(s) or the Compilation of all contributions collected so far on "LC-MS Behaviour", click on the TABS below:

Tabs with YOUR contributions show the prefix "Yours". You can edit your data sets by clicking on "Edit". Tabs with the compilation of ALL contributions have the prefix "All".

Yours - General Info

ALL - General Info

Yours - MS Ionization

ALL - MS Ionization

Yours - Interferences

ALL - Interferences

Yours - Sensitivity

ALL - Sensitivity

ALL - Sensitivity

[Advanced Search](#) [export](#)

User	Compound	Ionization Mode	Detector	Remark	Ions / MS/MS-Transition(s) / Accurate Mass(es) Used (1)	Sens. (1)	Ions/... (2)
Norbert	3-Hydroxycarbofuran	ESI (neg)	Triple Quad.	bad reproducibility of Peak area in ESI (neg) mode			
Sabine	3-Hydroxycarbofuran	ESI (pos)	(Q-)Orbitrap (High Resol.)	§64 L00.00 115/1 Q-Exactive	260,08933	+++ (0.005< C ≤0.01 mg/kg)	

PestiPedia | Practical/Legal Aspects

Stability of Pure/Neat Standards

Stability of Standard Solutions

Stability in Matrix-Extracts

LC-MS Behaviour

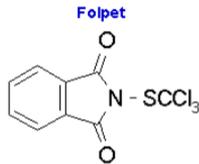
GC Behaviour

Losses during Extraction/Cleanup

Practical/Legal Aspects

Folpet

[More Details from DataPool](#)



1

To add NEW or ADDITIONAL data sets on Practical/Legal Aspects, click on the button below:

[Add New Data on Practical/Legal Aspects](#)

To see Your Contribution(s) or the Compilation of all contributions collected so far on "Practical/Legal Aspects", click on the TABS below:

Tabs with YOUR contributions show the prefix "Yours". You can edit your data sets by clicking on "Edit". Tabs with the compilation of ALL contributions have the prefix "All".

Yours - Practical/Legal Aspects

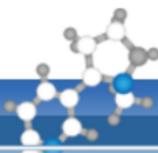
ALL - Practical/Legal Aspects

2

ALL - Practical/Legal Aspects

Advanced Search

User	Compound	Name Relevant Commodities for this Compound	Compound Originates from Other Sources	Remark (Other ...)	Compound or Degradation Products thereof may Originate from a
Anna	Folpet	hops, wine	Generated from the degradation of other pesticides, From a non-pesticide related contamination, As a natural product in food, Formed during food processing, Formed as an artefact in GC inlet, Formed as an artefact during Extraction, Formed as an artefact during Cleanup	under "Compound Originates from Other Sources" phthalimide, the metabolite of folpet is meaning:	drifts of phthalic acid from fruit plantations (Captan, Folpet applications) the prevalent presents of phthalic acid during drying is possible
Andreas	Folpet	processed dried food product			
Günter	Folpet	Herbs and spices, tea, fruit and herbal teas, processed (dried) food products		Phthalimid (PI) as the major metabolite might derive from environmental impact (Phthalic anhydrid or Phthalic acid) and might be formed during processing of food products and during injection process in GC.	



You are here: [Home](#) : Single Residue Methods

- [EURL Portal](#)
- [EURL for Fruits and Vegetables](#)
- [EURL for Cereals and Feeding Stuff](#)
- [EURL for Food of Animal Origin](#)
- [EURL for Single Residue Methods](#)



- Topics**
- [EURL-SRM Network](#)
NRL-SRM Network
 - [Proficiency Tests](#)
EUPT-SRM Overview
EUPT-SRM12 (Straw)
EUPT-SRM11 (Spinach)
EUPT-SRM10 (Corn)
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Workshop AO/SRM
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ILISS Distribution Service
Check Your Scope-Service
SRM-Board Service
List of methods
List of observations
Downloads
 - [Interest](#)
EURL DataPool
EURL DataPool (Test)
QuEChERS - Website

PestiPedia

Login

Enter your email address and password to login.

Email Address

Password (forgot?)

Remember me

Sign In



Metabolite AMTT by QuEChERS Method using LC-MS/MS

Interested?

Please contact:

eurl-srm@cvuas.bwl.de



[Analysis of Residues of Carbofuran - Analytical Observations and Method Report](#)
 Analysis of Carbofuran by QuEChERS methodology - an Analytical Observations Report and a Method Protocol

Take Home Message

**PestiPedia = website to share
experiences/observations/...
with other pesticide experts.
Give/Take-Concept!**



Collection of CS₂-Findings non-Originating from DTC-Pesticides

- Re-evaluation of dithiocarbamate-MRLs is planned for 2019
- DTCs are usually analyzed by using **common moiety methods involving the release of carbon disulfide (CS₂)** via an acid digestion/hydrolysis step (using a mixture of tin(II)-chloride and hydrochloric acid)
- Some crops **naturally contain compounds** (e.g. mustard oil glycosides) **that do release CS₂** (either spontaneously or) during the digestion/hydrolysis step of DTC analysis (=> background CS₂-levels):
 - crops belonging to *Brassicaceae* + *Alliaceae* family
 - Papaya

CS₂-Background Levels | Some Results

Common Name	Genus	MRL (CS ₂) [mg/kg]	CS ₂ Findings by the EURL-SRM			
			[mg/kg]			
			n	Homogenized and analyzed frozen	Homogenized at room temp. and analyzed after ...	
					15 min	2 h
Arugula (rocket/rucola)	Eruca	5	3	0,37±0,06 - 0,82±0,08	2,6±0,07 - 8,33±0,3	2,2±0,2 - 7,24±0,9
Caper	Capparis	25				
Caper Berries (canned)			1		1,40	
Brine of Caper Berries (canned)			1		0,35	
Capers (edible flower buds; canned)			1		5,24	
Brine of Capers (...)			1		0,20	
Cabbage	Brassica	Head cabbages: 3	1	0,18±0,004	0,23±0,02	0,20±0,05
Cauliflower	Brassica	1	1	0,08±0,01	0,12±0,02	0,07±0,01
Champignon mushroom	Agaricus	0.05*	1	≤0,01	≤0,01	≤0,01
Chinese cabbage, napa cabbage	Brassica	Chinese cabbages/pe-tsai: 0,5	1	0,08±0,01	0,15±0,04	0,11±0,02
Collard greens	Brassica	Kales: 0,5				
Garden cress	Lepidium	Cresses and other sprouts and shoots: 5,0	1	(≈1,1)	(≈5,9)	(≈3,6)
Moringa	Moringa	0.1*Processing Factor 0.1 (from 2018 onwards)	7		0,70±0,08 – 11,2±0,09	

CS₂-Background Levels | Some Results

Common Name	Genus	MRL (CS ₂) [mg/kg]	CS ₂ Findings by the EURL-SRM			
			[mg/kg]			
			n	Homogenized and analyzed frozen	Homogenized at room temp. and analyzed after ...	
15 min	2 h					
Mustard	Brassica	seeds: 0,1*				
Black mustard seeds	Brassica	seeds: 0,1*	1		0,93	
Table Mustard (medium-strength)	Brassica	seeds: 0,1*	1		30	
Table Mustard (hot)	Brassica	seeds: 0,1*	1		263	
Radish (black)	Raphanus	2	1	0,17±0,02	1,22±0,05	1,1±0,03
Radish (white)		2	1	0,04±0,01	0,22±0,09	0,22±0,07
Turnip cabbage	Brassica	1	1	0,012	0,09±0,1	0,05±0,03
May turnip	Brassica		1	0,38±0,03	0,59±0,04	0,7±0,1
Onions	Allium	1	2	0,09±0,02	0,055±0,003	0,055±0,006
Shallots	Allium	1	1	0,24±0,03	0,24±0,01	0,25±0,03
Spring onions/green onions and Welsh onions	Allium	1	1	0,15±0,01	0,07±0,006	0,09±0,01

=> Need to collect data on non-pesticide related CS₂ levels of ORGANIC products

CS₂-Background Levels | Priority List (by EFSA & EURL-SRM)

Final Decision	Keep Product	Priority	on CS ₂ relevance	Confirmation by UPL-experiments	EFSA conclusion whether further data need to be generated to derive MRL proposal	Crop suspicious to CS ₂ -release from matrix during	Based on EFSA data	Based on EURL-SRM	Based on other Info	Product Name	SUMMARY of CS ₂ -Results submitted by EFSA, EURL-SRM and other sources					EU monitoring 2013/2014/2015 (EFSA)			MRLs		CS ₂ -Findings by EURL-SRM [mg/l]		
											CS ₂ -Commodity Group	N° of samples to be analyzed (group OR individual)	N° of samples still to be analyzed	% positive CS ₂ -samples (only calc. for n>5)	Total-N° of CS ₂ -Results >LOQ	Total-N° of organic-samples analyzed for CS ₂	# of CS ₂ results MACP13-16	# of CS ₂ results >0.01 MACP13-16	Max. Conc. MACP13-16	Dithiocarbamates (DTC expr. as CS ₂ , including maneb, mancozeb, metiram, propineb, thiram)	# of samples analyzed	# of pos. samples (>LOQ)	Homogenized and analyzed frozen
X	high	Strong		Y (2)	Yes	Strong	Flowering brassica	Brassica (flower)	59	36	65.2	15	23	23	15	0.52	1 (F)						
X	high	Strong				Strong	Broccoli	Brassica (flower)	59	59		0	0										
X	high	Strong				Strong	Calabrese	Brassica (flower)	59	59		0	0										
X	high	Strong				Strong	Chinese broccoli/kai-lan	Brassica (flower)	59	59		0	0										
X	high	Strong				Strong	Choi sumtsoi sam	Brassica (flower)	59	59		0	0										
X	high	Strong				Strong	Rapini/brocchetto/broccoli	Brassica (flower)	59	59		0	0										
X	high	Strong	Yes	Y (2)	Yes	Strong	Cauliflowers	Brassica (flower)	59	56		1	3										
X	high	Strong				Strong	Romanesco cauliflowers	Brassica (flower)	59	59		0	0	2	0		1 (F)		1	0.08±0.01	0.12±0.02	0.07±0.01	
X	high	Strong		Y (2)		Strong	Other flowering brassica	Brassica (flower)	59	59		0	0				1 (F)						
X	high	Strong				Strong	Head brassica	Brassica (leaf)	59	59		0	0										
X	high	Strong		Y (2)		Strong	Brussels sprouts	Brassica (leaf)	59	58		1	1	1	1	5.39	2 (F)						
X	high	Strong				Strong	Flower sprouts	Brassica (leaf)	59	59		0	0										
X	high	Strong	Yes	Y (2)	Yes	Strong	Head cabbages	Brassica (leaf)	59	32	40.7	11	27	26	10	0.41	3 (F)	1	1	0.18±0.004	0.23±0.02	0.20±0.05	
X	high	Strong				Strong	Pointed head cabbages	Brassica (leaf)	59	59		0	0										
X	high	Strong				Strong	Red cabbages	Brassica (leaf)	59	59		0	0										
X	high	Strong				Strong	Savoy cabbages	Brassica (leaf)	59	59		0	0										
X	high	Strong				Strong	White cabbage	Brassica (leaf)	59	59		0	0										

Priority # of crops Exemplary crops

High

91

Radish, turnips, broccoli, cauliflower, caper, papaya, guava

Medium

46

Figs, sweet potatoes, pomegranate, mango, maracuja, chamomile, ginger

Low

186

Almonds, berries & small fruits, avocado, lentil

>5300 organically grown crops have theoretically to be analyzed to quantify CS₂-background levels (*)



(*) For relevant commodities data from 59 samples is needed

PestiPedia

Home

Observations on Properties of Pesticides

Compilation of CS₂ Data

Additional Info

Products Intended to be Analyzed for CS₂

Cs₂ Intended Products Evaluation

Welcome to PestiPedia!

PestiPedia was designed to make the compilation of data relevant to value analysts straightforward.

Find below information and links to currently ongoing projects.

Compilation of Carbon Disulphide

A large number of commodities naturally contain CS₂. Some of these compounds cannot be detected and evaluating CS₂-levels more reasonably.

In 2017, the EURL-SRM and EFSA jointly elaborated a list of crops suspicious to release CS₂ during analysis. This list was distributed to regional control programs.

You can enter the number of samples you intend to analyze for CS₂ by using the following link:

Number of Samples Intended to be Analyzed for CS₂

Select „Products Intended to be Analyzed for CS₂“ from the tab „Compilation of CS₂ Data“.

CS₂-Background Levels | Coordination via PestiPedia

Products Intended to be Analyzed for CS₂

The table "Number of samples you intend to analyze for CS₂" will be evaluated and a coordination will take place to ensure good representation of important products.

You can use [this link](#) to get an actual list of products intended to be analyzed for CS₂.

Preferably enter the number of samples you intend to analyze for CS₂.

Number of samples you intend to analyze for CS₂

How to proceed?

(1) Search for a product by using the search function.

(2) Click into the column "Number of samples you intend to analyze for CS₂".

In case you do not find a product in the list, you can click on the link "Add new product" and fill in the necessary information.

[Click here, in case you do not find a product in the list.](#)

E.g. Search for products of high priority.

All products of high priority are listed.

1.

high

Showing 1-31 of 31 [Advanced Search](#) [export](#)

Product Code	Product Group	Product	Priority	Number of samples your lab intends to analyze for CS ₂
0251080-000	Baby leaf crops (including brassica species)	Baby leaf crops (including brassica species)	High	
0241010-000	Broccoli	Broccoli	High	6
0242010-000	Brussels sprouts	Brussels sprouts	High	
0850020-000	Capers	Capers	High	
0241020-000	Cauliflowers	Cauliflowers	High	
0243010-000	Chinese cabbages/pe-tsai	Chinese cabbages/pe-tsai	High	
0256020-000	Chives	Chives	High	
0251070-000	Cress and other sprouts and shoots	Cress and other sprouts and shoots	High	

2.

Background CS₂-Levels | Results

N° of participating labs	N° of different crops intended to be analyzed by Member State	N° of samples intended to be analyzed per crop-priority		
		High	Medium	Low
11	34	194	16	39

Could be shifted to crops of higher priority!



Background CS₂-Levels | Results

Crop	Number of samples to be analyzed					N° of intended samples to be analyzed per Member State
	Required	Done	Missing	Intended to be analyzed	Still missing	
Broccoli	59	23	36	28	8	DE (23), GR (4), PT (1)
Brussels sprouts	59	1	58	1	57	PT (1)
Cauliflowers	59	3	56	27	29	DE (22), GR (4), PT (1)
Chinese cabbages	59	2	57	13	44	DE (12), PT (1)
Chives	59	0	59	2	57	DE (2)
Cress & similar	59	2	57	1	56	PT (1)
Garlic	59	1	58	5	53	DE (5)
Head cabbages	59	27	32	7	25	DE (3), GR (4)
Horseradishes	59	0	59	1	58	PT (1)
Kales	59	1	58	6	52	DE (6)
Kohlrabies	59	2	57	9	48	DE (9)
Land cress	59	0	59	5	53	DE (5)
Leeks	59	62	/	23	-	DE (21), PT (2)
Onions	59	10	49	10	39	DE (4), GR (4), PT (2)
Papayas	59	1	58	21		DE (20), PT (1)
Parsnips	59	0	59	5	5	DE (5)
Radishes	59					
Rucola	59					
Spring onions	59					
Turnips	59					

Enough CS₂-background data for leek!

EURL DataPool is used to run surveys:

- **Update of Sample Scope** by OFLs
-> invitation will be sent at the end of October
- **Survey on Analytical Capabilities** (currently ongoing)

Surveys on Analytical Capabilities

- Surveys conducted on behalf of COM (2016, 2017, 2018 (ongoing))
- **Goal of Surveys:**
how many EU-OFLs **routinely analyze for full residue definition of pesticides** that are included in MACP Working Document (chapter 4 of SANCO/12745/2013 Rev)?
- **Participation (FV-OFLs):** 69 % in 2017
51 % in 2016

Survey on Analytical Capabilities | Survey 2018 is ongoing

Official Control Program (MACP; national; regional) for Germany - Edit Individual Pesticides here

✓ Save changes

⊘ Cancel changes

Official Controls

Survey	Compound Group	Compound	Within Lab Scope	Routinely Analyzed
Yes <input checked="" type="radio"/> No <input type="radio"/>	<input type="text"/>	<input type="text"/>	Yes <input type="radio"/> No <input type="radio"/>	Yes <input type="radio"/> No <input type="radio"/>
Yes	Amitraz	Dimethylphenylformamide, 2,4-	Yes	Yes
Yes	Amitraz	Dimethylanilin, 2,4-	No	<input checked="" type="checkbox"/>
Yes	Amitraz	Amitraz	Yes	Yes
Yes	Amitraz	Dimethylphenyl-N-methylformamidine, N-2,4-	Yes	Yes
Yes	Amitraz	Amitraz (sum: following hydrolysis)	Yes	Yes

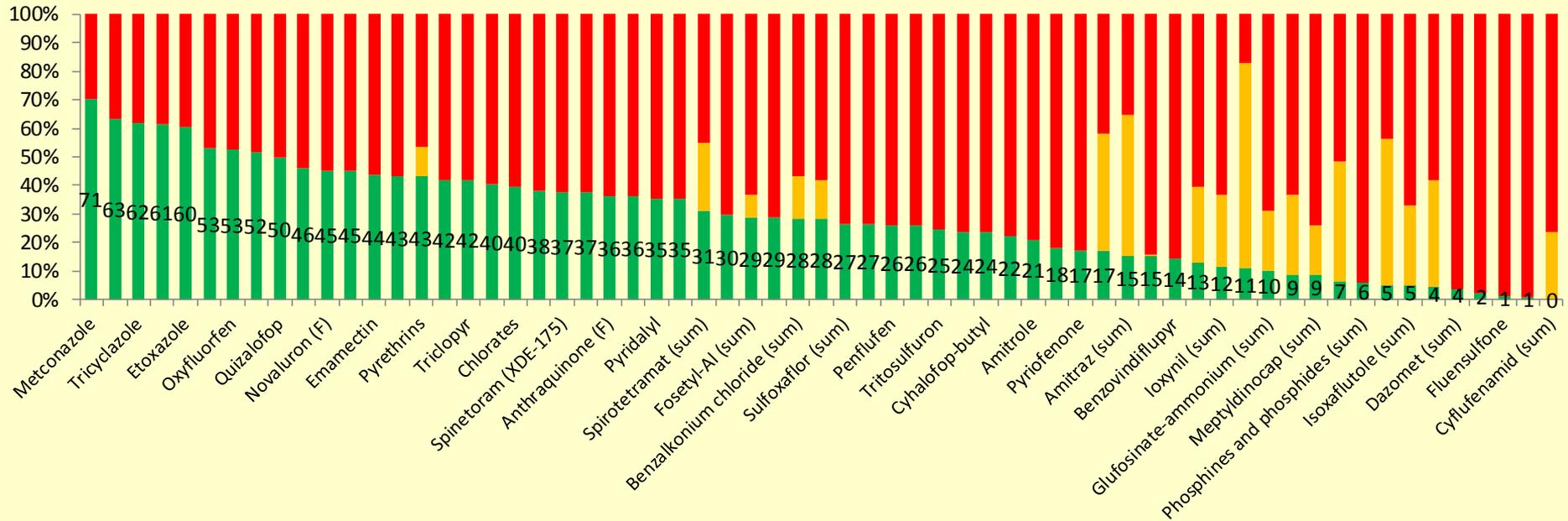
Detailed instructions were sent to participants.

We hope for a lively participation!

Survey on Analytical Capabilities: Results from 2017-Survey

% of official EU-Pesticide Labs analyzing for ... (n = 139; PLANTS)

■ Full RD ■ Partial RD ■ Not Analyzing RD



Survey on Analytical Capabilities: Results from 2017-Survey

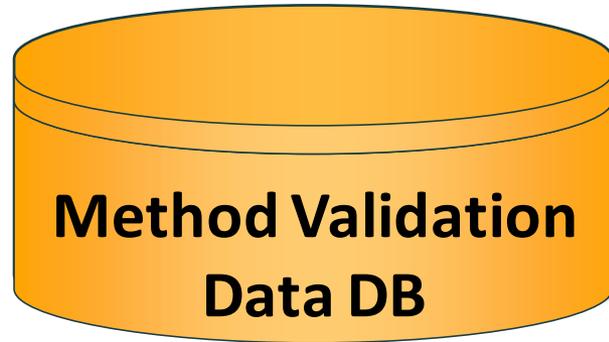
- **FULL RD** is covered by $\geq 70\%$ of participating OFLs
 - Metconazole
- **FULL RD** is covered by $\geq 50\%$ and $< 70\%$ of participating OFLs
 - Metrafenone (F)
 - Tricyclazole
 - Cyazofamid
 - Etoxazole
 - Glyphosate
 - Oxyfluorfen
 - Proquinazid (R)

Survey on Analytical Capabilities: Results from 2017-Survey

- FULL RD is covered by **less than 20%** of participating OFLs:
in total: 22 compounds; excerpt from the list:

RDs	# of OfLs intending to introduce RD/compound in 2018
Oxasulfuron	18
Pyriofenone	10
Amitraz (not approved)	DMF: 6; Amitraz: 5; DMPF: 6
MCPA and MCPB	Various MCPA esters: 4 MCPA: 2 MCPB: 3
Benzovindiflupyr	15
loxynil (sum of loxynil, its salts and its esters, expressed as loxynil (F))	loxynil: 5 loxynil-heptanoate: 4 loxynil-octanoate: 5
Bifenazate	Bifenazate: 4 Bifenazate-Diazene: 15
Sulfuryl fluoride	6
Fluensulfone	11
Cyflufenamid: sum of cyflufenamid (Z-isomer) and its E-isomer	0

Method Validation DB



- ≈500.000 recoveries
- submitted by 46 labs



EURL-DataPool

EU Reference Laboratories for Residues

[Home](#) [Compound Data](#) [Regulatory](#) [myLab](#) [EURL Network](#) [Administration](#) [Reference Labs](#) [Tutorials](#)

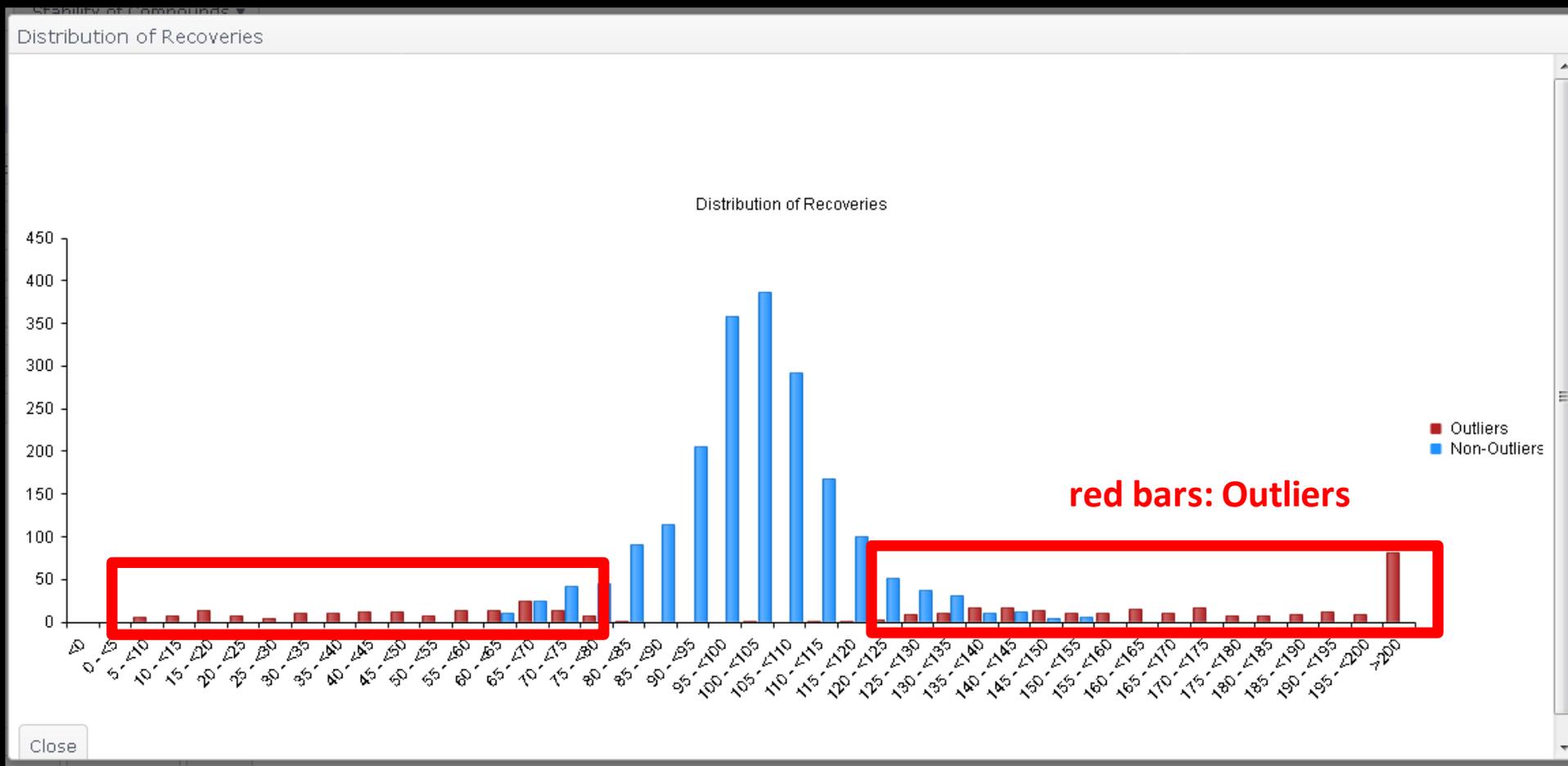
Compounds ▾ Method Validation Data ▾ Stability of Compounds ▾

Detailed Query

Commodity Information	Method Information	Compound Information
Commodity <input type="text" value="Search Commodity (min. 3 chars)"/>	Extraction Method <input type="text" value="Select..."/>	Compound (spiked) <input type="text" value="1,8-Diaminooctane"/>
Commodity Group <input type="text" value="Select..."/>	Spiking Step <input type="text" value="Select..."/>	Spiking Level From <input type="text" value="Select..."/>
Water Content <input type="text" value="Select..."/>	Extraction pH <input type="text" value="Select..."/>	Spiking Level To <input type="text" value="Select..."/>
Fat Content <input type="text" value="Select..."/>	ISTD <input type="text" value="Search ISTD (min. 3 chars)"/>	
Sugar Content <input type="text" value="Select..."/>	ISTD Addition Step <input type="text" value="Select..."/>	General Information
pH Value <input type="text" value="Select..."/>	Cleanup <input type="text" value="Select..."/>	Lab <input type="text" value="Search Lab (min. 3 chars)"/>
	Cleanup Details <input type="text" value="Select..."/>	Date From <input type="text"/>
	Post Cleanup Details <input type="text" value="Select..."/>	Date To <input type="text"/>
	Chromatography <input type="text" value="Select..."/>	Validation Context <input type="text" value="Select..."/>
	Interface <input type="text" value="Select..."/>	Context Details <input type="text"/>
	Calibration <input type="text" value="Select..."/>	Exclude Outliers <input type="checkbox"/>
	Calibration Details <input type="text" value="Select..."/>	Experiment No. <input type="text"/>

[Detailed Result List](#) [Aggregate by Spiking Level](#) [Recoveries](#) [Clear](#)

Method Validation DB | Distribution of Recoveries



Query:

- Extraction Method: QuPPE
- Water Content: 30-80%
- Exclude Outliers: No

Outlier – How do we calculate the Outliers?

- Grubbs Outlier Test:
 - Recoveries: 95% | 98% | 96% | 97% | 90% (=> outlier)
-> too strict for pesticide residue analysis!

1. Group the data by
 - Compound
 - Extraction Method
 - Commodity Group (according to AQC Guideline)
 - Extraction pH (of method)
 - Cleanup Principle
2. Exclude groups with less than 5 recoveries
3. Calculate the median for each group: “**Global Median**”
(only for groups with $n(\text{labs}) > 2$)

4. Compare “Global Median” with Experiment-Median:

- $N(\text{recoveries}) > 2$:

if Experiment-Median $> 1 + 0.4 * \text{“Global Median”}$

OR

if Experiment-Median $> 1 - 0.4 * \text{“Global Median”}$

then whole Procedure \Rightarrow outlier

- $N(\text{recoveries}) < 3$:

if Experiment-Median $> 1 + 0.6 * \text{“Global Median”}$

OR

if Experiment-Median $> 1 - 0.6 * \text{“Global Median”}$

then whole Procedure \Rightarrow outlier

- All recoveries $< 1 \Rightarrow$ outliers

5. Calculate the “Global Rel. Standarddeviation” (**Global RSD**) for each group:
 - Group the data by
 - Compound
 - Extraction Method
 - Commodity Group (according to AQC Guideline)
 - Extraction pH (of method)
 - Cleanup Principle

6. Compare the “**Global RSD**” with recovery-data set belonging to each group:
- For **Global RSD \leq 10%**
 - If recovery $<$ Global Median $\cdot (1 - 3 \cdot \text{Global RSD}/100) \Rightarrow$ outlier
 - If recovery $>$ Global Median $\cdot (1 + 3 \cdot \text{Global RSD}/100) \Rightarrow$ outlier
 - For **Global 10% $<$ RSD \leq 25 %**
 - If recovery $<$ Global Median $\cdot (1 - 2 \cdot \text{Global RSD}/100) \Rightarrow$ outlier
 - If recovery $>$ Global Median $\cdot (1 + 2 \cdot \text{Global RSD}/100) \Rightarrow$ outlier
 - For **Global RSD $>$ 25 %**
 - If recovery $<$ Global Median $\cdot (1 - 1 \cdot \text{Global RSD}/100) \Rightarrow$ outlier
 - If recovery $>$ Global Median $\cdot (1 + 1 \cdot \text{Global RSD}/100) \Rightarrow$ outlier

- Search Tool for **Accurate Mass Data**
- **PestiPedia** = Tool to share experiences with other pesticide experts
- EURL DataPool is used to **run surveys**:
 - Analytical Capabilities on Pesticides
 - Update of official sample scope
- **Outlier-Test** in Method Validation DB:
-> open for discussion/contributions

**Thank You
for Your Attention**



www.eurl-pesticides-datapool.eu