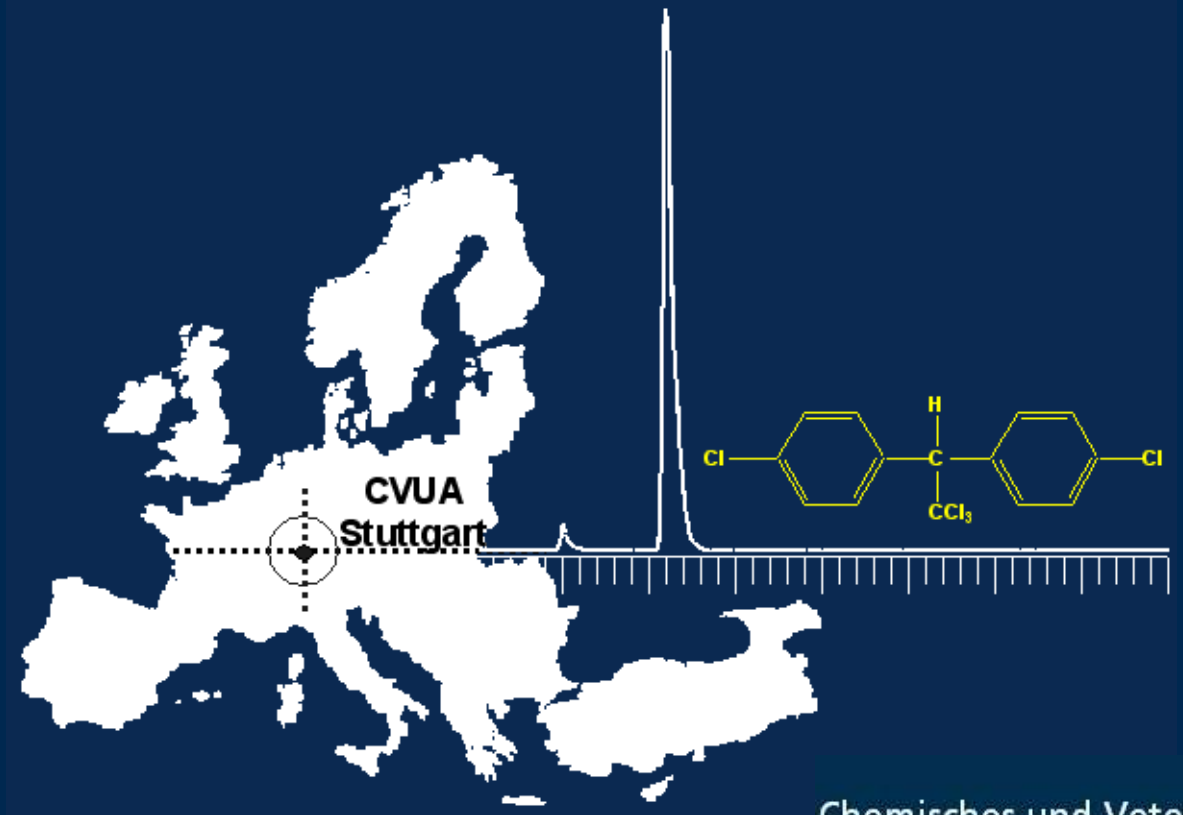
CRL-SRM

Working Plan and Lab Presentation



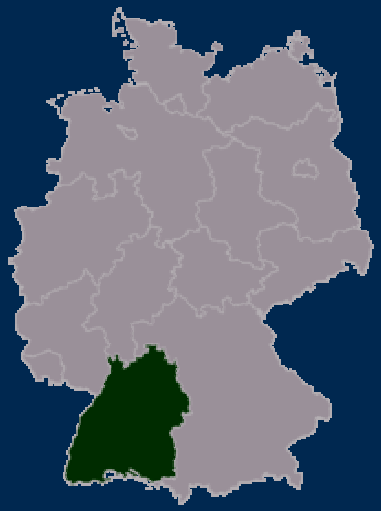
Michelangelo
Anastassiades

Chemisches und Veterinäruntersuchungsamt | Stuttgart

Our Laboratory - Development

Up to 2001:
Regional Lab (4 mio)

Since 2002:
Central Lab (10 mio)



From 2006 on:
EU-CRL (380 mio)

Mainly Routine
Surveillance Work

More Personnel ➔ Specialization

- Research
- Strategy Work
- International Activities (EU, CODEX etc.)
- Dissemination of Knowledge

Our Laboratory - Some Numbers…

Entire CVUA:

ca. 240 Employees, ca. 24,000 Samples per Year, Budget: ca. 13 mio. €

Pesticide Residue Section (Food of Plant Origin) :

22 Employees (6 Chemists+16 Technicians),
ca. 2500 Samples / Year (mainly fresh produce)

Analytical Instruments

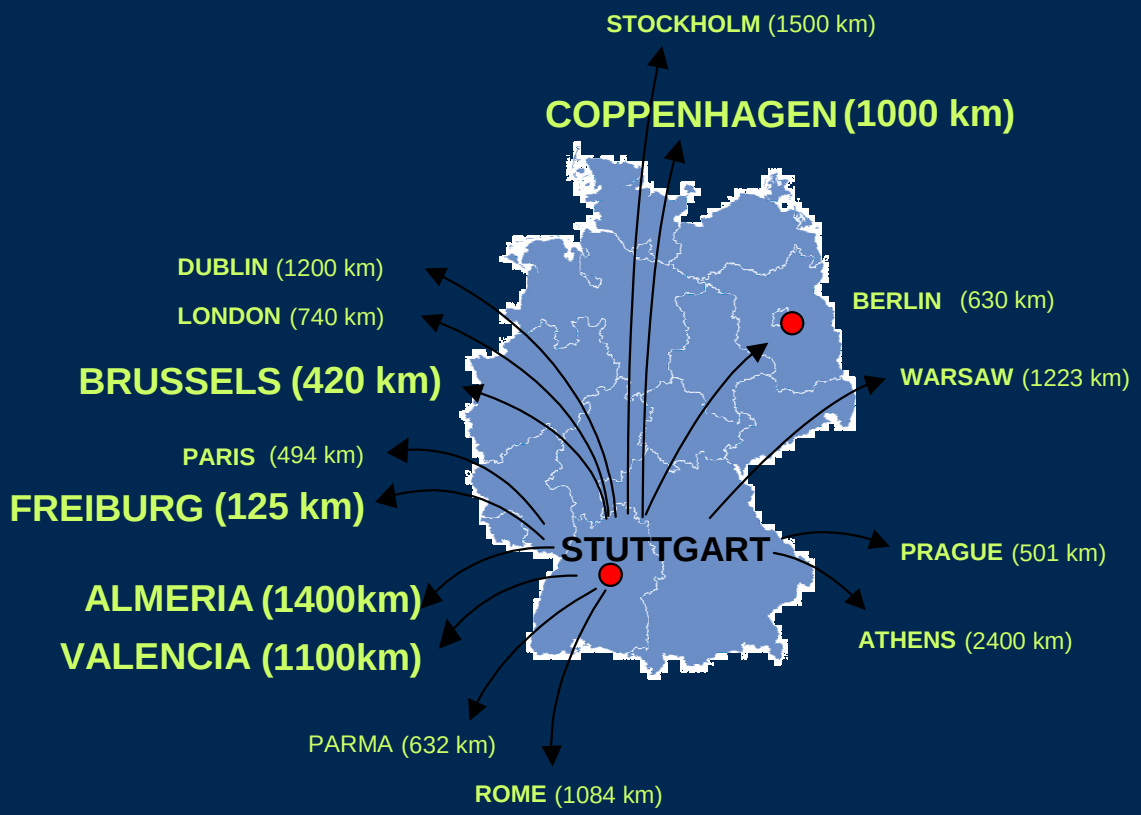
GC: 3 x MSD (EI+CI), 1x MS/MS, 1x ToF-MS, 1x ECD/NPD

LC: 2 x MS/MS, 2x Qtrap

Scope

> 500 pesticides and Metab. / Sample using MS-methods

Our Laboratory - Distances...



To Airport ca. 40 min by Metro (door to door)

The Staff

Working Tasks (some of)

Method Development

Method Validation

Proficiency Tests

Advisory Duties

Information Management
- Website
- Document Managem. (CIRCA)
- Databases

Administrative Duties

Technical Assistance
- Training
- Missions

CRL/NRL/ Official Labs Networking

Guideline Drafting
- AQC
- Validation

Working Tasks

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Method Validation

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Method Development

Aim:

The methods should be:

- Reasonable (concerning pesticides of relevance)
- Technically Easily Adaptable by other Laboratories
- Attractive (cost effective, easy to perform)

Need to Set Priorities:

Taking into account:

- Importance (risk, relevant Pesticides etc.)
- Feasibility (analytical difficulties, limited resources)

⇨ **Search in Literature**

⇨ **Questionnaire Evaluation**

Method Development - Polar Pesticides by LC-MS/MS

What has been done by now?

First Project:

Polar pesticides by (logKow<-2) LC-MS/MS

- Aim to develop a simple “multiresidue method”
- Literature Research
- MS/MS-Detection
- Chromatographic Separation
- Use of labelled ISTDs (some have to be synthesized)

Method Development

Future Plans:

Compound Class	Examples	Pre-examination Period	Decision for Priorities
Polar Compounds	Quats, Glyphosate, certain metabolites,	2006/7-2006/12	
Dithiocarbamates	Maneb, Propineb	2007/1-2007/12	2007/12
Volatile compounds	Ethyleneoxide,	2007/1-2007/12	2007/12
Compounds amenable to Multiresidue Methods after modification	Labile compounds, chromatographically challenging compounds	As required	As required

Working Tasks

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CRL/NRL/ Official Labs Networking

Guideline Drafting
- AQC
- Validation

Method Validation

What has been done by now?

Interlaboratory Method Validation for Acidic Pesticides:

- Use of Modified QuEChERS-Method or ChemElut Method
- Recovery Experiments
- 32 Analytes
- 2 Levels (0.01 mg/kg and 0.1 mg/kg)
- 4 Repesentative Commodities (Cucumber, Lemon, Raisin, Flour)
- 15 Labs volunteered to Participate
- 6 Labs already submitted Results so far

Pesticide	Recovery								% RSD								No of Labs each 5 replicates							
	Cucumber 0,1	Cucumber 0,01	Lemon 0,1	Lemon 0,01	Flour 0,1	Flour 0,01	Raisins 0,1	Raisins 0,01	Cucumber 0,1	Cucumber 0,01	Lemon 0,1	Lemon 0,01	Flour 0,1	Flour 0,01	Raisins 0,1	Raisins 0,01	Cucumber 0,1	Cucumber 0,01	Lemon 0,1	Lemon 0,01	Flour 0,1	Flour 0,01	Raisins 0,1	Raisins 0,01
2,4,5-T	102%	103%	95%	107%	92%	94%	101%	98%	10%	11%	8%	14%	8%	8%	5%	14%	5	5	6	6	4	4	4	4
2,4-D	103%	106%	93%	106%	91%	108%	100%	97%	11%	14%	9%	4%	13%	17%	2%	3%	5	5	5	4	4	4	4	3
2,4-DB	99%	100%	98%	93%	82%	86%	102%	103%	5%	5%	20%	32%	24%	39%	3%	6%	4	4	3	3	2	3	3	3
4-CPA	98%	94%	99%	105%	92%	97%	95%	99%	9%	20%	11%	12%	9%	22%	7%	6%	5	4	6	5	4	5	4	3
Bentazone	107%	104%	100%	98%	89%	86%	96%	91%	15%	11%	10%	7%	5%	19%	9%	20%	6	4	6	4	4	5	4	2
Bromoxynil	106%	100%	106%	105%	89%	100%	100%	91%	14%	13%	4%	16%	10%	8%	5%	13%	5	5	6	5	4	5	4	3
Clopyralid	62%	73%	73%	76%	61%	57%	53%	49%	57%	6%	26%	0%	21%	47%	10%	20%	3	2	3	2	2	3	3	2
Cycloxydim	86%	73%	97%	463%	152%	142%	97%	99%	21%	31%	11%	136%	55%	37%	12%	5%	5	4	5	3	4	5	4	3
Dicamba	95%	76%	87%	94%	78%	87%	87%	78%	22%	28%	12%	30%	15%	21%	13%	0%	5	3	4	2	2	3	3	2
Dichlorprop	106%	103%	94%	101%	97%	104%	106%	100%	12%	16%	7%	11%	9%	14%	6%	9%	6	5	6	5	4	5	4	3
Fenoprop	103%	98%	99%	99%	100%	97%	100%	99%	3%	9%	7%	10%	7%	10%	4%	6%	6	5	6	5	4	4	4	3
Fenoxaprop-P	106%	99%	106%	108%	97%	105%	104%	101%	10%	10%	6%	6%	5%	10%	8%	7%	5	5	5	4	3	4	3	2
Fluazifop	105%	99%	105%	104%	107%	94%	108%	107%	3%	6%	10%	2%	27%	7%	8%	6%	5	4	6	5	4	3	4	3
Fludioxonil	106%	102%	101%	100%	96%	92%	107%	95%	18%	14%	9%	3%	5%	10%	7%	17%	6	5	6	5	4	5	4	4
Fluroxypyr	105%	109%	96%	101%	94%	100%	99%	104%	14%	23%	14%	11%	4%	11%	9%	17%	4	4	6	4	4	3	4	4
Fomesafen	102%	99%	104%	95%	92%	88%	105%	103%	3%	7%	4%	22%	8%	16%	3%	8%	5	4	5	5	3	4	4	3
Haloxyfop	100%	98%	108%	97%	104%	104%	104%	93%	3%	9%	5%	18%	25%	0%	3%	11%	5	4	6	4	4	2	4	3
Imazapyr	86%	77%	92%	91%	89%	82%	86%	80%	26%	39%	5%	25%	13%	4%	10%	9%	5	4	5	4	3	3	4	3
Imazaquin	88%	91%	97%	98%	99%	92%	99%	97%	31%	14%	7%	7%	19%	18%	5%	4%	6	4	5	5	4	5	4	4
Imazethapyr	97%	91%	96%	90%	98%	97%	96%	91%	8%	11%	5%	11%	7%	11%	5%	7%	6	5	6	6	4	4	4	4
Imazosulfuron	84%	102%	86%	99%	86%	78%	73%	80%	23%	13%	21%	12%	40%	34%	22%	43%	6	4	6	6	4	5	4	4
Ioxynil	103%	97%	101%	97%	94%	98%	98%	95%	7%	10%	6%	3%	5%	5%	3%	8%	6	5	6	6	4	5	4	4
MCPA	104%	99%	101%	103%	91%	96%	101%	100%	15%	17%	8%	4%	10%	12%	6%	2%	6	5	6	6	4	5	4	4
MCPB	105%	96%	108%	99%	98%	106%	106%	99%	3%	10%	9%	10%	17%	22%	4%	9%	6	4	6	6	4	5	4	3
MCPP	103%	101%	95%	101%	95%	104%	102%	100%	11%	10%	5%	2%	6%	13%	2%	5%	6	5	6	6	4	5	4	4
Metosulam	101%	99%	105%	99%	108%	95%	99%	99%	6%	10%	4%	8%	10%	6%	10%	13%	6	5	6	6	4	5	4	4
Metsulfuron-Methyl	98%	94%	102%	98%	103%	98%	99%	91%	5%	8%	10%	9%	11%	13%	5%	14%	6	5	6	6	3	5	4	4
Naphthoxyacetic acid, 2-	99%	96%	97%	106%	95%	112%	92%	99%	11%	9%	10%	18%	8%	18%	9%	7%	6	4	6	6	4	5	4	4
Picloram	61%	88%	79%	75%	48%	53%	68%	64%	74%	26%	14%	4%	6%	8%	18%	22%	3	2	3	3	2	2	3	2
Quinmerac	82%	82%	88%	95%	81%	96%	83%	78%	36%	37%	8%	29%	14%	19%	19%	9%	5	4	5	4	3	4	4	4
Thifensulfuron-Methyl	98%	98%	101%	102%	106%	111%	98%	95%	4%	10%	10%	8%	10%	14%	5%	13%	6	5	6	6	4	4	4	4
Triclopyr	102%	102%	94%	103%	88%	86%	102%	101%	5%	17%	11%	12%	13%	10%	9%	4%	5	4	5	4	3	2	4	3
AVERAGE	**97%**	**95%**	**97%**	**109%**	**93%**	**95%**	**96%**	**93%**	**15%**	**15%**	**10%**	**16%**	**14%**	**16%**	**8%**	**11%**								

Method Validation

Future Plans:

- **Interlaboratory Method Validation for Glyphosat in Cereals in collaboration with CRL for Cereals**
- **Interlaboratory Method Validation for Polar Compounds in Fruits and Vegetables**

Working Tasks

Method Development

Method Validation

Proficiency Tests

Information Management
- Website
- Document Managem. (CIRCA)
- Databases

Advisory Duties

Administrative Duties

Technical Assistance
- Training
- Missions

CRL/NRL/ Official Labs Networking

Guideline Drafting
- AQC
- Validation

Proficiency Test

EUPT-SRM01

…a nice collaboration between CRL - FV and CRL - SRM

University of ALMERIA

CVUA STUTTGART

Proficiency Test

Commodity:

Apple Juice

Proficiency Test –List of Potential Pesticides

10 Acidic Pesticides

Pesticide	MRPL (mg/Kg)
2,4-D (2,4-Dichlorophenoxy acetic acid) (free acid)	0.05
Dichloroprop (2,4-DP, 2,4- Dichlorophenoxy propionic acid) (free acid, including Dichlorprop-P)	0.05
2-Naphthoxyacetic acid	0.05#
4-CPA (4-Chlorophenoxy acid)	0.05#
Bentazone (with conjugates of 6-hydroxy-bentazone)	0.1
Dicamba (free acid)	0.05#
Fluazifop (free acid, Fluazifop + Fluazifop-P)	0.05#
MCPA (free acid)	0.05#
Mecoprop (MCPP) (free acid, Mecoprop + Mecoprop-P)	0.05
Quizalofop (free acid, Quizalofop + Quizalofop-P)	0.05#

- **Not amenable to classical MRMs**
- **Require special attention in pH of extraction and cleanup**
- **Require LC/MS-Analysis or derivatisation**

Proficiency Test –List of Potential Pesticides

4 Organotin Pesticides

Pesticide	MRPL (mg/Kg)
Azocyclotin (see Cyhexatin)	**0.05**
Cyhexatin (Azocyclotin + Cyhexatin, expressed as Cyhexatin)	
Fenbutatin oxide	**0.05**
Fentin (Fentin hydroxide+ Fentin acetate, expressed as Fentin)	**0.05**

- **Give low recoveries with traditional MRMs,**
- **Require LC/MS or derivatisation**

Proficiency Test –List of Potential Pesticides

2 "Quats"

Pesticide	MRPL (mg/Kg)
Chlormequat (expressed as Chlormequat cation)	**0.05**
Mepiquat (expressed as Mepiquat cation)	**0.05#**

- **Not amenable to traditional MRMs,**
- **Require LC/MS and use of isotopically labeled ISTDs**
- **Chlormequat is included in the EU-monitoring list**

Proficiency Test

Participation was optional , but...

Labs analyzing chlormequat within the EU co-ordinated monitoring program, were urged to participate at least for this analyte.

Proficiency Test - Participants

	Labs Participating/Reporting
Austria	2/2
Czech Republic:	2/2
Denmark:	2/1
Finland:	1/1
France:	2/1
Germany:	8/8
Italy:	1/1
Latvia:	1/1
Norway:	1/1
Slovakia:	1/0
Slovenia:	2/2
Spain:	1/1
Sweden:	1/1
United Kingdom:	2/2
The Netherlands:	1/1
SUM:	27/24

Proficiency Test – Homogeneity Test

8 portions in duplicate
N=16

Analyte	Mean	% RSD
Chlormequat	0.127 mg/kg	3.3
Fenbutatin Oxide	0.474 mg/kg	1.2
MCPA	0.366 mg/kg	3.2

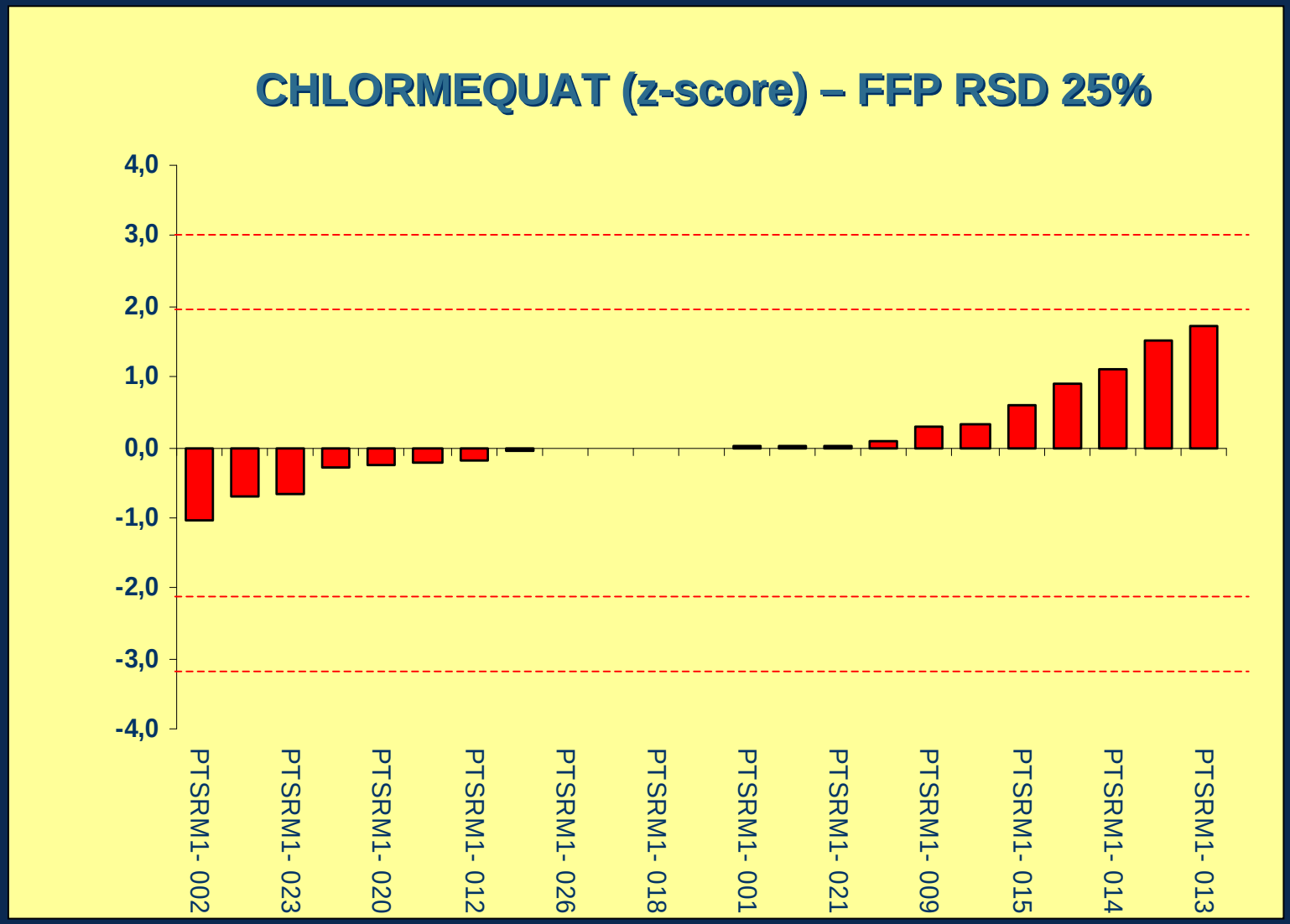
Stability test was also OK !

Proficiency Test- Results

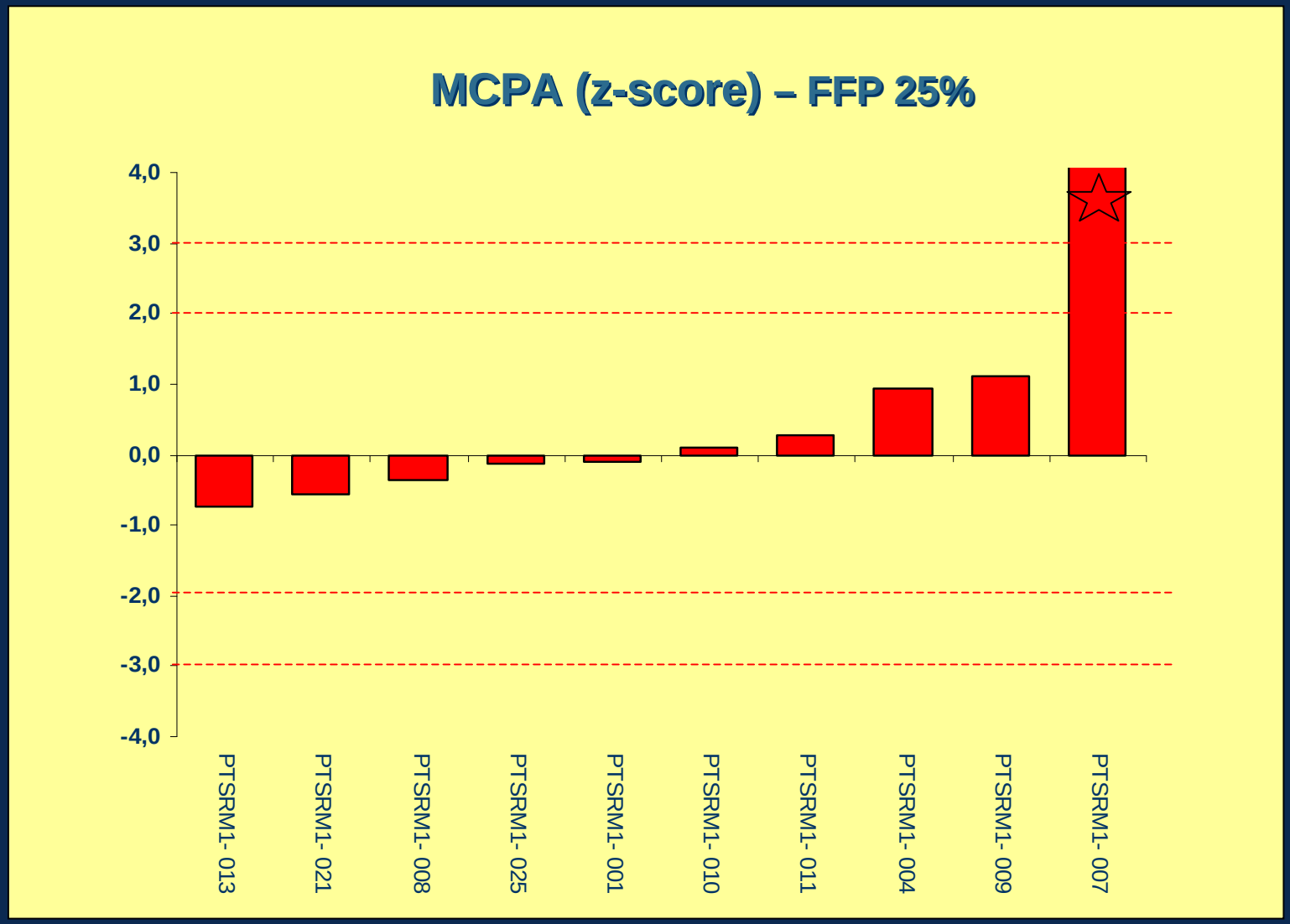
Using FFP - RSD of 25%

Lab Code	Chlormequat	*z-score*	Fenbutatin oxide	*z-score*	MCPA	*z-score*
PTSRM1- 001	0,172	**0,0**	0,482		0,306	**-0,1**
PTSRM1- 002	0,126	**-1,1**	NA		NA	
PTSRM1- 004	NA		NA		0,39	**1,0**
PTSRM1- 005	0,185	**0,3**	NA		NA	
PTSRM1- 006	0,236	**1,5**	NA		NA	
PTSRM1- 007	0,210	**0,9**	NA		0,71	**5,0**
PTSRM1- 008	0,158	**-0,3**	0,464		0,286	**-0,4**
PTSRM1- 009	0,183	**0,3**	0,490		0,402	**1,1**
PTSRM1- 010	0,172	**0,0**	NA		0,324	**0,1**
PTSRM1- 011	0,141	**-0,7**	NA		0,337	**0,3**
PTSRM1- 012	0,163	**-0,2**	NA		NA	
PTSRM1- 013	0,189	**0,4**	0,400		0,257	**-0,7**
PTSRM1- 014	0,218	**1,1**	NA		NA	
PTSRM1- 015	0,197	**0,6**	NA		NA	
PTSRM1- 016	0,174	**0,1**	NA		NA	
PTSRM1- 018	0,171	**0,0**	NA		NA	
PTSRM1- 019	0,162	**-0,2**	0,61		NA	
PTSRM1- 020	0,160	**-0,3**	NA		NA	
PTSRM1- 021	0,172	**0,0**	NA		0,271	**-0,6**
PTSRM1- 023	0,142	**-0,7**	NA		NA	
PTSRM1- 024	0,131	**-0,9**	NA		NA	
PTSRM1- 025	0,171	**0,0**	NA		0,305	**-0,1**
PTSRM1- 026	0,170	**0,0**	NA		NA	
PTSRM1- 027	0,132	**-0,9**	NA		NA	
Median (labs)	**0,171 (23)**		**0,482 (5)**		**0,315 (10)**	
Fortif. level	**0,156**		**0,500**		**0,361**	

Proficiency Test- Results



Proficiency Test- Results



Proficiency Test- Methods Employed

Analyte Group	Extraction	Measurement	Σ
Acids	6x QuEChERS 3x In-house 1x Dilution	8x LC-MS(/MS) 2x GC-MS (deriv.)	**10**
O-Tins	3x QuEChERS 1x National 1x Dilution	4x LC-MS/MS 1x GC-FPD (deriv.)	**5**
Quats	21x MeOH/water 1x Acetone 1x No data	23x LC-MS(/MS) (16x D4-labelled ISTD)	**23**

Proficiency Test - Conclusions

- **Many labs do not cover important SRM-Analytes**
  - **Existing Methods laborious time-consuming and expensive**
  - **Many Labs lack sophisticated Instrumentation required for simple methodologies**

- **What should/will be done by CRL?**
  - **Identify Lab shortcomings (Survey)**
  - **Collect information on SRM-Analytes and set priorities**
  - **Develop simple cheap and thus attractive methods**
  - **Inform labs in advance about analytes to be included in future PTs (i.e. animate labs to establish methods)**

Future Plans:

Proficiency Test for Single Residue Analytes in Flour-Matrix in collaboration with CRL for cereals and Feeding Stuff

Working Tasks

Method Development

Method Validation

Proficiency Tests

Advisory Duties

Information Management
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Guideline Drafting
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Information Management - Overview

Aim: Build an appropriate structure....
for Collection and Exchange of information within the network

CIRCA

Document-Management Tool

Member-Area [restricted access]

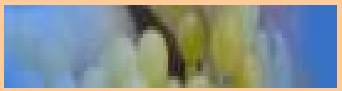
Member-Area [restricted access]

Links to

- Method Validation Database
- Pesticide Properties Database
- Commodity Database
- Network Database ....

CRL-Pesticides-Website (Homepage)
www.???.eu
[= website for experts]

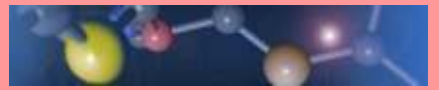
CRL-FV
Fruits & Vegetables



CRL-CF
Cereals & Feeding Stuff

CRL-FAO
Food of Animal Origin

CRL-SRM
Single Residue Methods



Information Management

What has been done by now?

Website:

- Base Structure has been programmed (by Stephan Böttcher)

Document Management Tool:

- Closed system based on CIRCA platform
- Contact has been established (we can use platform for free)
- CRL in Freiburg will take over the Administration

Databases:

- Database for Method Validation Data (first Version ready)
- Database for Pesticide Properties (in preparation)

Information Management

Future Plans:

Website:

- Fill with Information and Links (by Stephan Böttcher)
- Details to be decided in a CRL-Meeting shortly

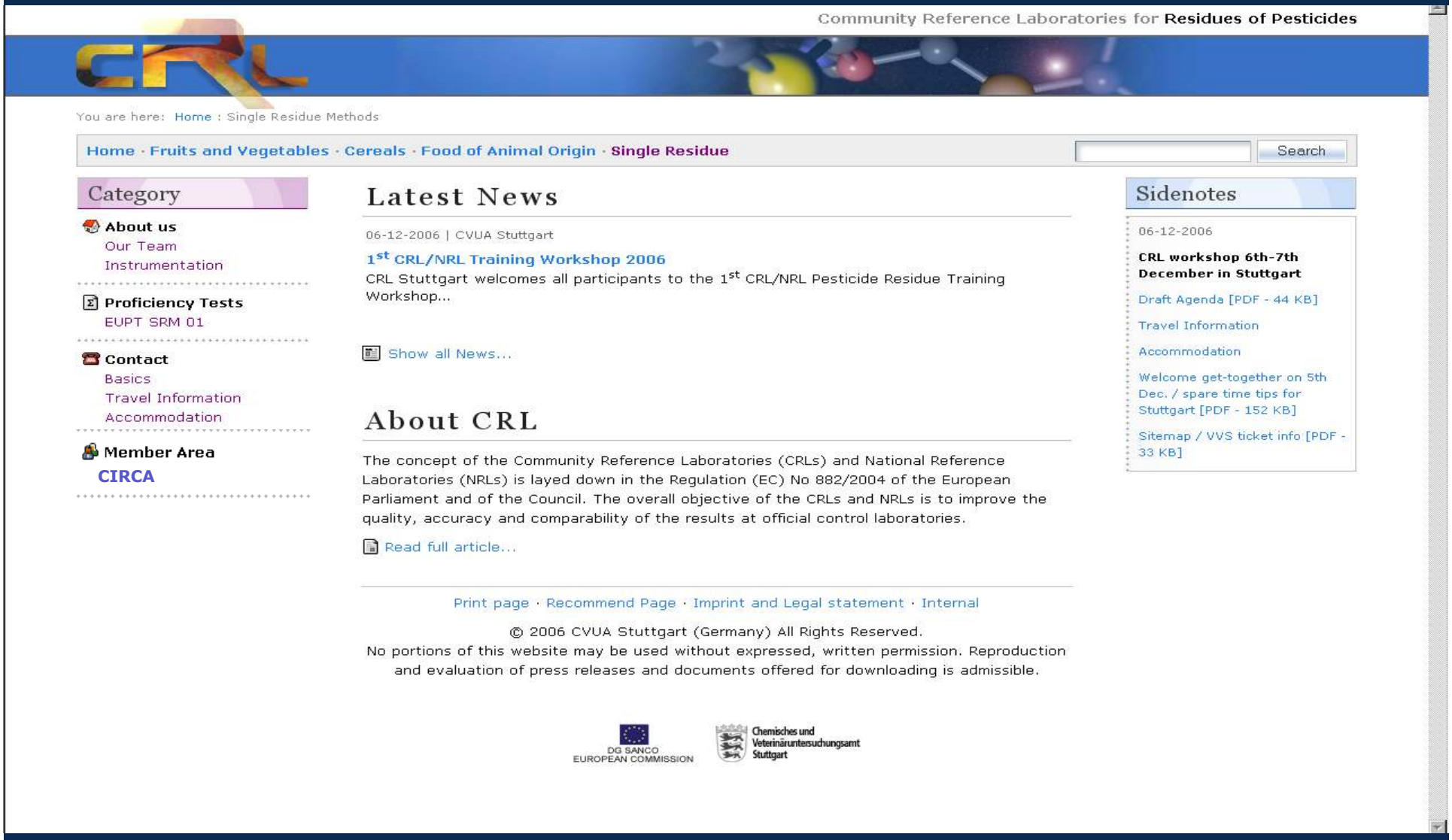
Document Management Tool (CIRCA Platform):

- Establish Common and CRL-specific Areas
- Colleagues from NRLs and Official Labs will get access

Databases:

- Feed Method-Validation and Pesticide-Properties Databases
- Create Commodity-Database
- Create NETWORK Database (Lab-Profiles, Contact Points)

Website


Community Reference Laboratories for Residues of Pesticides
You are here: Home : Single Residue Methods
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Basics
Travel Information
Accommodation
Member Area
CIRCA
Latest News
06-12-2006 | CVUA Stuttgart
1st CRL/NRL Training Workshop 2006
CRL Stuttgart welcomes all participants to the 1st CRL/NRL Pesticide Residue Training Workshop...
Show all News...
About CRL
The concept of the Community Reference Laboratories (CRLs) and National Reference Laboratories (NRLs) is layed down in the Regulation (EC) No 882/2004 of the European Parliament and of the Council. The overall objective of the CRLs and NRLs is to improve the quality, accuracy and comparability of the results at official control laboratories.
Read full article...
Sidenotes
06-12-2006
CRL workshop 6th-7th December in Stuttgart
Draft Agenda [PDF - 44 KB]
Travel Information
Accommodation
Welcome get-together on 5th Dec. / spare time tips for Stuttgart [PDF - 152 KB]
Sitemap / VVS ticket info [PDF - 33 KB]
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Chemisches und Veterinäruntersuchungsamt Stuttgart

Information Management – Databases

➢ **Pesticide Database , Commodity Database**

Aims:

- Create a Pool with analytically valuable information
- Exploit synergy potentials in Information Management
- Spend less time in retrieving information
- Facilitate Decision-Making (knowledge Based planning)
  - Define Priorities
  - Targeted Sampling and Analysis
  - Targeted Research
- Allow grouping (profiling) and thus selection of Representative Pesticides and Commodities based on sound information

Information Management – Databases

Not only Data collected from Literature…
…but also experimentally generated data where reasonable

- **Pesticide Database:**
  - Recovery data with different methods
  - Degradation behaviour of pesticides
  - Behaviour in Analysis (partitioning, cleanup, Chr/phy)
- **Commodity Database:**
  - Amount of co-extracted components
  - Behaviour in cleanup
  - Matrix Effects

Need for simple Standardized Testing Schemes

so that experimental data can be generated by various labs

Information Management – Databases

In addition: Network Database

- **With information about Laboratories:**
  - Contact Information (contact persons…)
  - Instrumentation available
  - Specializations
  - Link to web-site
  - Link to annual report
  - Expression of Interest to send or receive trainees
  - Photo
  - …

Aim:

strengthen the Network between official Laboratories

Working Tasks

Method Development

Method Validation

Proficiency Tests

Advisory Duties

Information Management
- Website
- Document Managem. (CIRCA)
- Databases

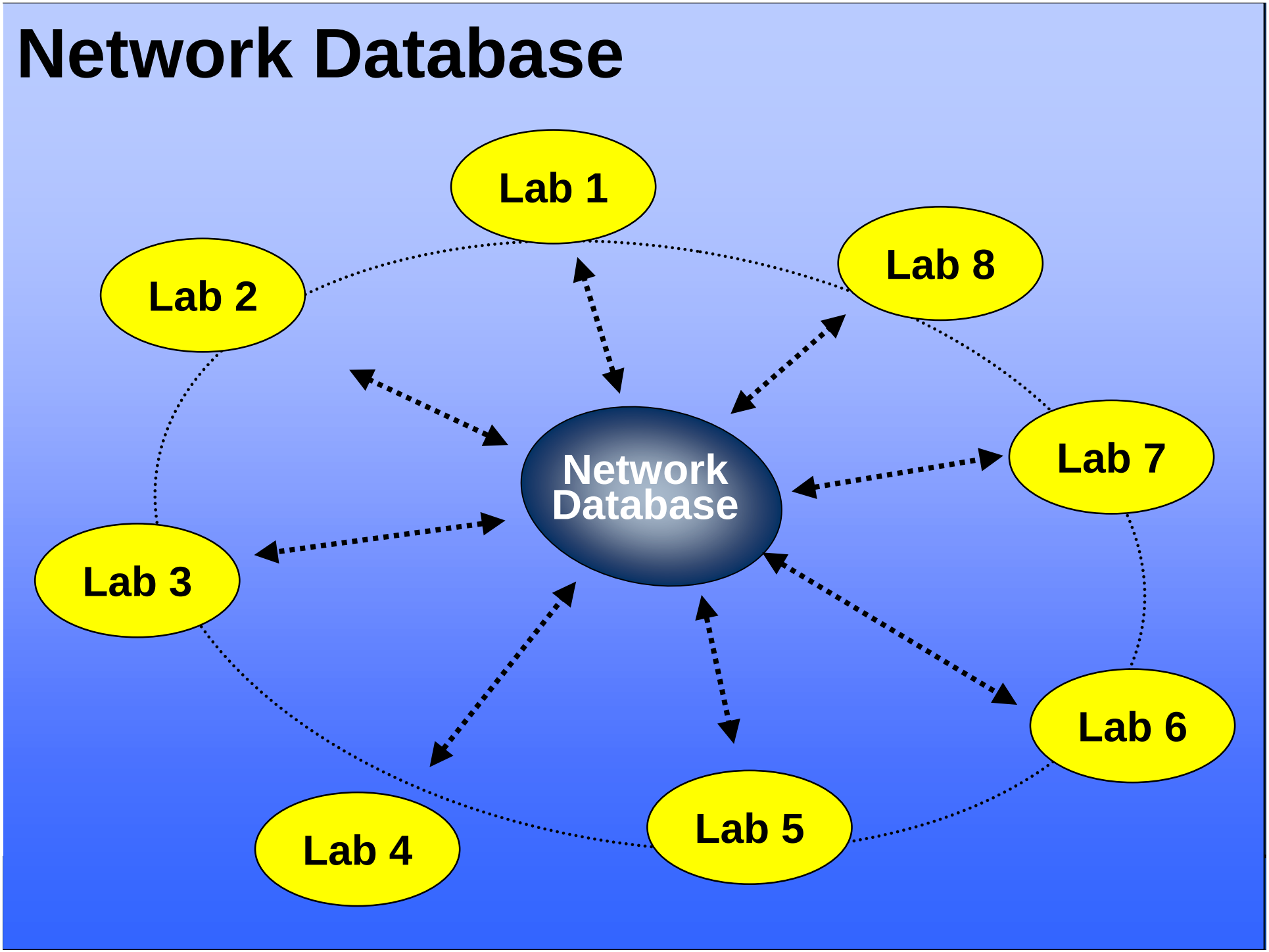
Administrative Duties

Technical Assistance
- Training
- Missions

CRL/NRL/ Official Labs Networking

Guideline Drafting
- AQC
- Validation

Network Database



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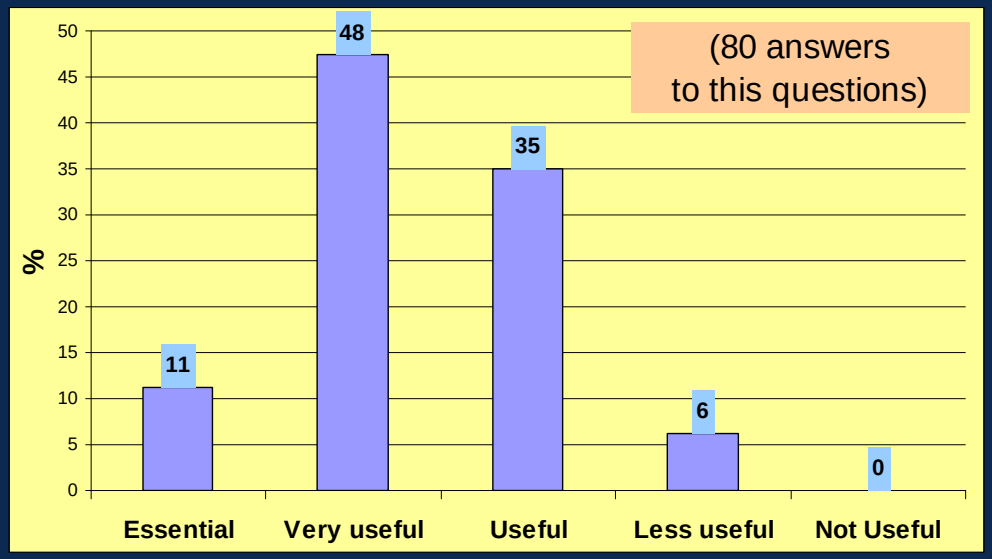
We look forward to having a Good Collaboration with you !!

Results of Lab-Questionnaire 2006

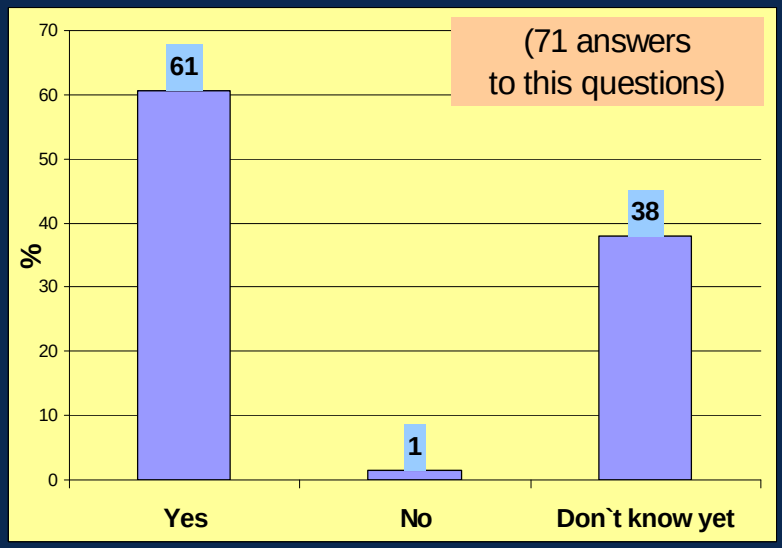
- **Website-section of lab-questionnaire:**

What types of data would you like to see in our common CRL website?

A RESIDUE FINDINGS Database containing residue findings collected from various labs?



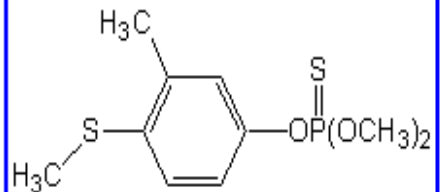
Would you be willing to contribute data to such as database?



FENTHION 55-38-9		Pesticide Class:	Organophosphorous
		Mode of Action:	Insecticide
PHYSICOCHEMICAL AND TOXICOLOGICAL DATA			
MW / Molecular Formula	278,3 / C10H15O3PS2		
Water Solubility [mg/L] / pKow	4,2 / 4,84		
pKa			
Vapour pressure [Pa]	0,00074		
ARfD / ADI [mg/kg bw]	0,01 / 0,002		
Endocrine Disruption			
Add. Info	Forms oxidation products		
Residue Definition	Sum of fenthion, its oxygen analogue, and their sulfoxides and sulfones, expressed as fenthion		

Physicochemical Data

Fenthion

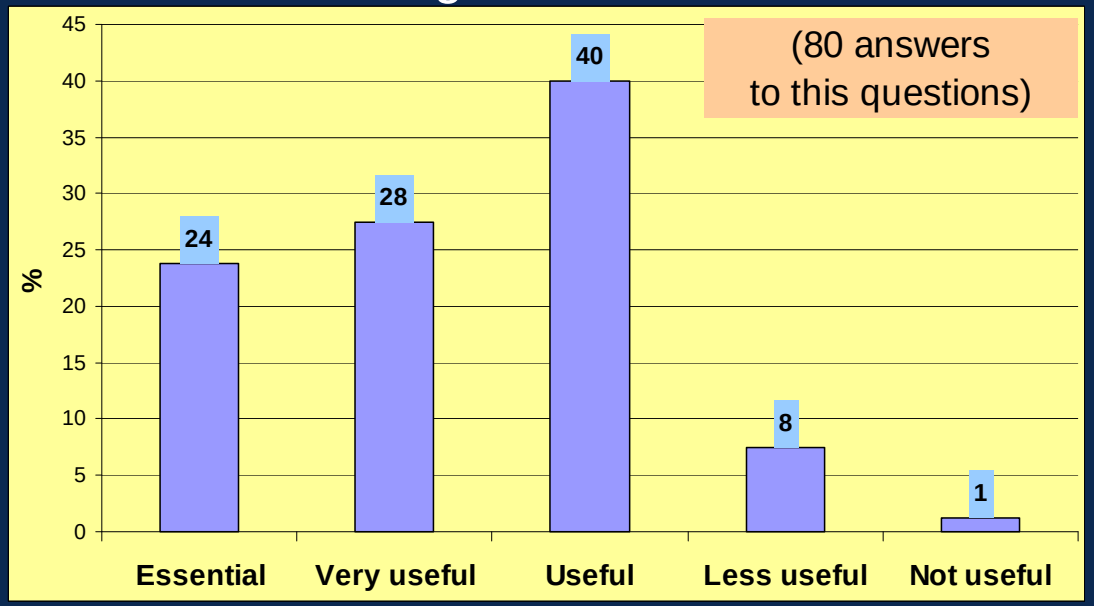


Questionnaire 2006 by the CRL for SRM: (85 Feedbacks, 01.12.06)

What types of data would you like to see in our common CRL website?

-> A PESTICIDE PROPERTIES Database containing ...

physicochemical properties of pesticides (pKa, solubility, logKow, ...)?



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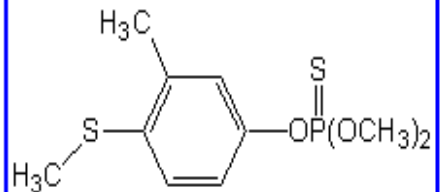
Residue Definition

Fenthion



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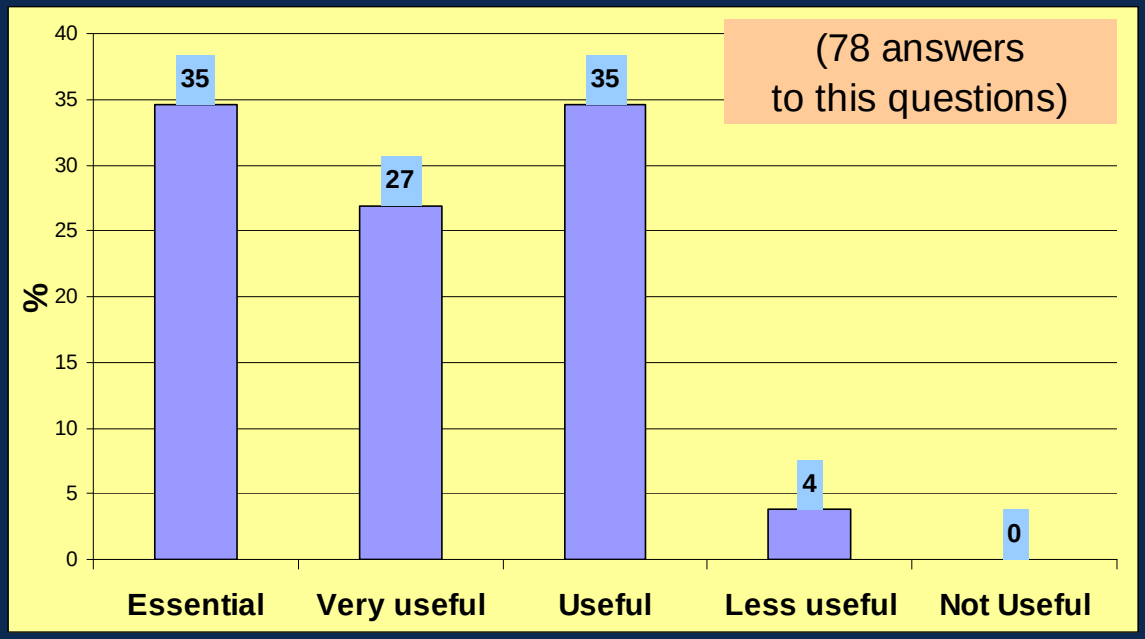
Residue definition?



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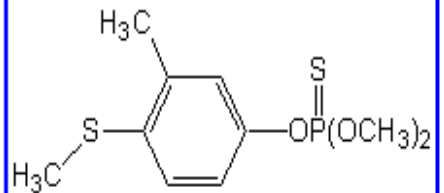
Add. Info	Forms oxidation products		
Residue Definition	Sum of fenthion, its oxygen analogue, and their sulfoxides and sulfones, expressed as fenthion		

Metabolites / Degradation products

Fenthion



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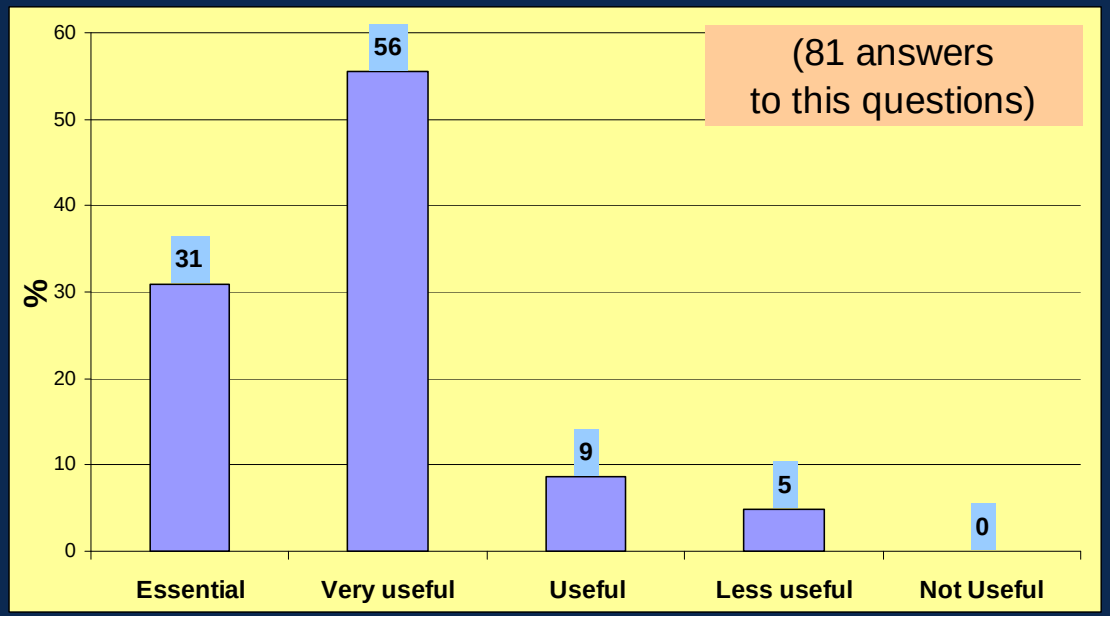
-> A PESTICIDE PROPERTIES Database containing ...

Important metabolites and degradation products?



ANALYTICAL DATA

TYPICAL RECOVERIES USING VARIOUS MULTIRESIDUE METHODS (in %)					
Method	0-20	20-50	50-70	70-110	Remarks
QuEChERS (MeCN)				X	
Stuttgart (Acetone)				X	
SFE (CO2)				X	
DFG S 19 (Acetone)				X	
Dutch (Acetone)					
Canadian (MeCN)				X	
CDFA (MeCN)					
Swedish (EtAc)					
L. Alder (MeOH)					
Stajnbaher (Acetone, SPE)				X	

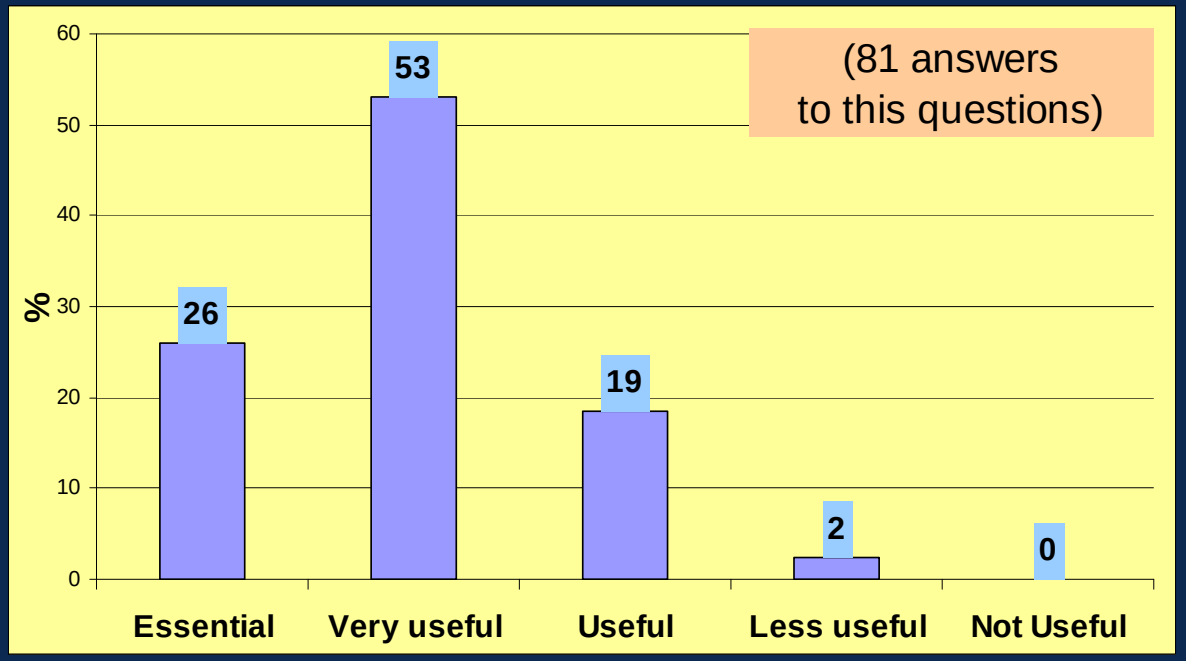
Typical recoveries with various multiresidue methods

GC-BEHAVIOR					
GC-amenable	Yes	Matrix Effects	NoData		
			0		
				m/z	
		CLICK	278	125	169
MSD CI (+)	+++	CLICK	279	307	
MSD CI (-)	0	CLICK			
TOF EI (+)		CLICK			
MS/MS EI (+)	+++	CLICK	278>109	278>169	
NPD / ECD / FPD	+++/0/+++				

What types of data would you like to see in our common CRL website?

-> A PESTICIDE PROPERTIES Database containing ...

typical recoveries with various methods?



ANALYTICAL DATA

TYPICAL RECOVERIES USING VARI… %)

Method	0-20	20-50			
QuEChERS (MeCN)					
Stuttgart (Acetone)					
SFE (CO2)				X	
DFG S 19 (Acetone)				X	
Dutch (Acetone)					
Canadian (MeCN)					
CDFA (MeCN)					
Swedish (EtAc)					
L. Alder (MeOH)					
Stajnbaher (Acetone, SPE)				X	

GC-behavior

GC-BEHAVIOR			
GC-amenable	Yes	Matrix Effects	NoData
Decomposition	0	Tailing	0
Decomposition Products			

LC-behavior

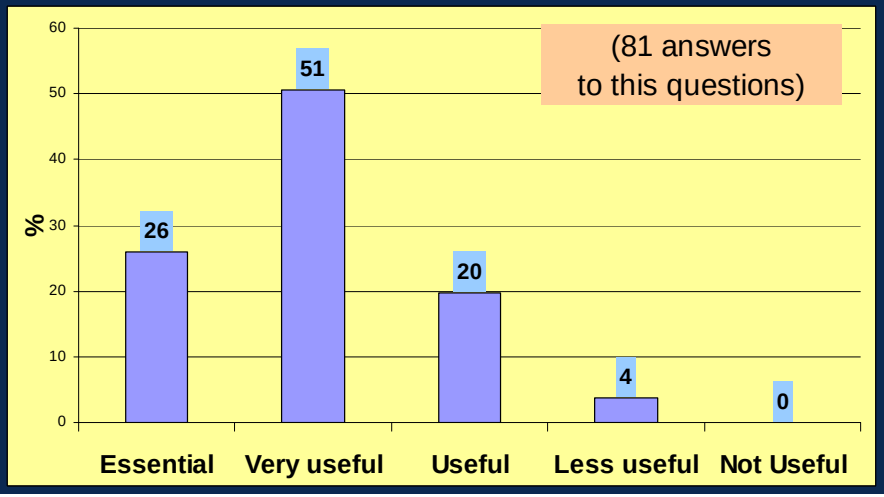
Detector	Sensitivity	Spectrum	m/z		
MSD EI (+)	+++	CLICK	278	125	169
MSD CI (+)	+++	CLICK	279	307	
MSD CI (-)	0	CLICK			
TOF EI (+)		CLICK			
MS/MS EI (+)	+++	CLICK	278>109	278>169	
NPD / ECD / FPD	+++/0/+++				

LC-BEHAVIOR

Ionization Source	Sensitivity	MS (m/z)			MS/MS-Transitions			MS/TOF		
ESI (+)	+++				279>169	279>247				
ESI (-)	NoData									
APCI (+)	NoData									
APCI (-)	NoData									

-> A PESTICIDE PROPERTIES Database containing ...

typical sensitivities achieved by various instrumental techniques?
(GC-ECD, NPD, FPD, GC-MS, LC-MS, ...)



ANALYTICAL DATA

TYPICAL RECOVERIES USING VARI… …%)

Method	0-20	20-50			
QuEChERS (MeCN)					
Stuttgart (Acetone)					
SFE (CO2)				X	
DFG S 19 (Acetone)				X	
Dutch (Acetone)					
Canadian (MeCN)					
CDFA (MeCN)					
Swedish (EtAc)					
L. Alder (MeOH)					
Stajnbaher (Acetone, SPE)				X	

GC-behavior

GC-BEHAVIOR

GC-amenable	Yes	Matrix Effects	NoData
Decomposition	0	Tailing	0
Decomposition Products			

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NPD / ECD / FPD	+++/0/+++				

LC-behavior

LC-BEHAVIOR

Ionization Source	Sensitivity	MS (m/z)			MS/MS-Transitions					
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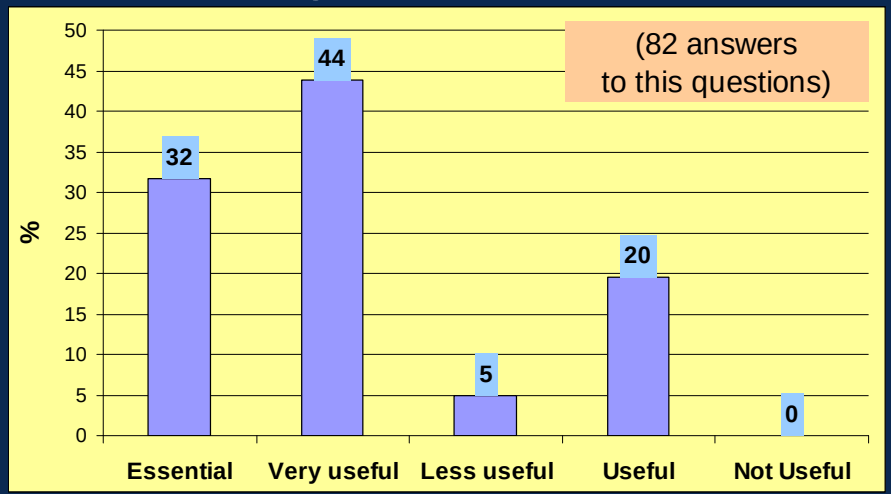
ESI (-)	NoData									
APCI (+)	NoData									
APCI (-)	NoData									

View MS-Spectra

-> A PESTICIDE PROPERTIES Database containing ...

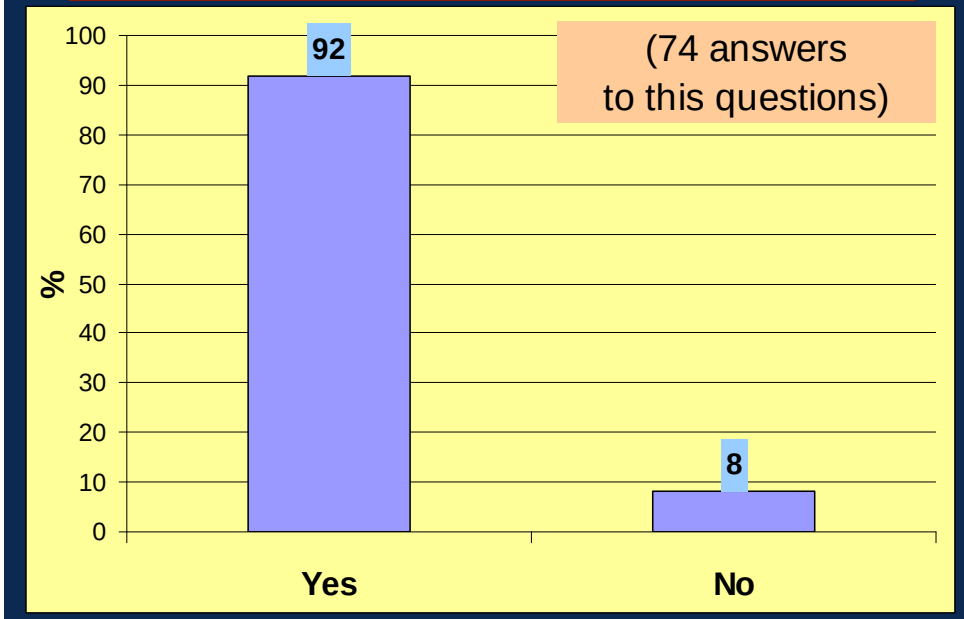
parameters required for programming Instruments (SIM masses, MRM transitions)?



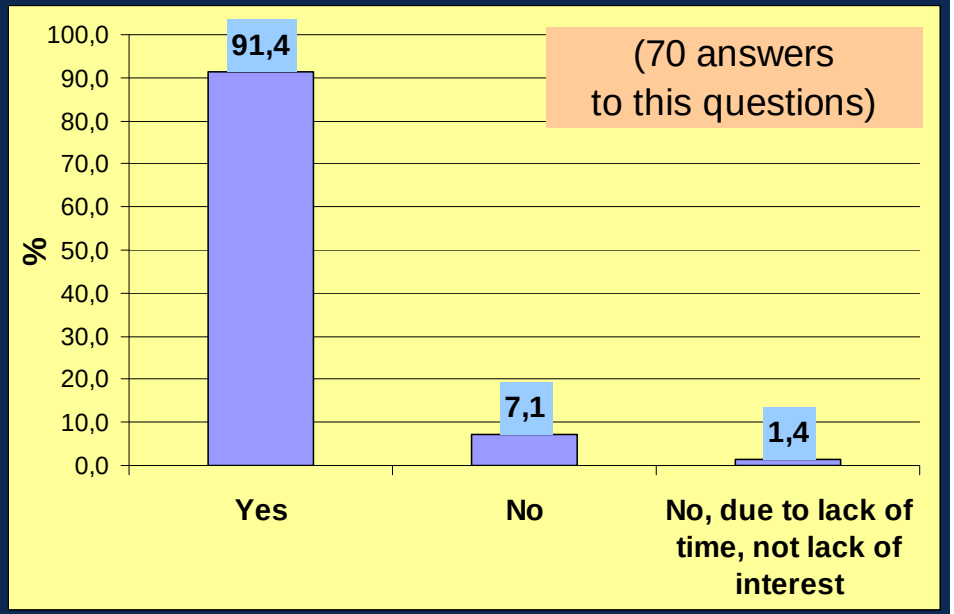
Results of Lab-Questionnaire 2006

What types of data would you like to see in our common CRL website?

Would you like a discussion forum to be established?

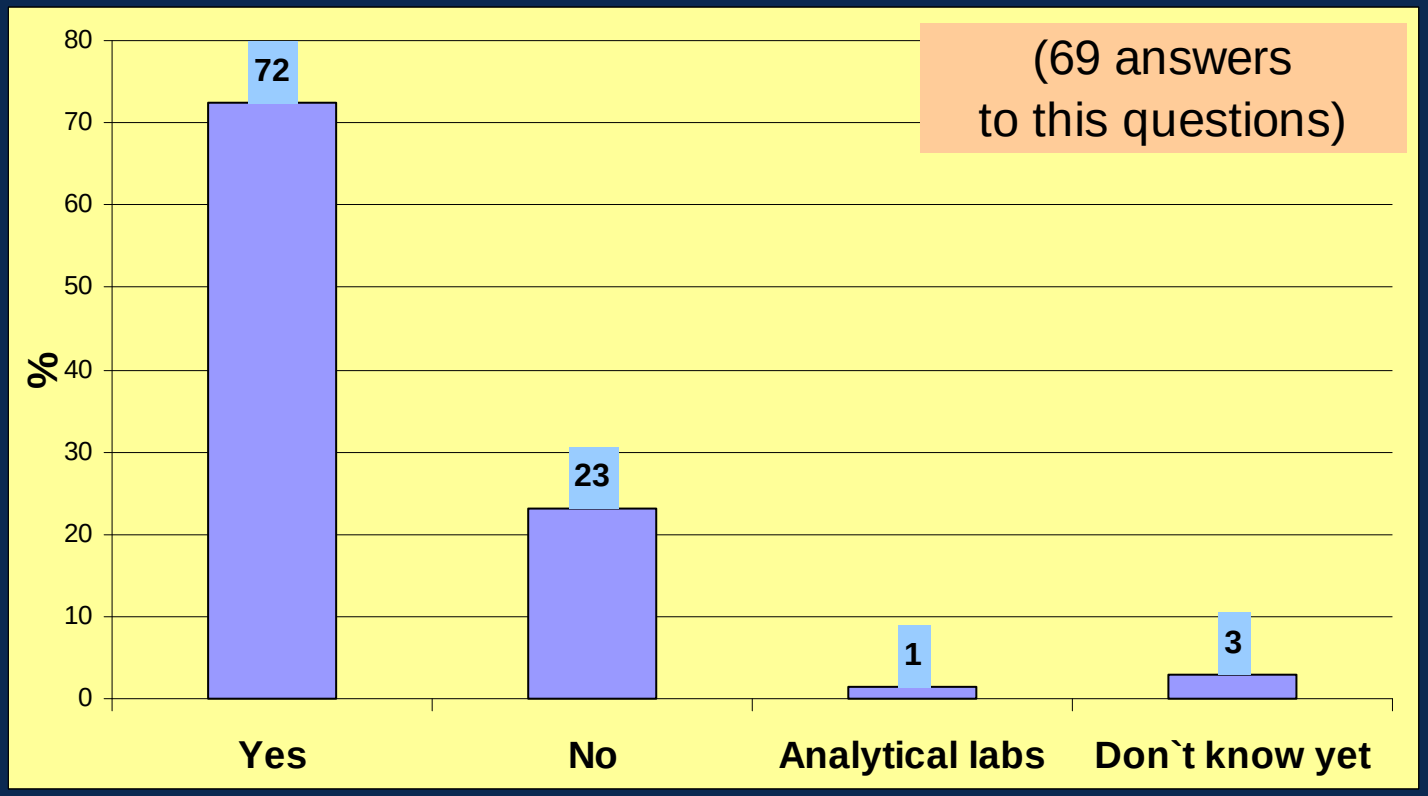


Would you be willing to use such a forum?



Results of Lab-Questionnaire 2006

Would you like the forum to be accessible also to colleagues outsite the CRL/NRL-Network (e.g. colleagues from countries outside the EU, from private labs...)?



Pesticide Profiling

Proposal:

Establish a default procedure to systematically generate and collect analytically important information about pesticides:

- Physicochemical properties
- Toxicological parameters
- Analytical behaviour
  - GC-, LC- Amenability
  - MS-Spectra,MS/MS-Transitions, TOF-Exact Masses
  - Recovery Rates with various Methods
  - Stability Data (pH, Storage etc.)

Collection of Pesticide Data

What Data is Analytically relevant:

- Pesticide Profiles
- Pesticide Use Information
- Pesticide Residue findings
- Pesticide Validation Data

➢ **Aim:**

- Spend less time in retrieving information (CRLs, NRLs)
- Facilitate Decision-Making (knowledge Based planning)
  - Define Priorities
  - Targeted Research (CRLs, NRLs, other labs)
  - Targeted Targeted Sampling and Analysis

- **Method Development**
  - Polar pesticides/metabolites,
  - Volatile pesticides
  - Susceptible Pesticides /metabolites
  - Chromatographically difficult Pesticides /metabolites
- **Systematic Pesticide Profiling** (with Spain?)
  - Study anal. behaviour of Pesticides (standard scheme)
  - Track analytically relevant data in DB (access to all off. labs)