NEW ANALYTICAL TOOLS FOR PESTICIDE RESIDUES IN FOOD CONTROL.

EXPERIENCE GAINED OVER THE LAST 15 YEARS AS THE EURL-FV.

Amadeo Rodríguez Fernández-Alba

European Commission
EURL-FV

EURL FV – European Union Reference Laboratory for Pesticide Residues in Fruits and Vegetables.
UNIVERSITY OF ALMERIA

OUTLOOK

History

Performance of MRM in OfLs network
Evaluation of MRM through EUPTs

Present

Improved technologies
High sensitve TQ (high benefits)
HRMS (impact and improvements)

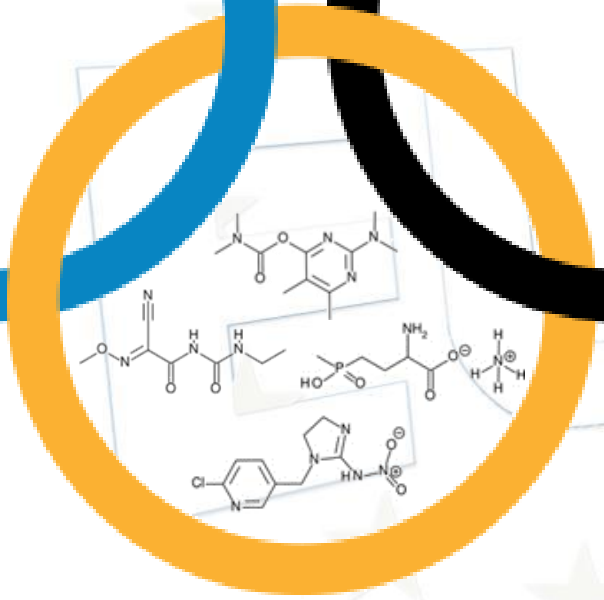
Future

Automation

Citius

Altius

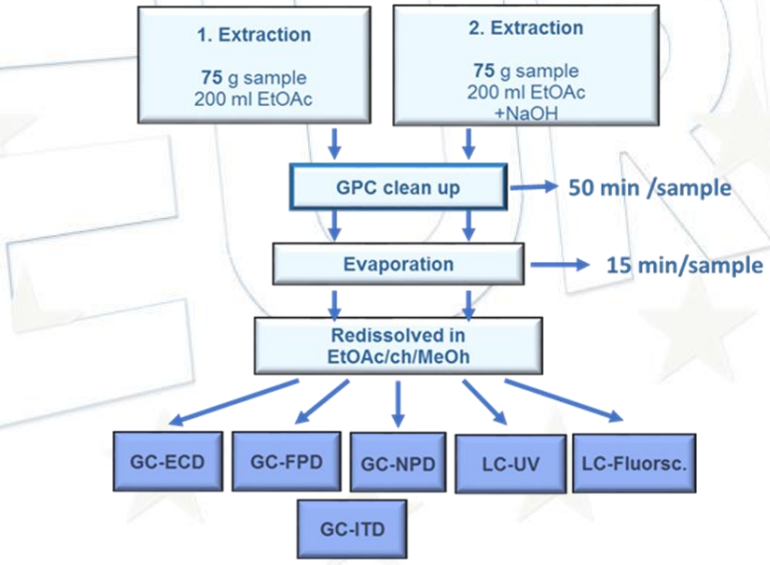
Fortius



Livsmedelsverket
Swedish Food Agency

2004

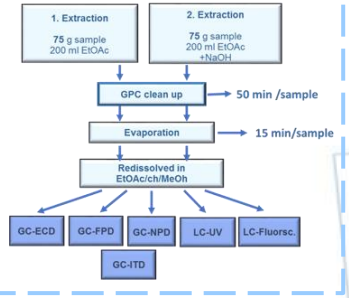
183 analytes



2022 The existing SweEt multi residue method in food

Livsmedelsverket Swedish Food Agency 2004

183 analytes



10 g/ml
(150 g)

0.5 g/ml
(10 g)

544

Extraction

10 g sample
20 ml EtOAc+$NaHCO_3$
3 min Spex shaker
Na_2SO_4

Centrifugation

Filtration

GC-MS/MS | UHPLC-MS/MS + HRMS

395

Extraction

5 g sample
10 ml water
10 ml EtOAc (1% HAc)
3 min Spex shaker
Na_2SO_4

Centrifugation

Filtration

GC-MS/MS | UHPLC-MS/MS

120

Extraction

5 g sample
PSA + C18
10 ml EtOAc
3 min Spex shaker
Na_2SO_4

Centrifugation

Filtration

GC-MS/MS | UHPLC-MS/MS

113

Extraction

2.5 g sample
5 ml EtOAc:ACN(80:20)
5 min Spex shaker
Na_2SO_4

Centrifugation/filtration

5 ml EtOAc:ACN(80:20)

Clean up EMR-Lipid 6 ml

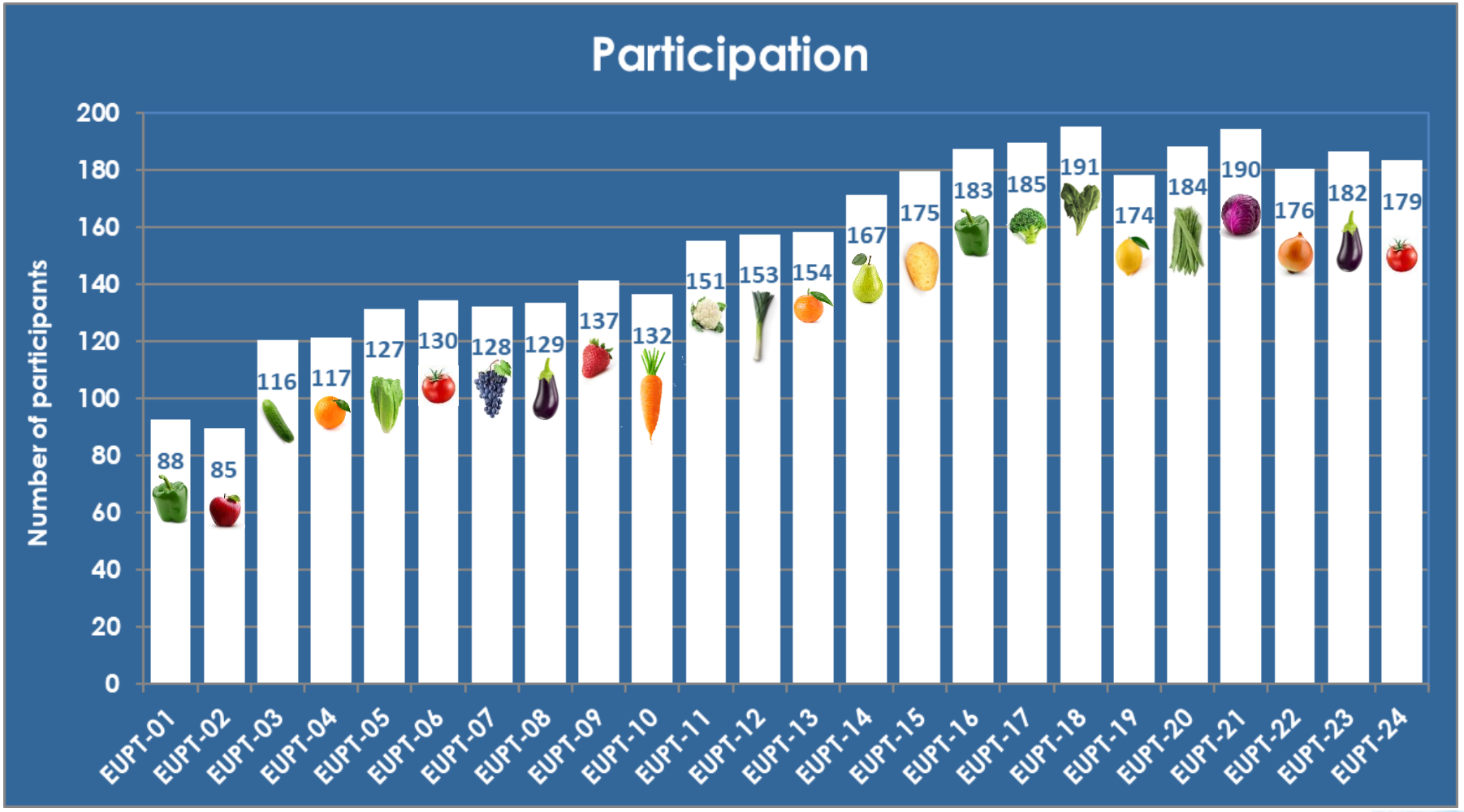
Elution EtOAc:ACN(20:80)

Centrifugation/filtration

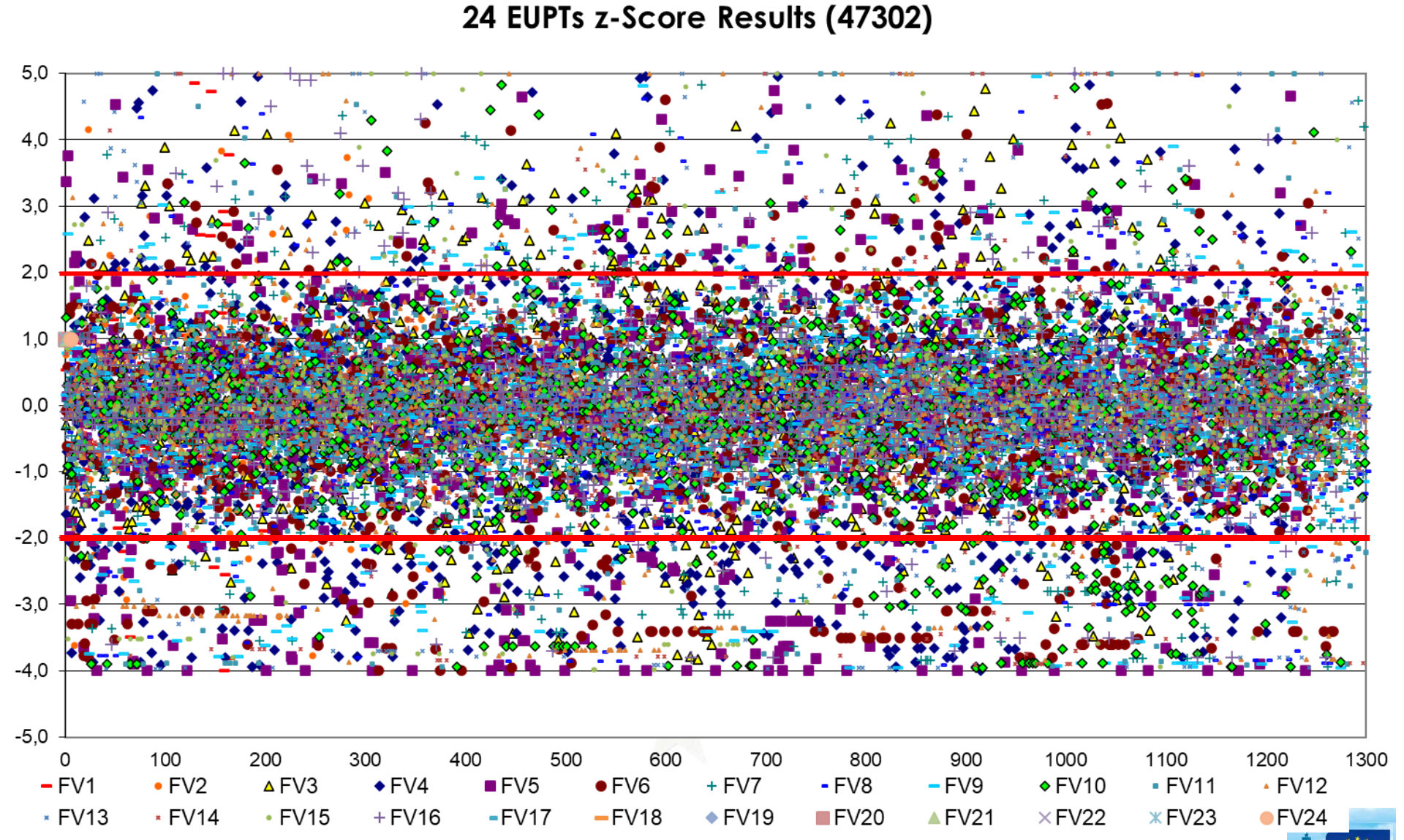
Sample conc. 0.2 g/ml

GC-MS/MS | UHPLC-MS/MS

EUPTs-FV

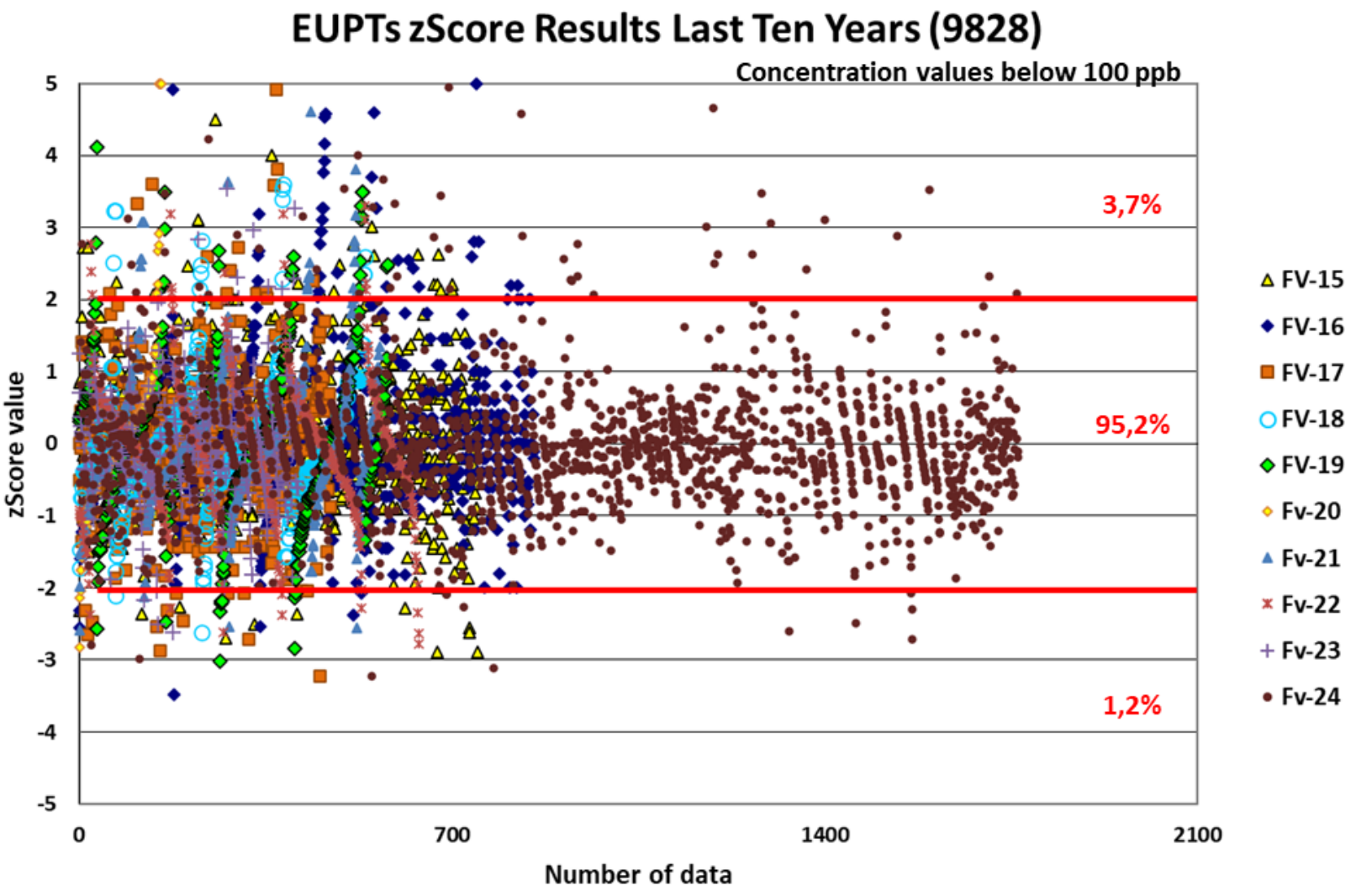

Participation
Number of participants
200
180
160
140
120
100
80
60
40
20
0
88
85
116
117
127
130
128
129
137
132
151
153
154
167
175
183
185
191
174
184
190
176
182
179
EUPT-01
EUPT-02
EUPT-03
EUPT-04
EUPT-05
EUPT-06
EUPT-07
EUPT-08
EUPT-09
EUPT-10
EUPT-11
EUPT-12
EUPT-13
EUPT-14
EUPT-15
EUPT-16
EUPT-17
EUPT-18
EUPT-19
EUPT-20
EUPT-21
EUPT-22
EUPT-23
EUPT-24

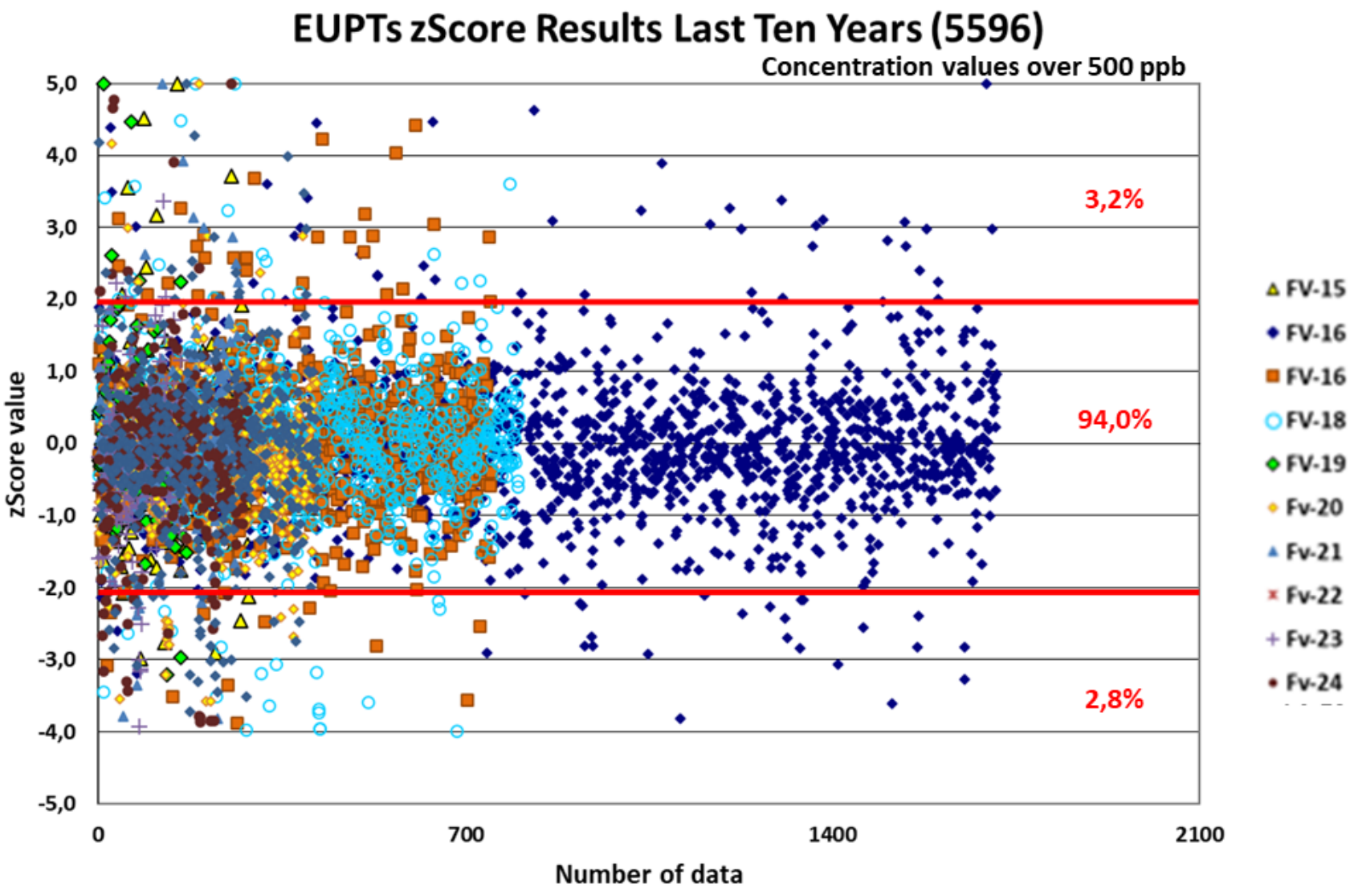
INFORMATION GAINED



EUPT-FV1 to EUPT-FV24 in numbers

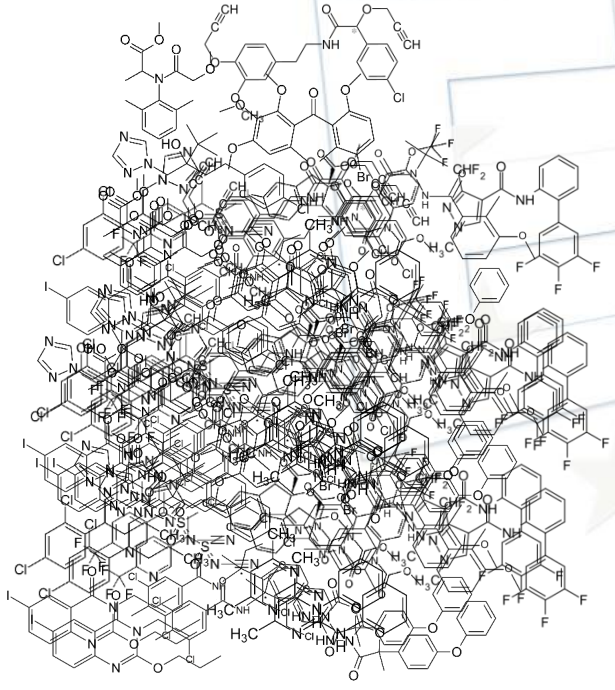
EUPT N°	Matrices	N° of Participants	N° of Possible Pesticides	N° of pesticides evaluated in test item
1	**Pepper**	88	**33**	6
2	**Apple**	85	**41**	6
3	**Cucumber**	116	**48**	14
4	**Orange**	117	**57**	14
5	**Lettuce**	127	**57**	15
6	**Tomato**	130	**57**	13
7	**Grape**	128	**65**	16
8	**Aubergine**	129	**68**	16
9	**Strawberry**	137	**82**	19
10	**Carrot**	132	**113**	18
11	**Cauliflower**	151	**128**	21
12	**Leek**	153	**144**	17
13	**Mandarin**	154	**144**	19
14	**Pear**	167	**175**	18
15	**Potato**	175	**175**	18
16	**Pepper**	183	**175**	22
17	**Broccoli**	185	**183**	11
18	**Spinach**	191	**190**	16 (14 mandatory + 2 voluntary)
19	**Lemon**	174	**192**	19 (17 mandatory + 2 voluntary)
20	**Green beans**	184	**195**	21 (19 mandatory + 2 voluntary)
21	**Red cabbage**	190	**205**	20 (17 mandatory + 3 voluntary)
22	**Onion**	176	**208**	19 (17 mandatory + 2 voluntary)
23	**Aubergine**	182	**215**	20 (18 mandatory + 2 voluntary)
24	**Tomato**	179	**215**	18 (16 mandatory + 2 voluntary)


EUPTs zScore Results Last Ten Years (9828)
Concentration values below 100 ppb
zScore value
Number of data
5
4
3
2
1
0
-1
-2
-3
-4
-5
0
700
1400
2100
3,7%
95,2%
1,2%
FV-15
FV-16
FV-17
FV-18
FV-19
Fv-20
Fv-21
Fv-22
Fv-23
Fv-24


EUPTs zScore Results Last Ten Years (5596)
Concentration values over 500 ppb
zScore value
5,0
4,0
3,0
2,0
1,0
0,0
-1,0
-2,0
-3,0
-4,0
-5,0
0
700
1400
2100
Number of data
3,2%
94,0%
2,8%
FV-15
FV-16
FV-16
FV-18
FV-19
Fv-20
Fv-21
Fv-22
Fv-23
Fv-24

LC-ESI

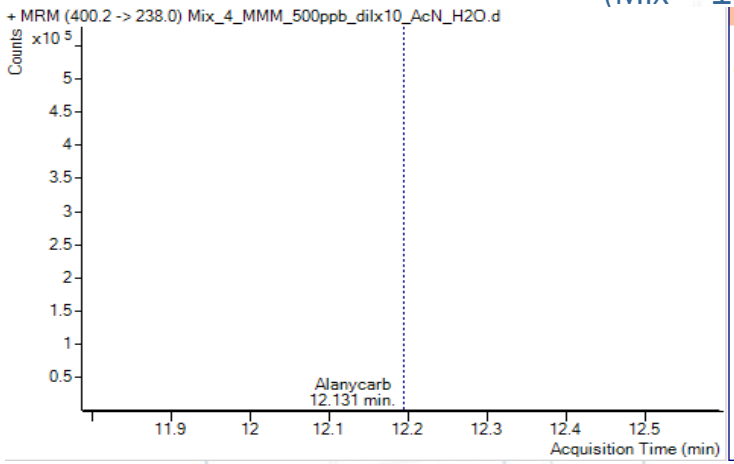
HUNDREDS OF COMPOUNDS

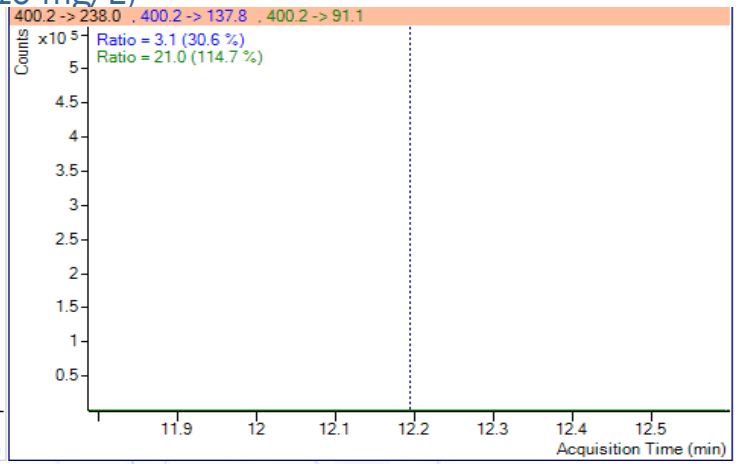


GC-EI

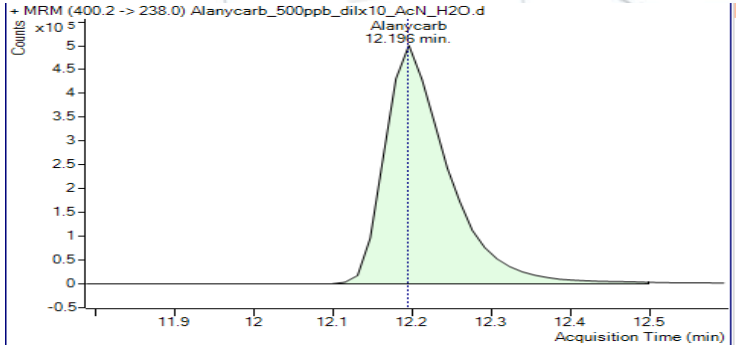
Degradation - Alanycarb

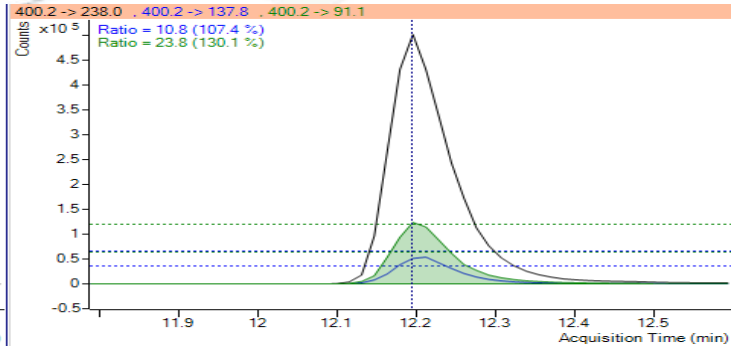
Alanycarb
(Mix – 10 mg/L)





Alanycarb
(Stock solution – 10 mg/L)

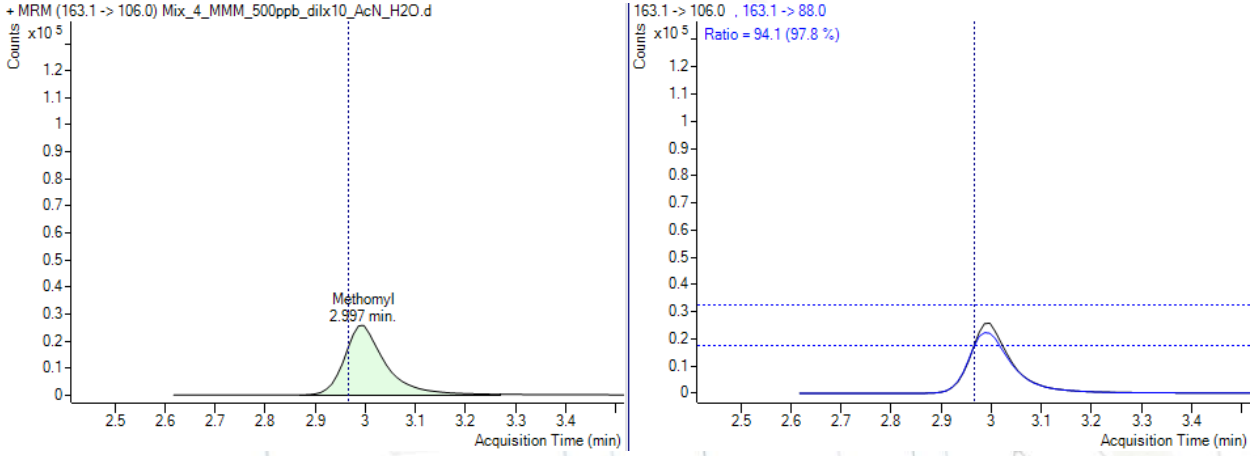




Degradation - Alanycarb

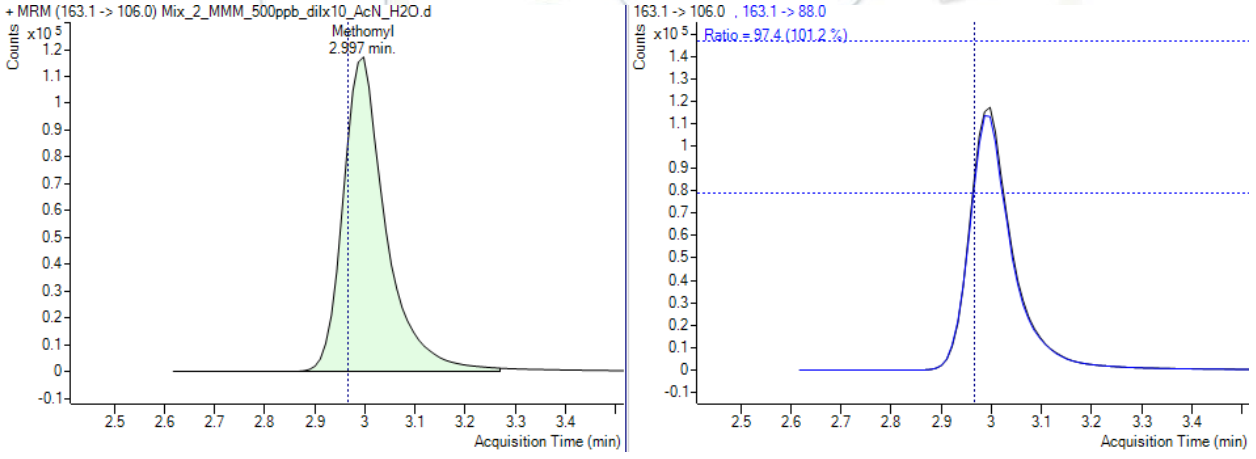
Methomyl

(Mix 4 – 20 mg/L)



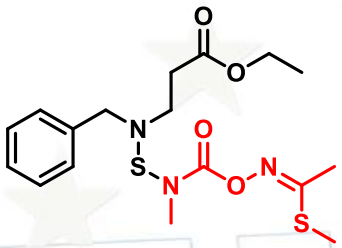
Methomyl

(Mix 2 – 10 mg/L)

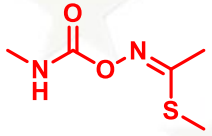


2.1 ppm of methomyl in mix 4?

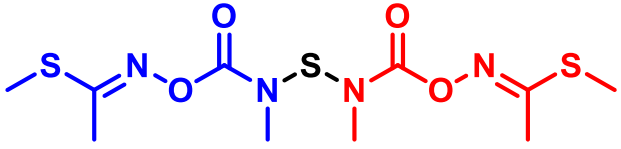
Degradation - Alanycarb



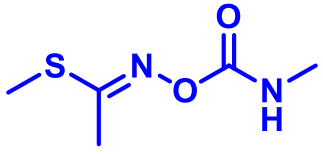
Alanycarb
t_R = 12,19 min
Chemical Formula: $C_{17}H_{25}N_3O_4S_2$
Exact Mass: 399,1286



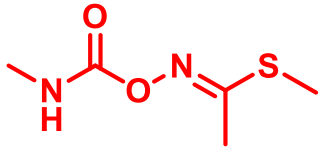
(*Z*)-Methomyl
t_R = 2,98 min
Chemical Formula: $C_5H_{10}N_2O_2S$
Exact Mass: 162,0463



thiodicarb



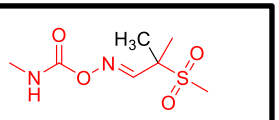
methomyl



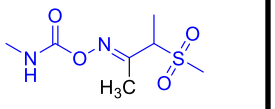
methomyl

Cocktail effect

Potential false positives and negatives: common mass transitions



Aldicarb-sulfone

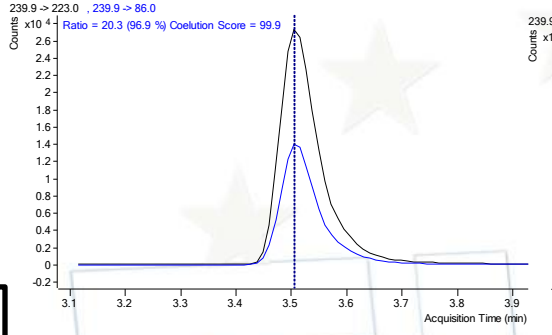


Butoxycarboxim

240 > 223

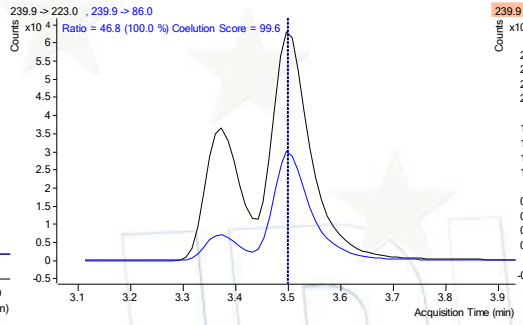
240 > 86

240 > 166



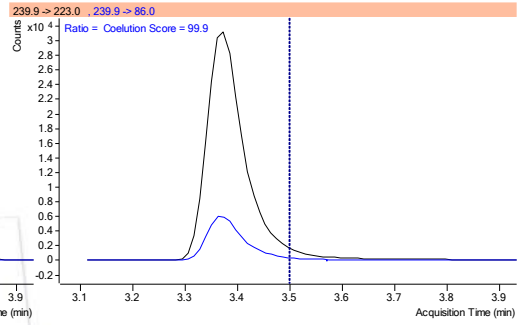
Aldicarb-sulfone

Aldicarb-sulfone monitored MRM transitions



Aldicarb-sulfone & Butoxycarboxim

Aldicarb-sulfone monitored MRM transitions

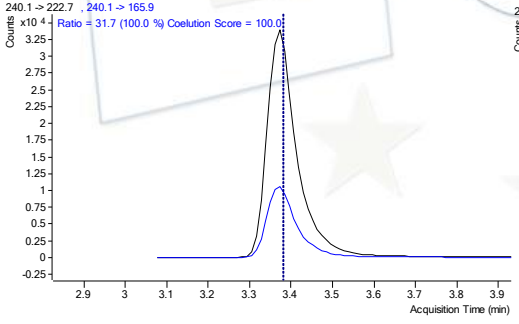


Butoxycarboxim

Aldicarb-sulfone monitored MRM transitions

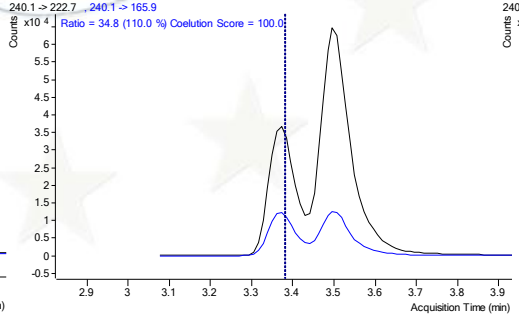
Butoxycarboxim

Butoxycarboxim monitored MRM transitions



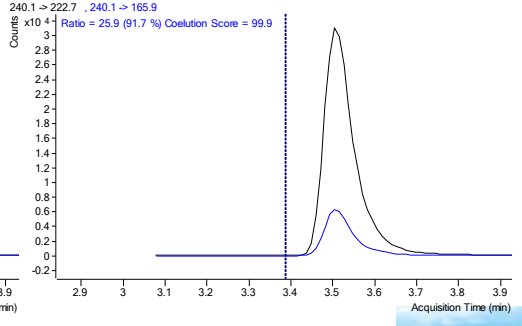
Butoxycarboxim & Aldicarb-sulfone

Butoxycarboxim monitored MRM transitions



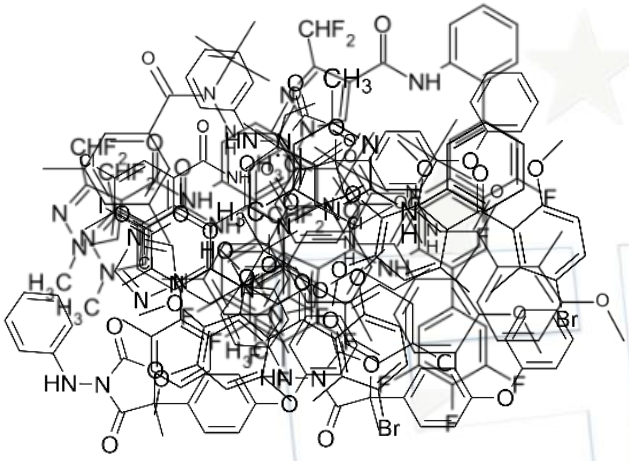
Aldicarb-sulfone

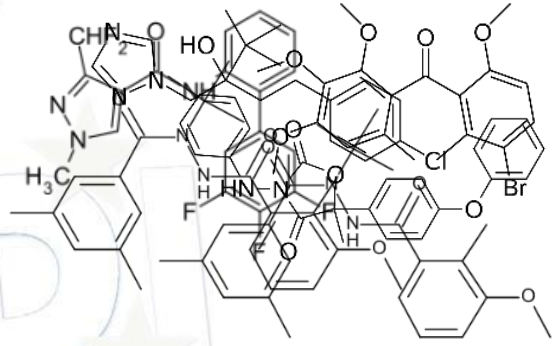
Butoxycarboxim monitored MRM transitions




vegetables

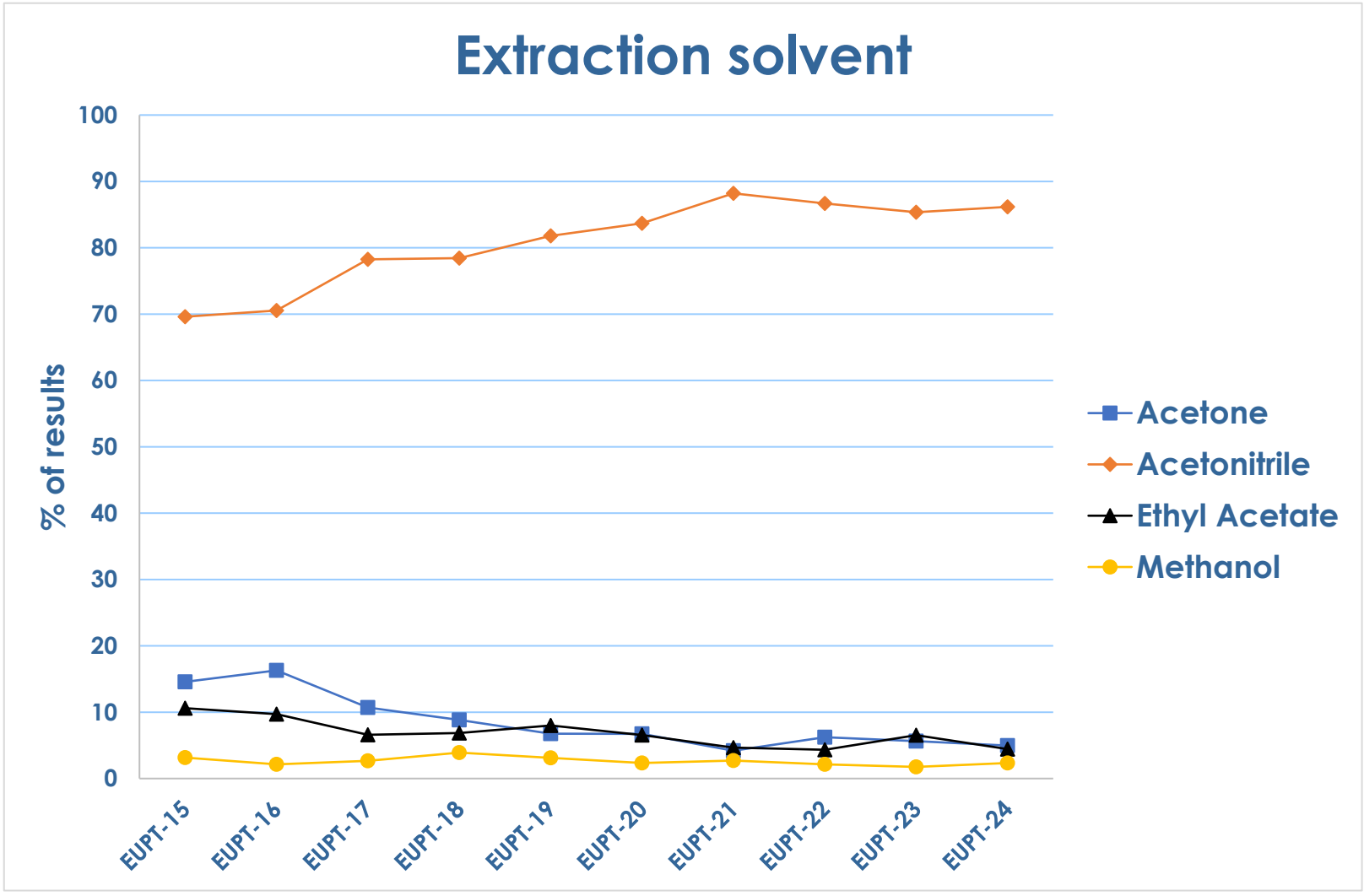
TARGET LIST



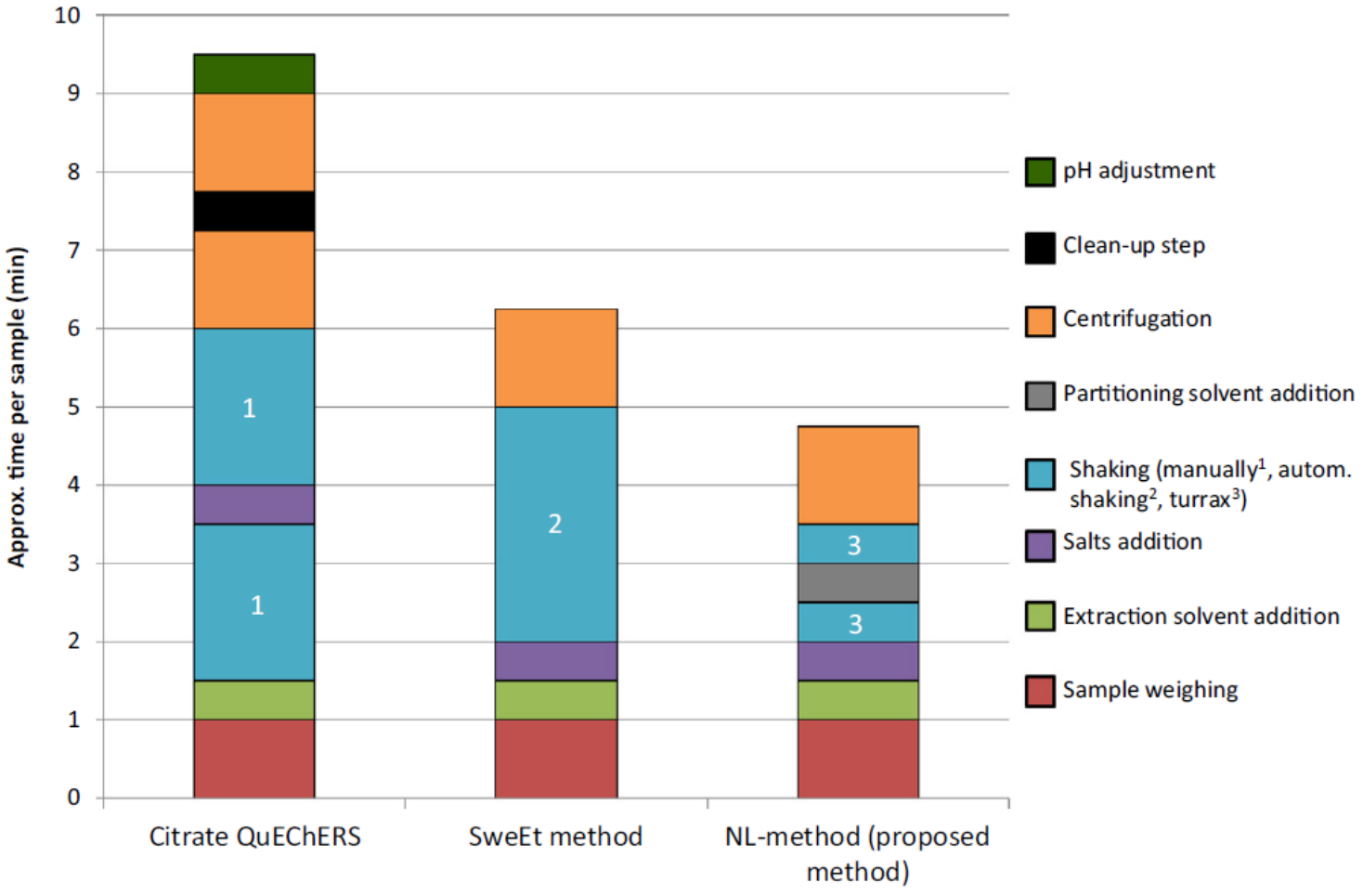


TARGET LIST

EXTRACTION

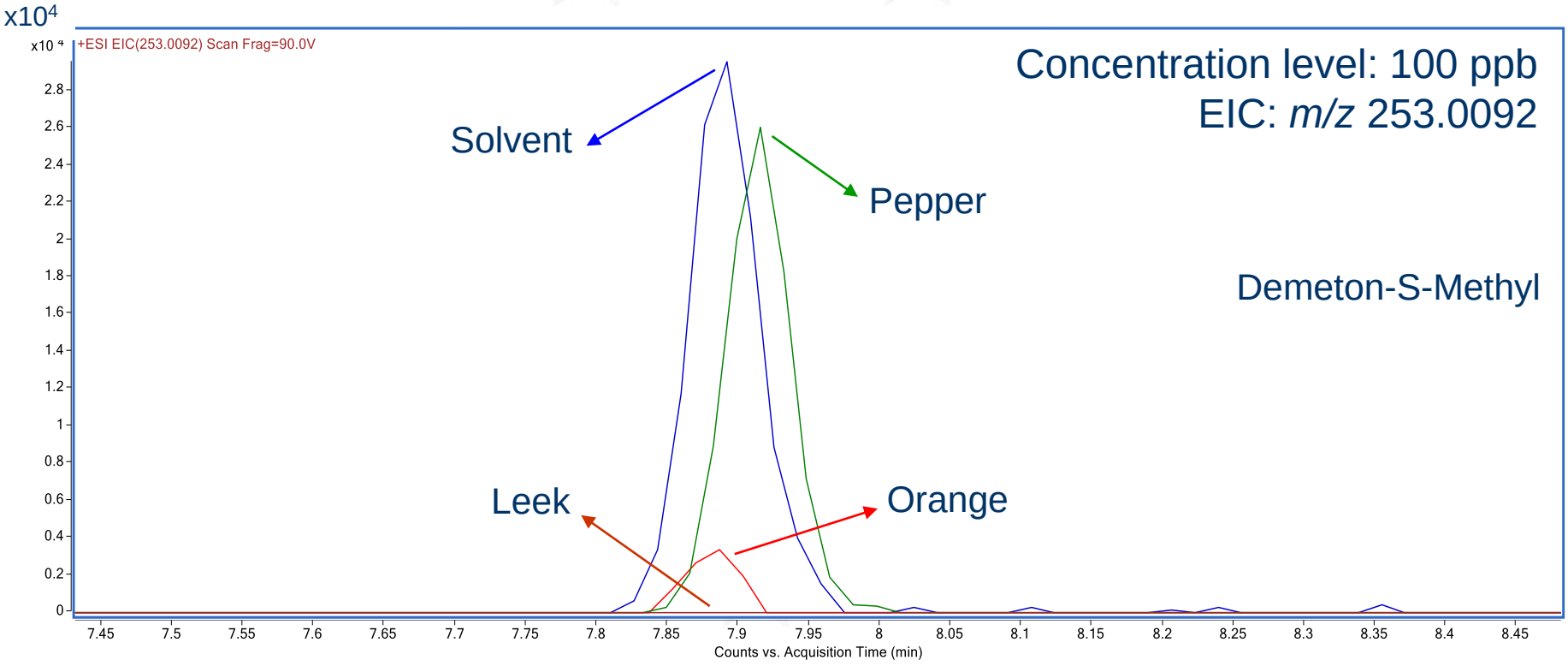

Extraction solvent
% of results
100
90
80
70
60
50
40
30
20
10
0
EUPT-15
EUPT-16
EUPT-17
EUPT-18
EUPT-19
EUPT-20
EUPT-21
EUPT-22
EUPT-23
EUPT-24
Acetone
Acetonitrile
Ethyl Acetate
Methanol

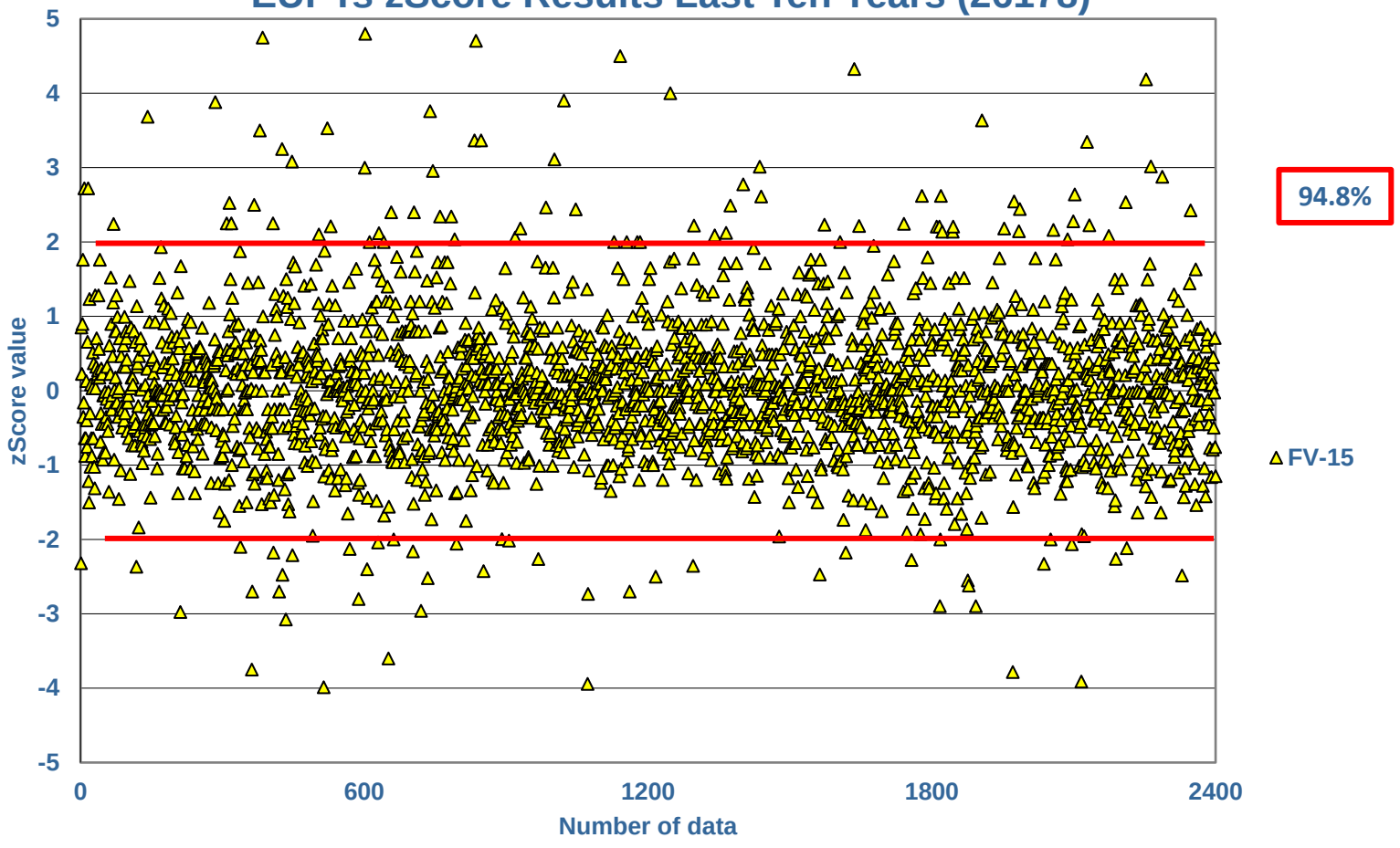
A. Lozano et al. / Food Chemistry 192 (2016) 668–681

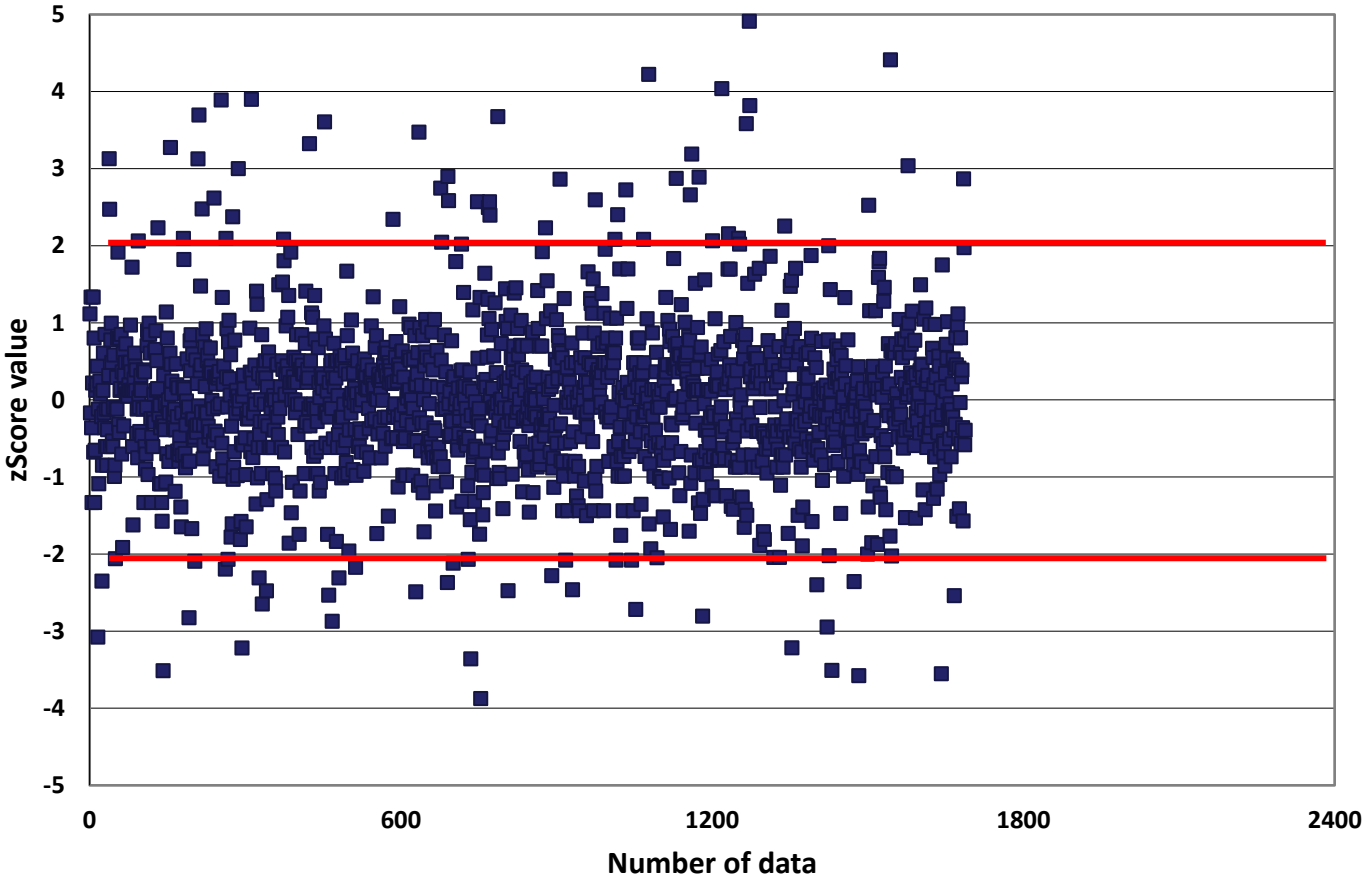


Signal supression due to matrix effects

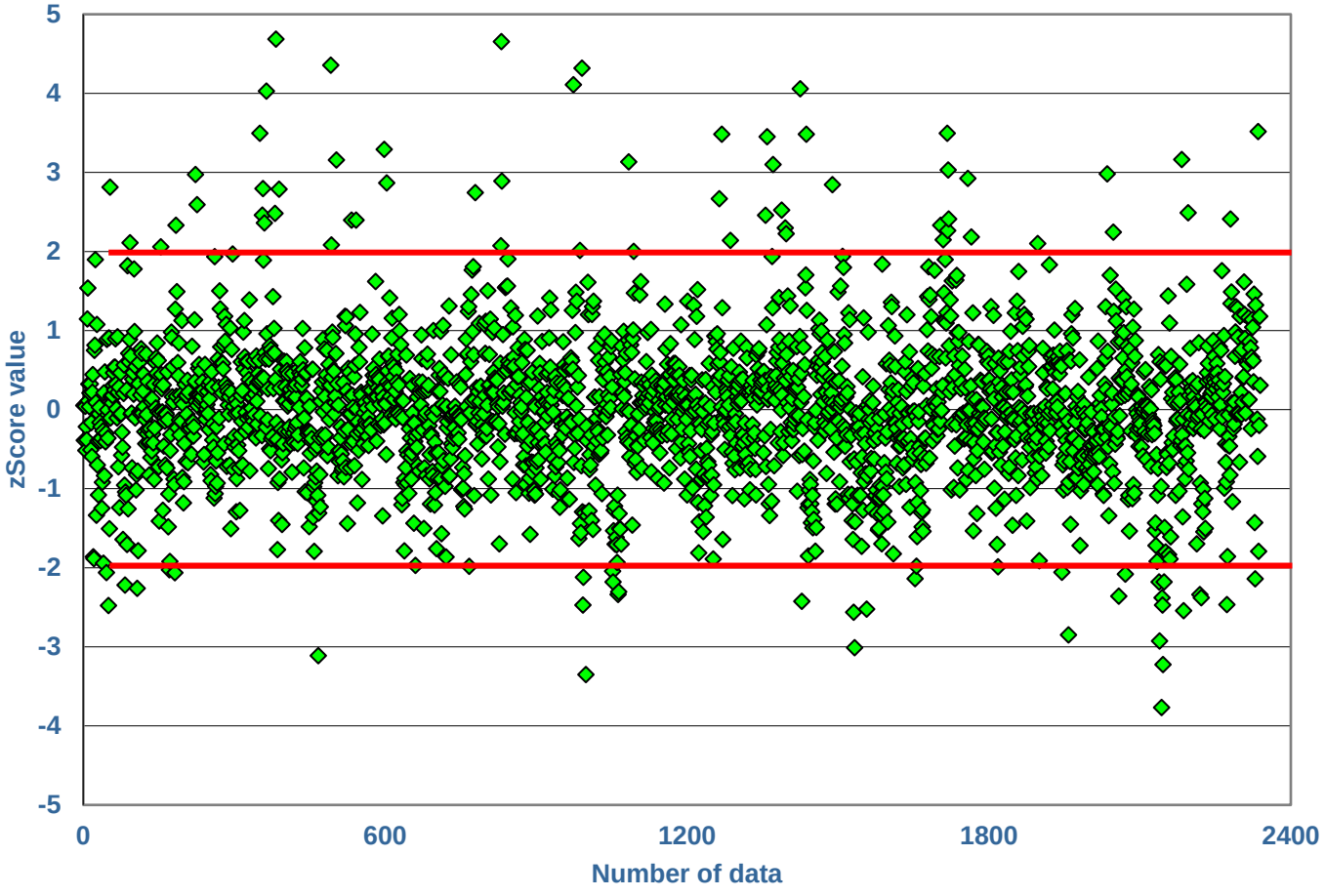
Injection 1g matrix/ml



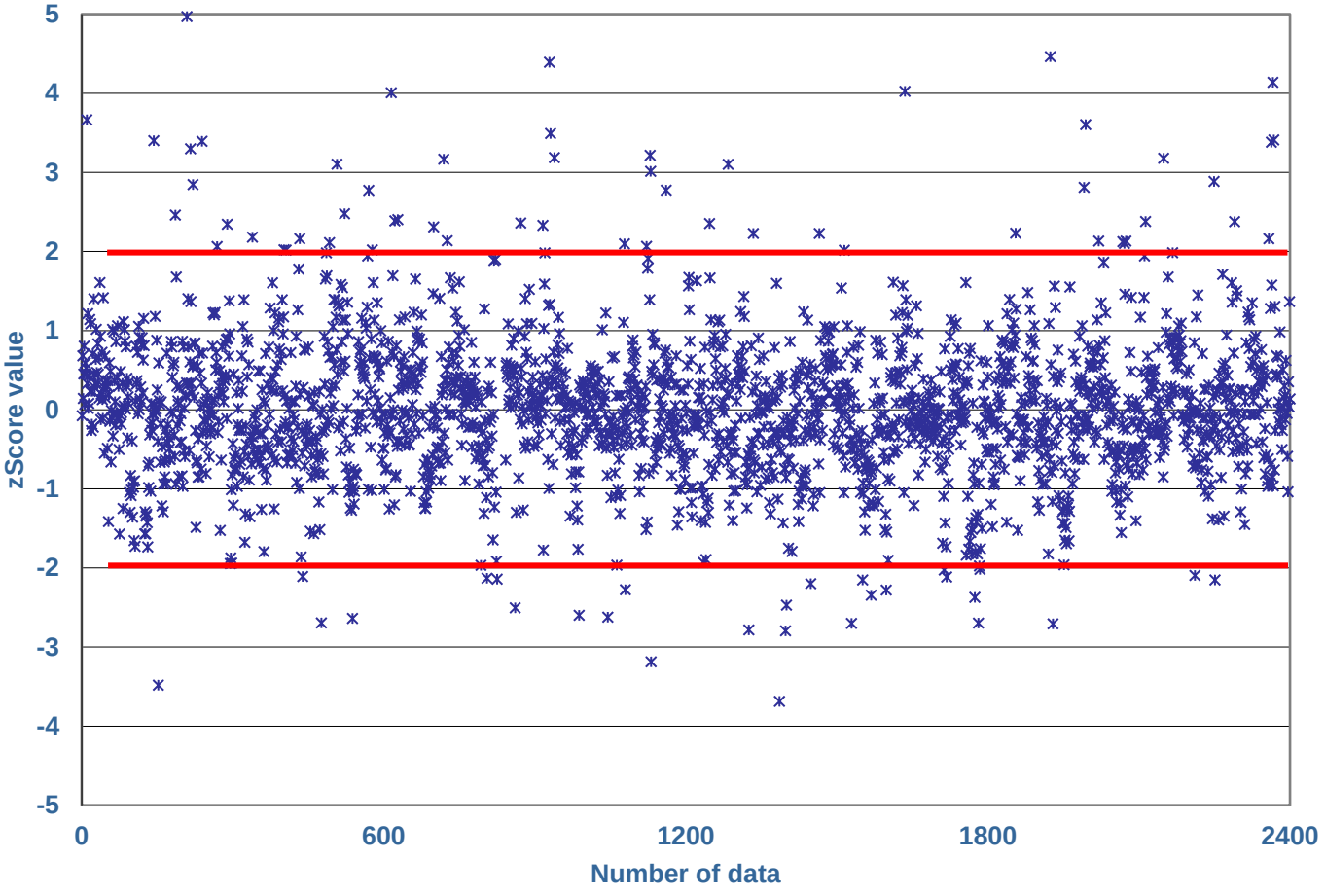

EUPTs zScore Results Last Ten Years (26178)
zScore value
5
4
3
2
1
0
-1
-2
-3
-4
-5
0
600
1200
1800
2400
Number of data
94.8%
FV-15


EUPTs zScore Results Last Ten Years (26178)
zScore value
5
4
3
2
1
0
-1
-2
-3
-4
-5
0
600
1200
1800
2400
Number of data
FV-17

92.1%

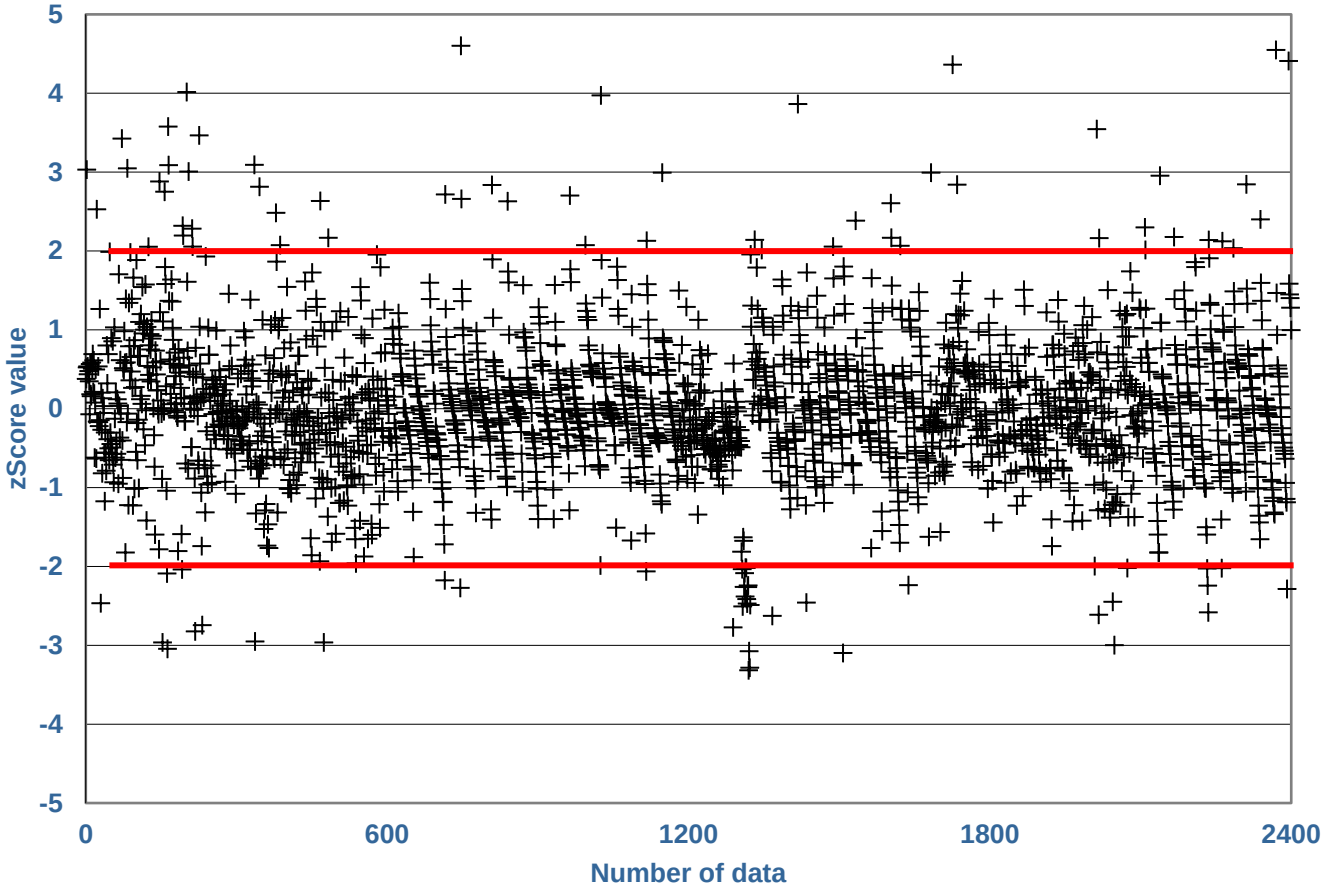

EUPTs zScore Results Last Ten Years (26178)
zScore value
5
4
3
2
1
0
-1
-2
-3
-4
-5
0
600
1200
1800
2400
Number of data
95.4%
FV-19

EUPTs zScore Results Last Ten Years (26178)



95.2%

EUPTs zScore Results Last Ten Years (26178)

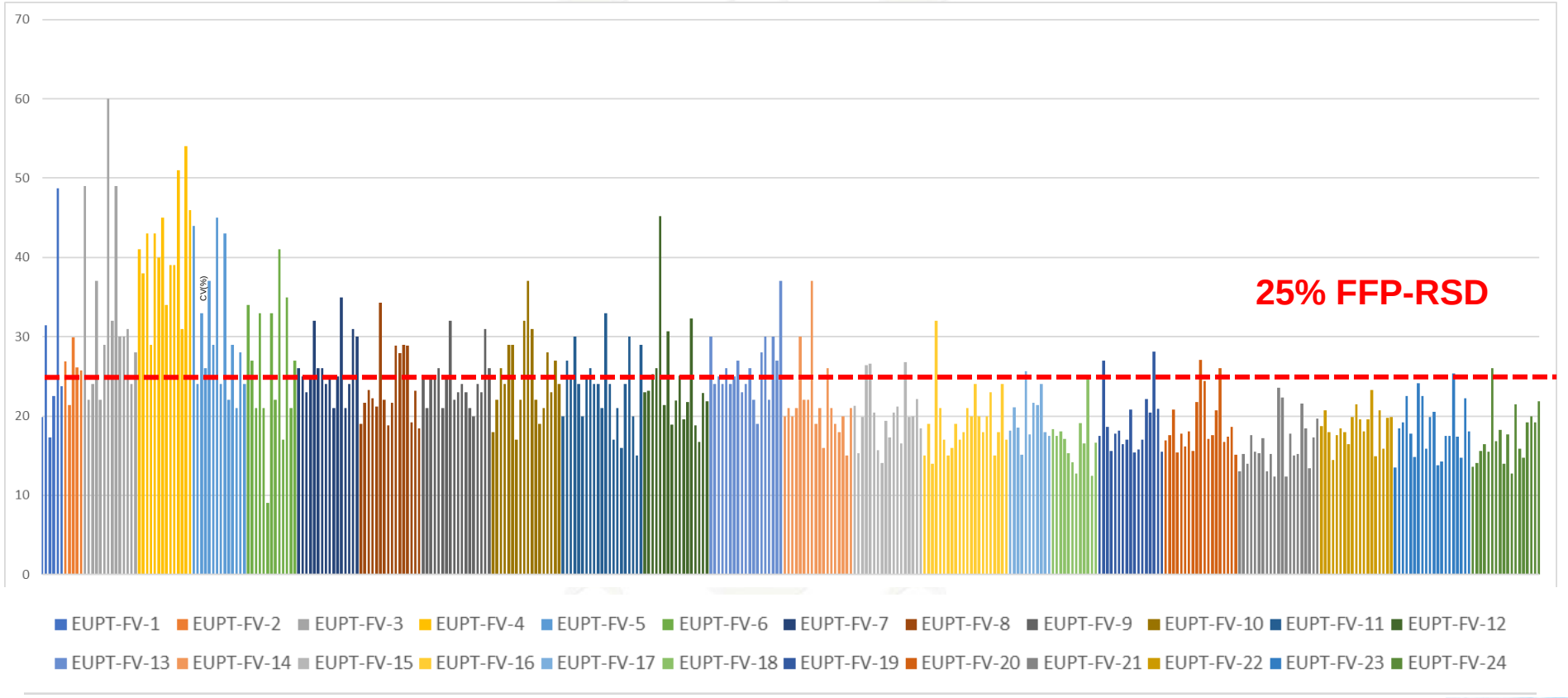


95.1%

+Fv-23

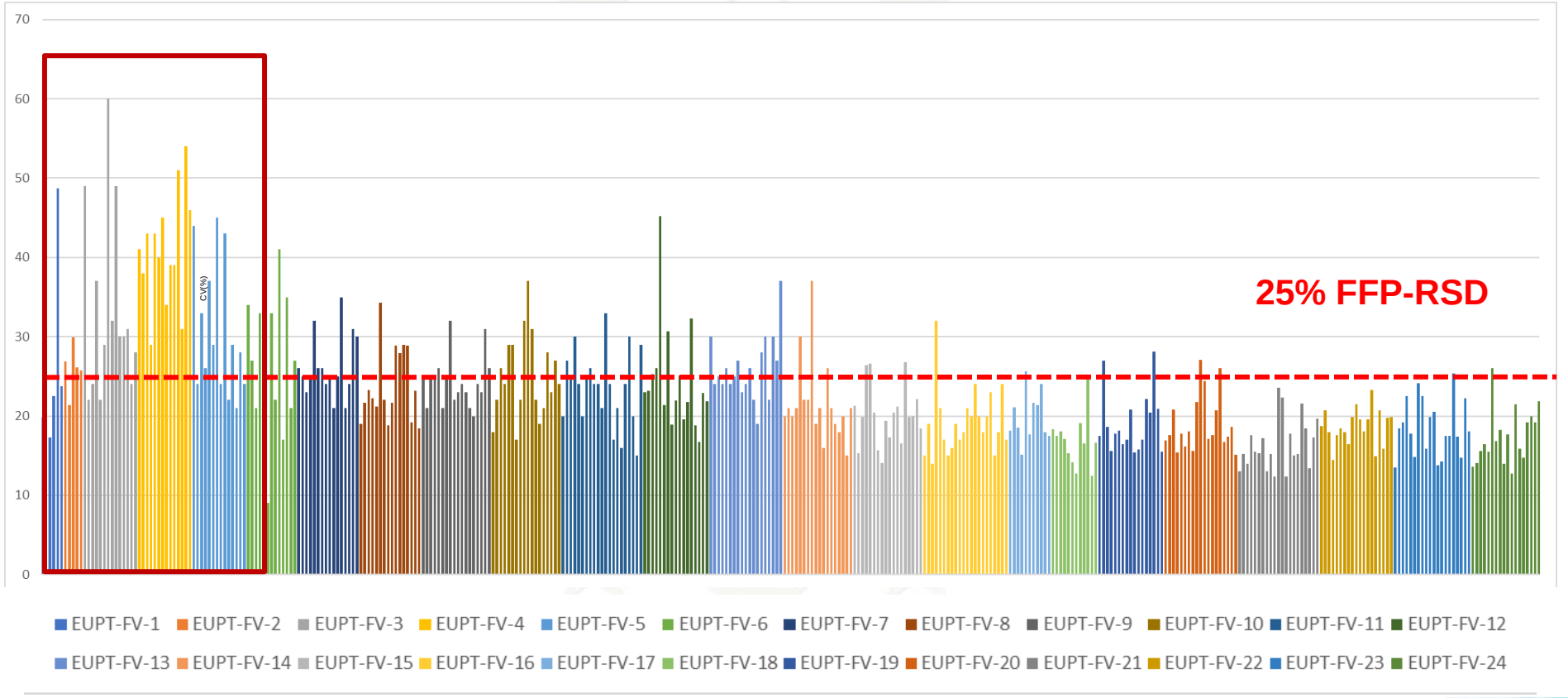
Global improvements
Quantification

Dispersion of results EUPT-FV1-FV24 (1996-2022)



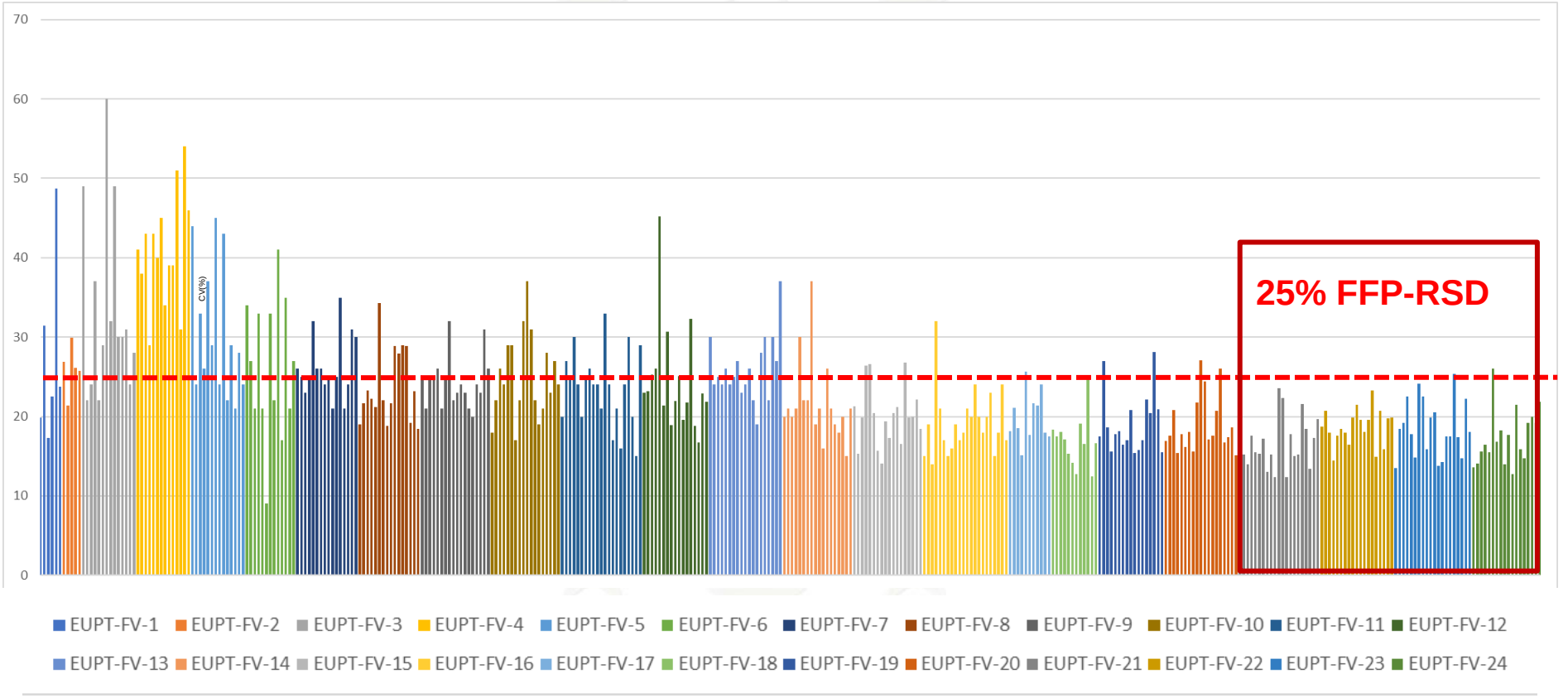
Global improvements
Quantification

Dispersion of results EUPT-FV1-FV24 (1996-2022)



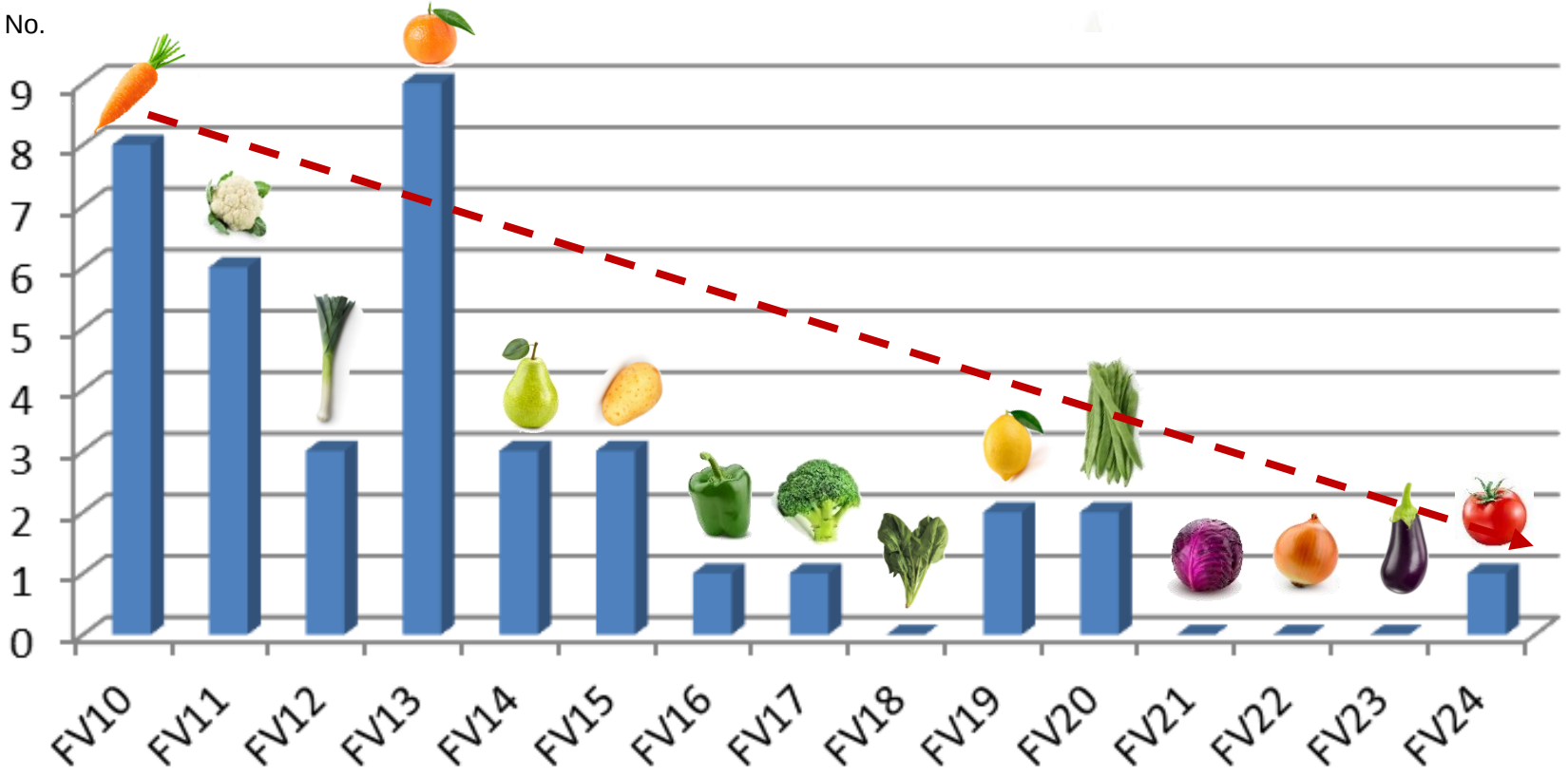
Global improvements
Quantification

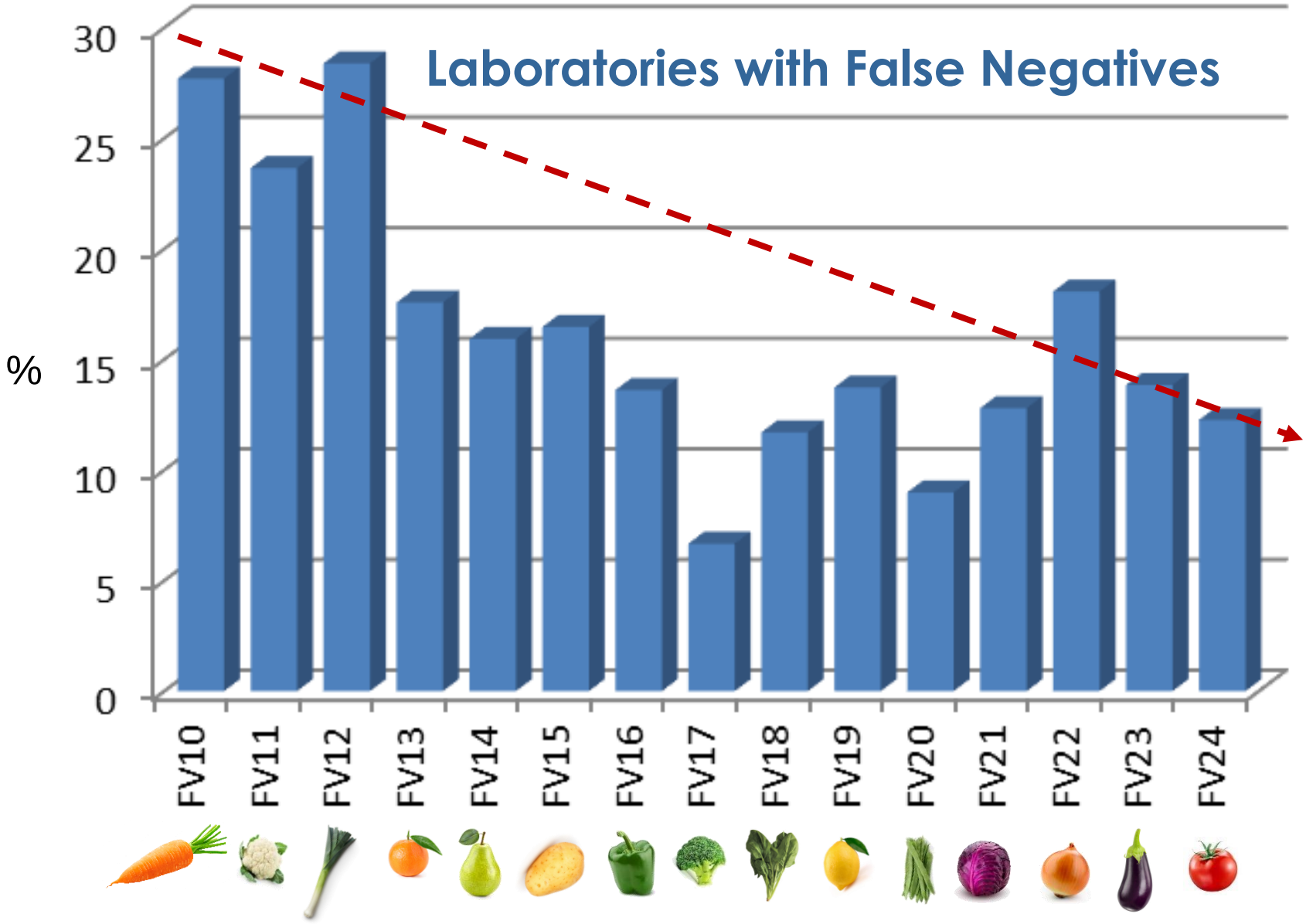
Dispersion of results EUPT-FV1-FV24 (1996-2022)



Global improvements
Quantification

Number of pesticides with CV > 25%




Laboratories with False Negatives
%
30
25
20
15
10
5
0
FV10
FV11
FV12
FV13
FV14
FV15
FV16
FV17
FV18
FV19
FV20
FV21
FV22
FV23
FV24

NEW TECHNOLOGIES

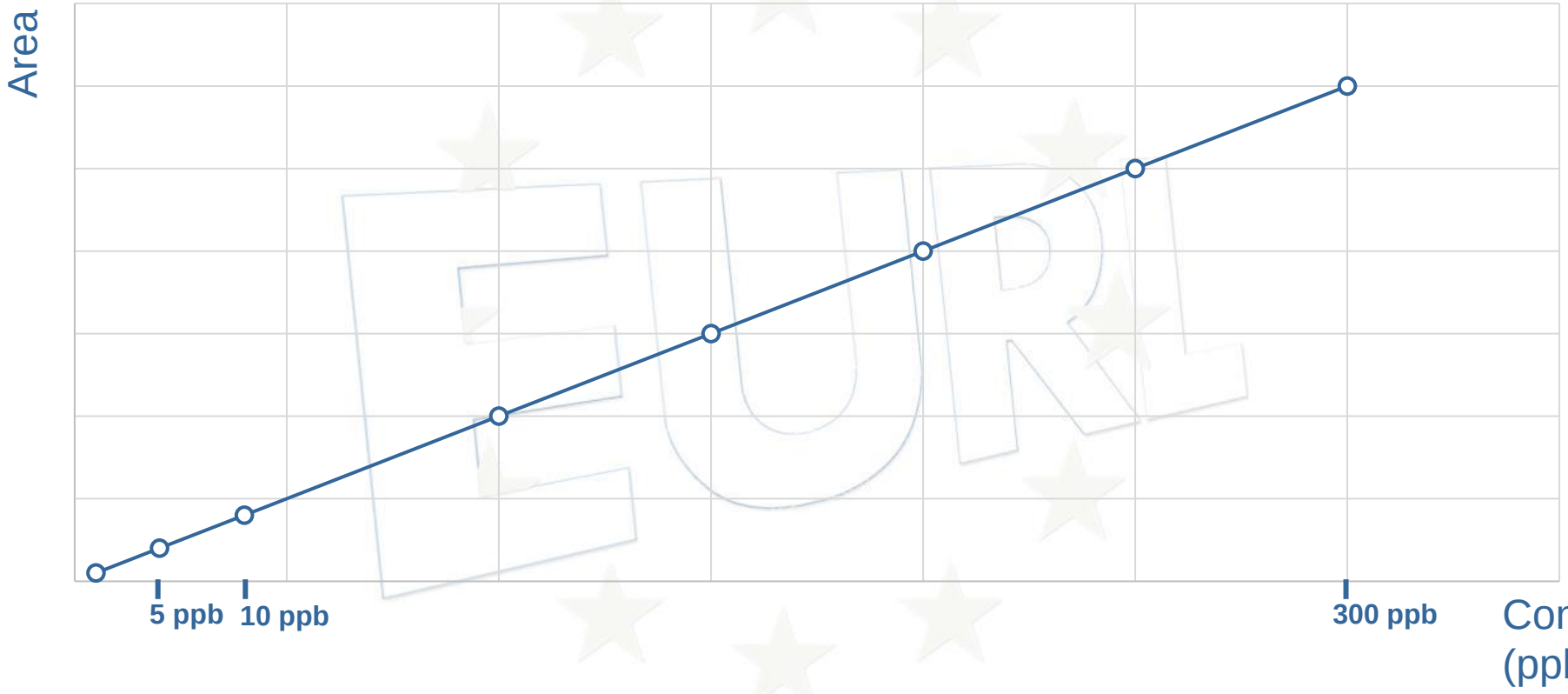
High sensitive LC/GC-TQ-MS/MS
High Resolution Mass Espectrometry
Automation

THEORETICAL IMPLEMENTATION

PRACTICAL IMPLEMENTATION

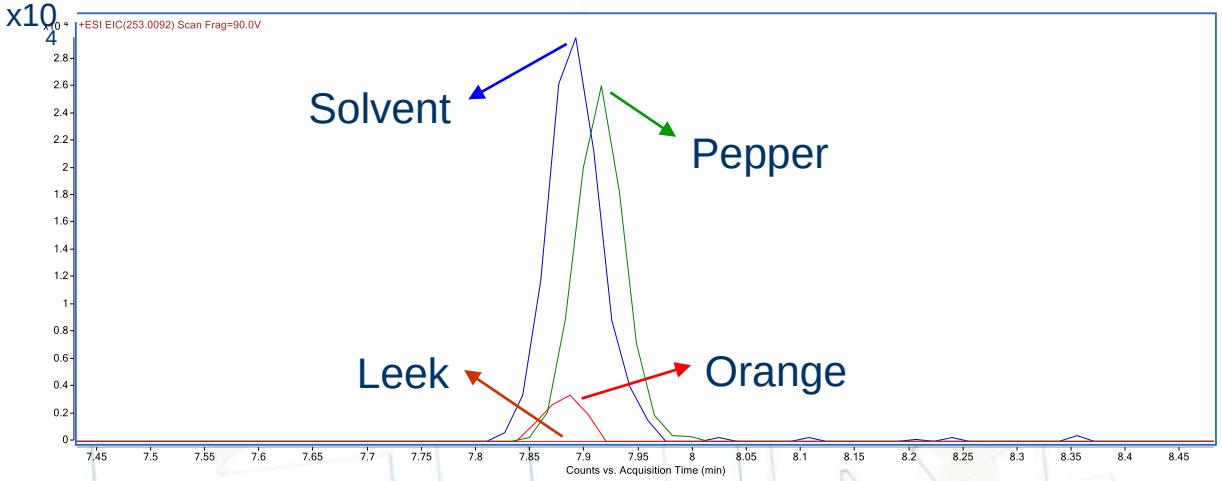
High sensitive LC/GC-TQ-MS/MS

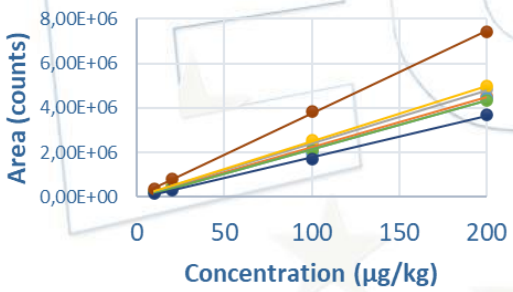
Calibration

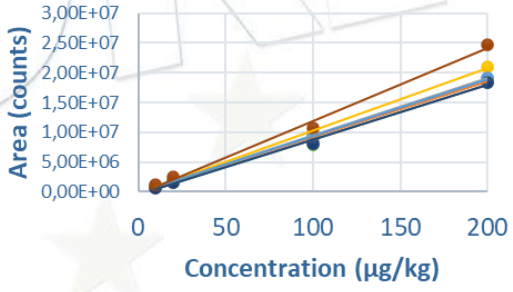


Signal supression due to matrix effects

Injection 1g matrix/ml (5µL-5 mg)





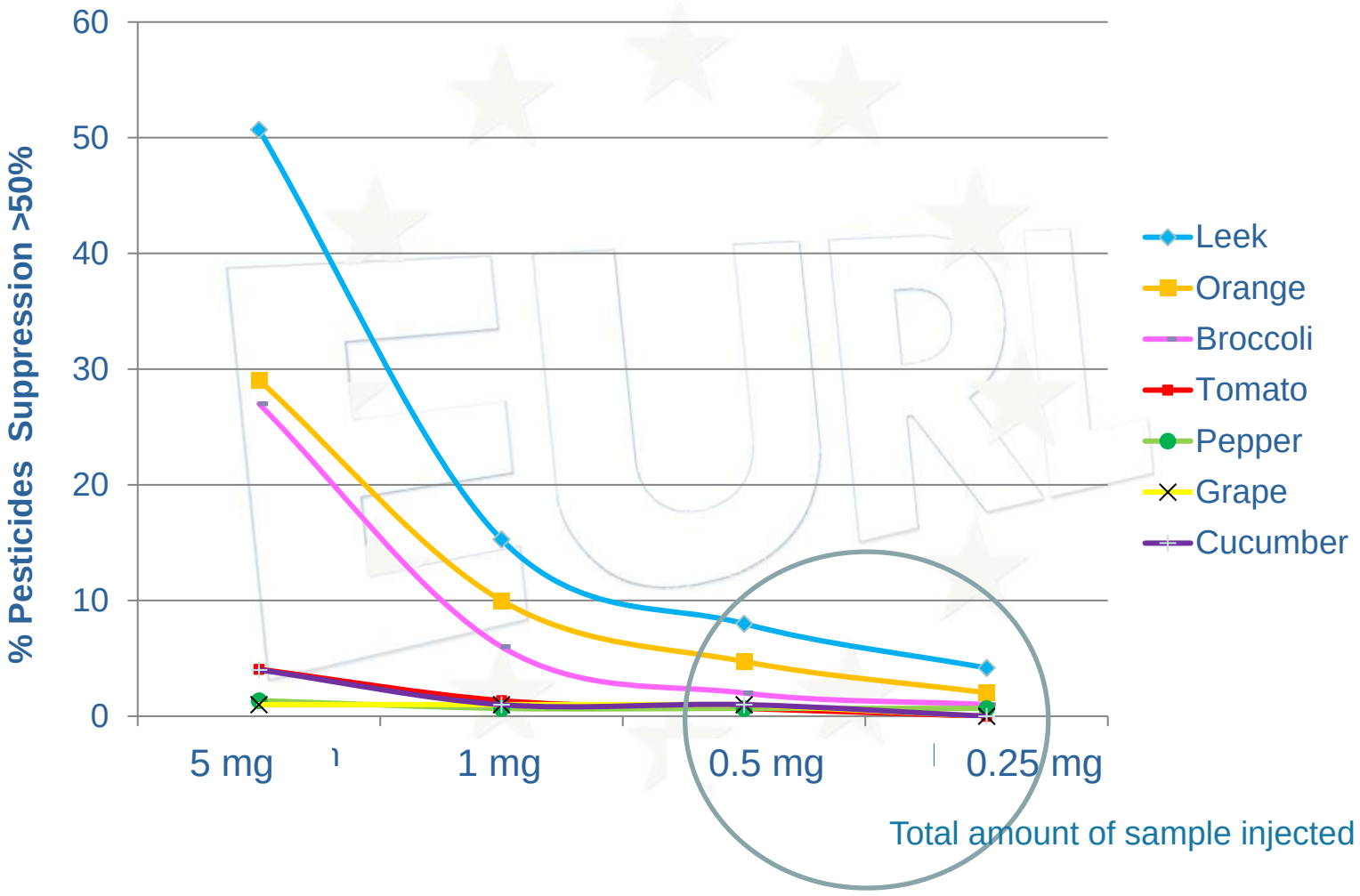


- Broccoli
- Lettuce
- Orange
- Pineapple
- Grapefruit
- Avocado

- Broccoli
- Lettuce
- Orange
- Pineapple
- Grapefruit
- Avocado

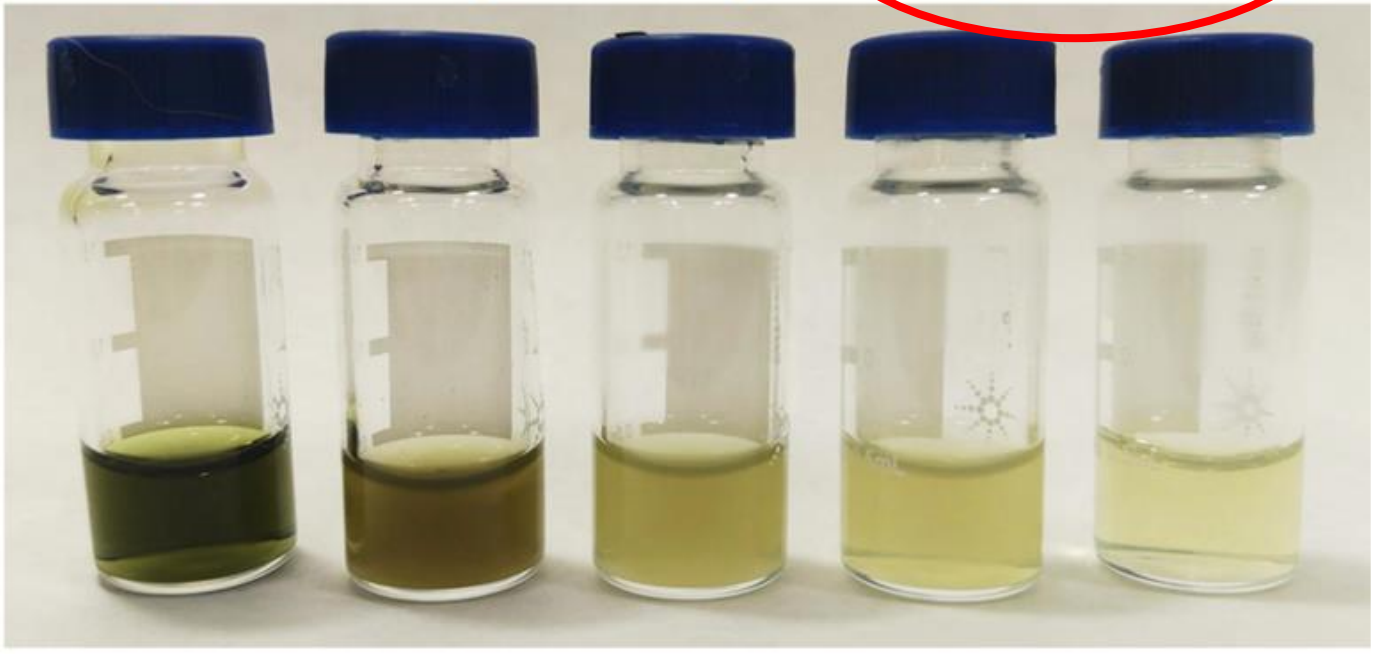
LC-MS

EFFECT OF DILUTION IN "EASY-MEDIUM" COMPLEX MATRICES



Injection volume	Matrix injected in column				
LC: 5 µL	5 mg	2.5 mg	1 mg	0.5 mg	0.25 mg
GC: 1 µL	1 mg	0.5 mg	0.2 mg	0.1 mg	0.05 mg

Green Tea



Dilx0	Dilx2	Dilx5	Dilx10	Dilx20
1 g/mL	0.5 g/mL	0.2 g/mL	0.1 g/mL	0.05 g/mL

Matrix effect of leek matrix over tomato matrix (250 compounds)

Relative matrix effect

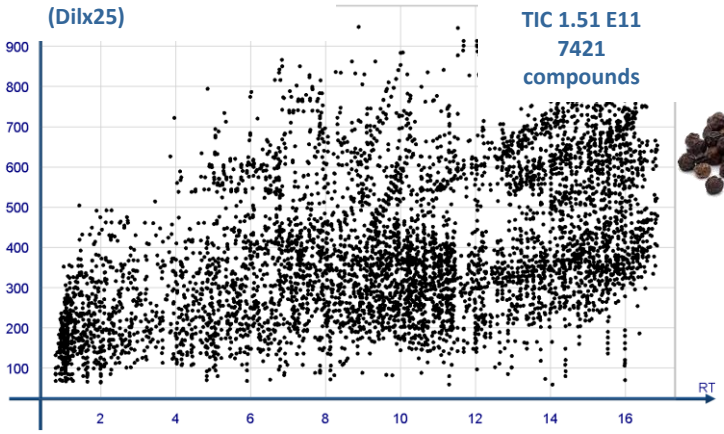
	Leek/Tomato (2.5 µL)	Leek/Tomato (5.0 µL)
Average (%)	-6.6 %	-19.4 %
Median (%)	-7.3 %	-20.9 %
<= |20 %|	168	111
> |20 %| & <= |50 %|	76	111
> |50 %|	6	28
<= |20 %| (%)	67.2 %	44.4 %
> |20 %| & <= |50 %| (%)	30.4 %	44.4 %
> |50 %| (%)	2.4 %	11.2 %

0.2 mg 0.5 mg

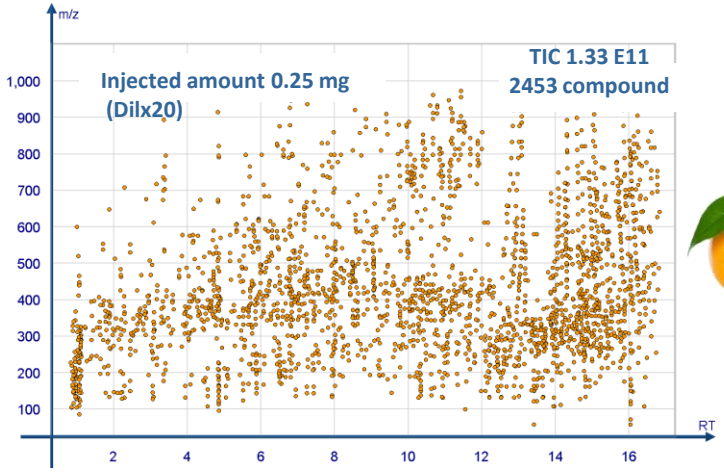
Many commodities

Injected amount 0.2 mg
(Dilx25)

TIC 1.51 E11
7421
compounds



Co-extracted matrix components of Black Pepper
Citrate QuEChERS+EMR clean-up



Injected amount 0.25 mg
(Dilx20)

TIC 1.33 E11
2453 compound

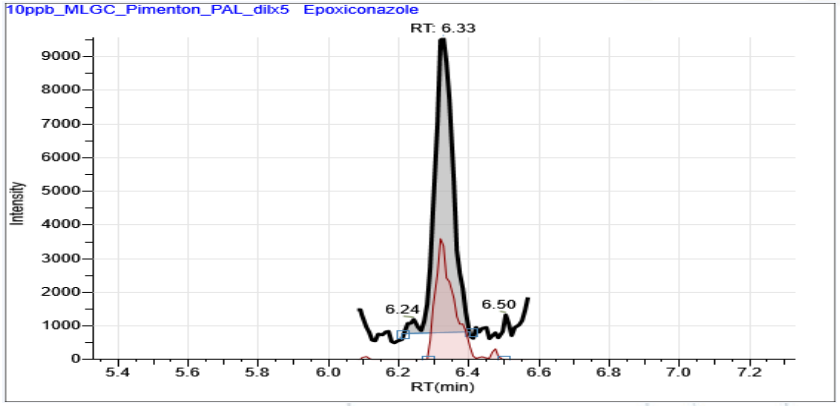
Co-extracted matrix components of Orange LC-TOF-MS, Citrate QuEChERS+PSA clean up

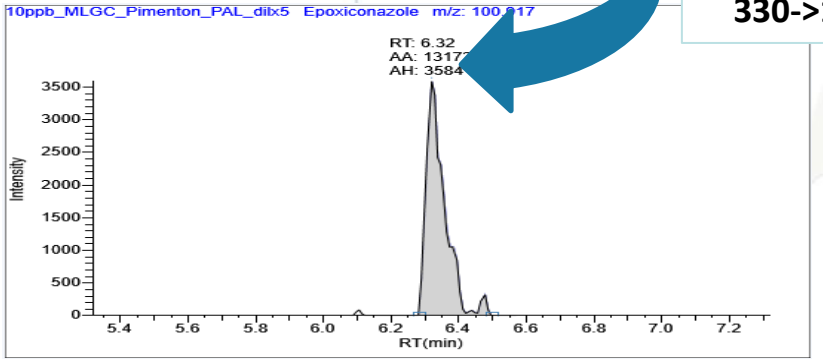
Epoxiconazole

High Sensitive TQ

Spiked standard 10 µg/kg

Total injected amount: 0.066 mg Paprika



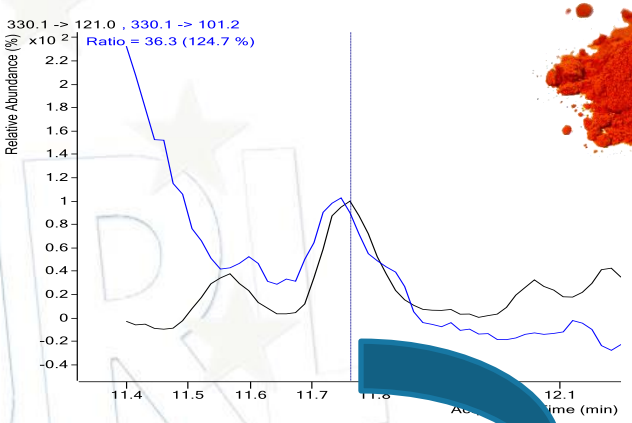


Qualifier transition: 330->101

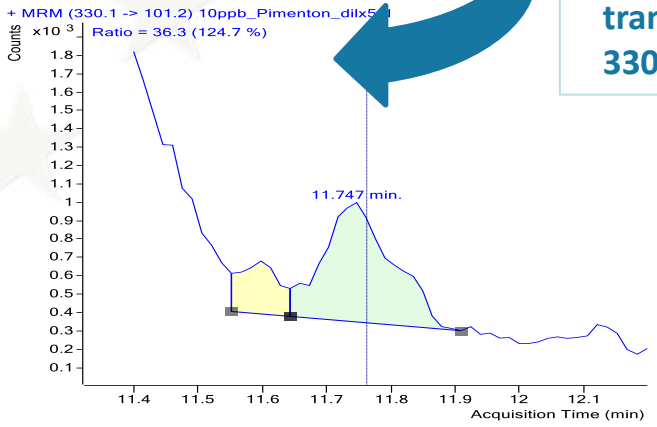
Regular

Spiked standard 10 µg/kg

Total injected amount: 0.13 mg Paprika



Qualifier transition: 330 -> 101

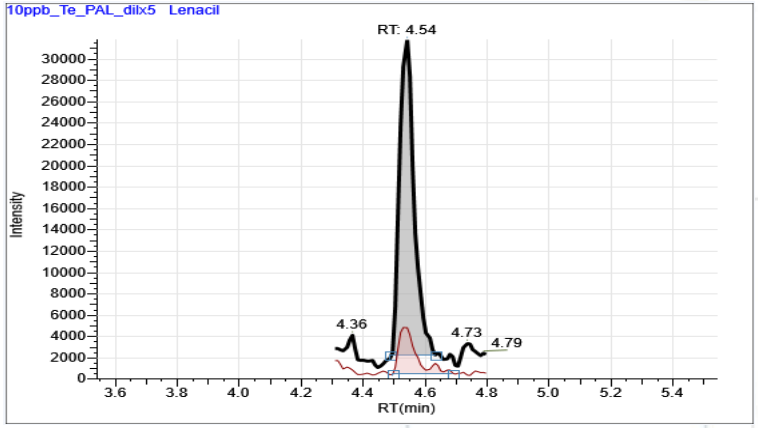


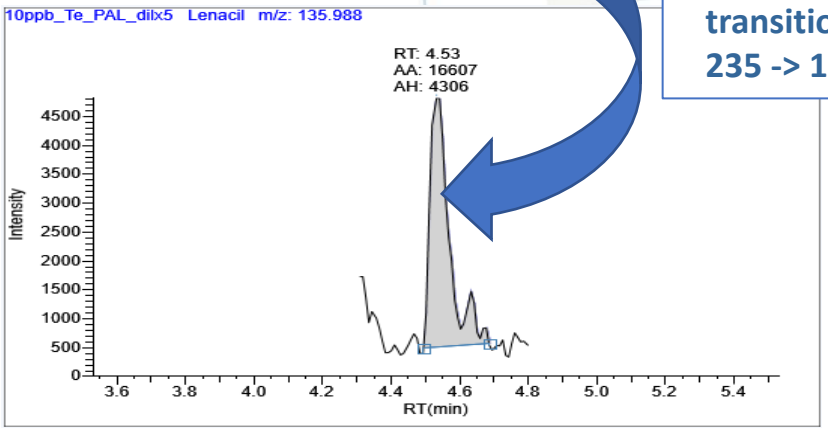
Lenacil

High sensitive TQ

Spiked standard 10 µg/kg

Total injected amount: 0.066 mg Tea

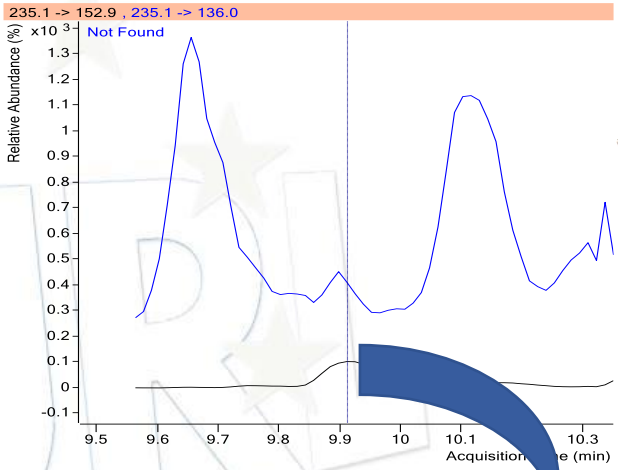




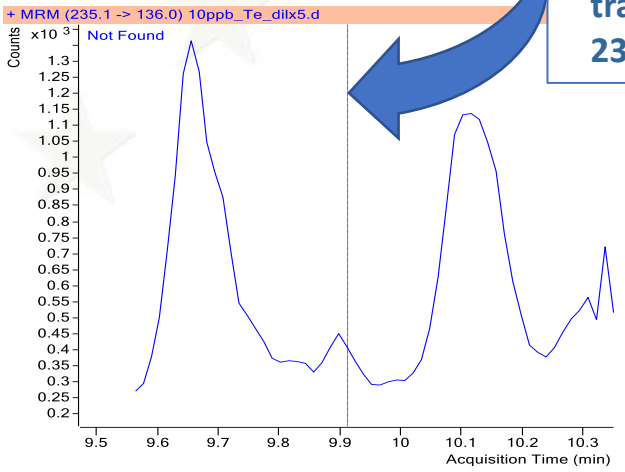
Qualifier transition: 235 -> 136

Spiked standard 10 µg/kg

Total injected amount: 0.13 mg Tea

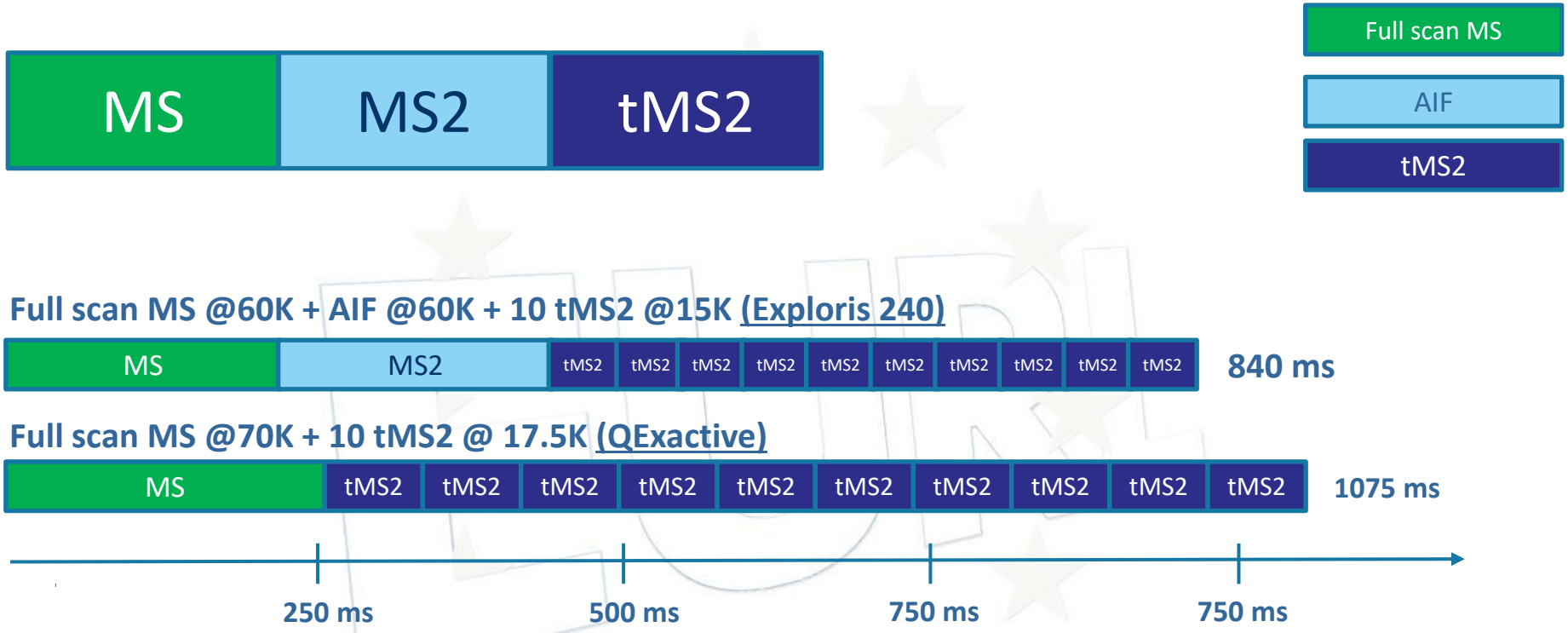


Qualifier transition: 235 -> 136



High Resolution Mass Spectrometry

Comparison of cycle times

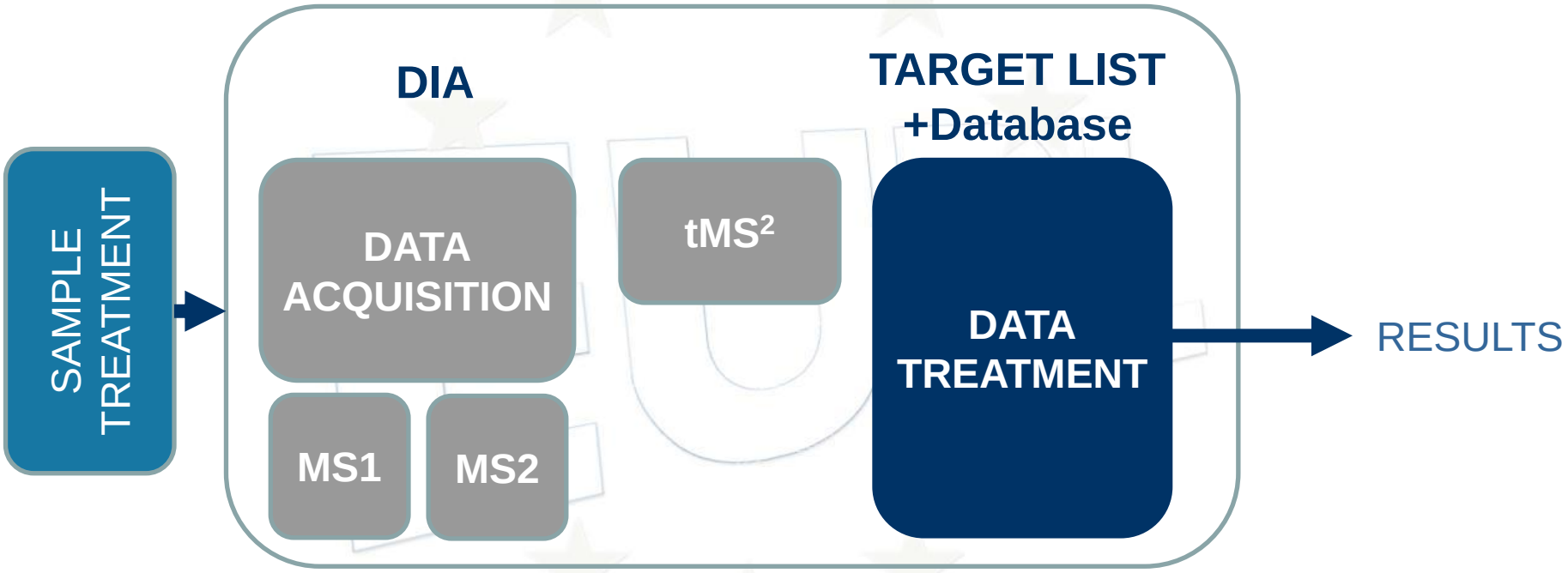


Orbitrap Exploris 240 MS

Vs

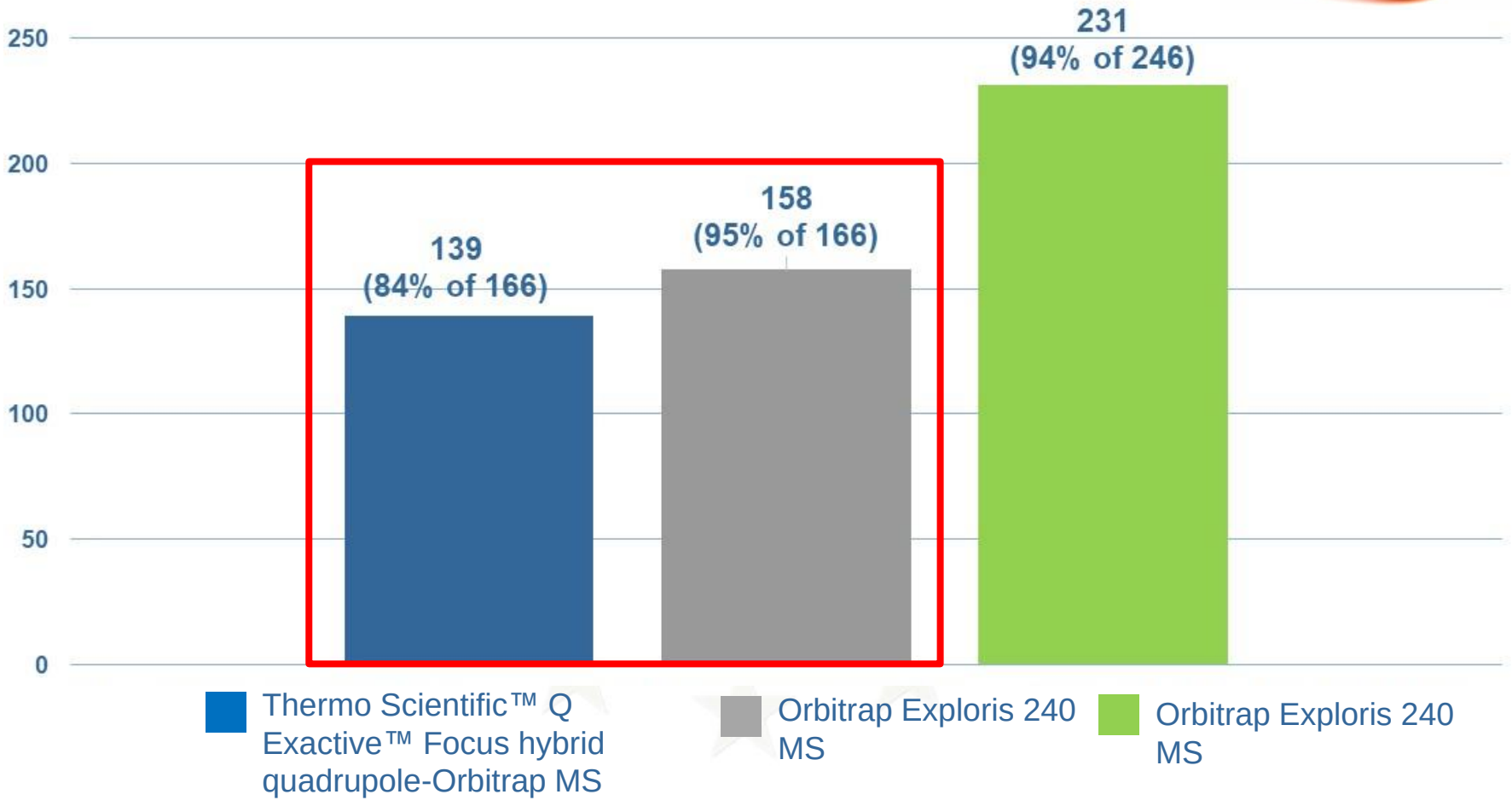
Thermo Scientific™ Q Exactive™ Hybrid Quadrupole-Orbitrap™ MS systems (Classic & Plus)

Parallel Reaction Monitoring (PRM) ≡ Target MS2 (tMS2)



Increasing the scope

Identified pesticides/10ppb in Orange

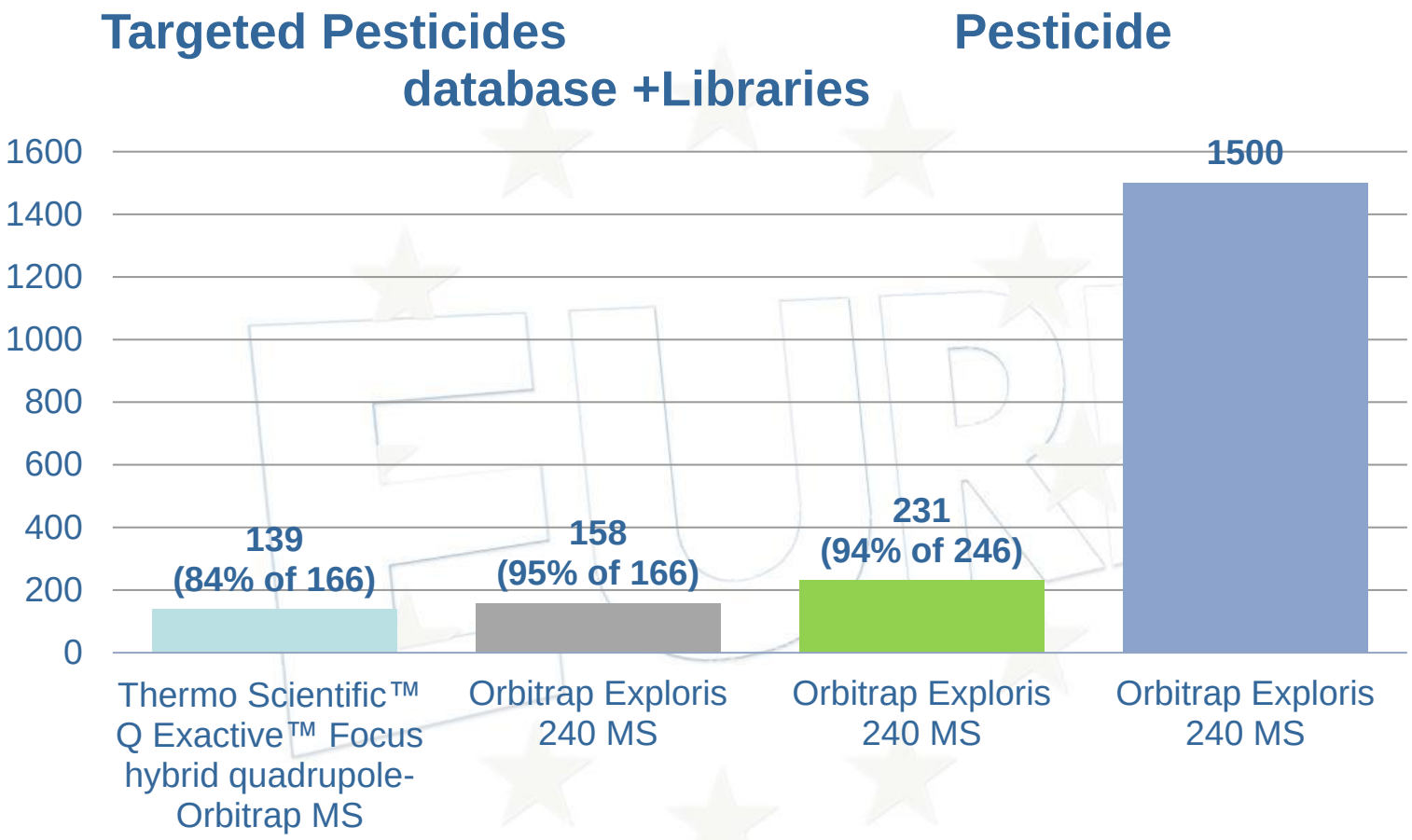


Acquistion modes: QE Focus (FS/AIF), Orbitrap Exploris 240 MS (FS/AIF/tMS2)

246 Compounds

Acephate	Chlorpyrifos	Fenamidone	Iprovalicarb	Paraoxon methyl	Quinoxyfen
Acetamiprid	Chromafenozide	Fenamiphos	Isocarbophos	Penconazole	Quizalofop-ethyl
Alachlor	Clofentezine	Fenamiphos-sulfone	Isoprocarb	Pencycuron	Rotenone
Albendazole	Clomazone	Fenamiphos-sulfoxide	Isoprothiolane	Pendimethalin	Simazine
Aldicarb	Clothianidin	Fenarimol	Isoproturon	Penflufen	Spinosyn A
Aldicarb-sulfone	Coumaphos	Fenazaquin	Isoxaflutole	Penthiopyrad	Spinosyn D
Aldicarb-sulfoxide	Cyazofamid	Fenbendazole	Kresoxim-methyl	Permethrin, trans-	Spinosyn J
Ametoctradin	Cyflufenamid	Fenbuconazole	Lenacil	Phenthoate	Spinosyn L
Anilofos	Cyhalofop-butyl	Fenhexamid	Linuron	Phosalone	Spirodiclofen
Atrazine	Cymoxanil	Fenobucarb	Malaoxon	Phosmet	Spiromesifen
Avermectin B1a	Cyproconazole	Fenoxycarb	Malathion	Phoxim	Spirotetramat
Azinphos-ethyl	Cyprodinil	Fenpropathrin	Mandipropamid	Pirimicarb	Spiroxamine
Azinphos-methyl	Cyromazine	Fenpropidin	Mepanipyrim	Pirimicarb, desmethyl-	Sulfoxaflor
Azoxystrobin	DEET	Fenpropimorph	Metalaxyl	Pirimiphos-methyl	Tebuconazole
BAC10	Demeton-S-methyl	Fenpyrazamine	Metamitron	Prochloraz	Tebufenozide
BAC8	Demeton-S-Methyl-Sulfone	Fenpyroximate	Metconazole	Profenofos	Tebufenpyrad
Benalaxyl	Demeton-S-methylsulfoxide	Fenthion	Methamidophos	Promecarb	Terbuthylazine
Bendiocarb	Diazinon	Fenthion-sulfone	Methidathion	Prometryn	Terbuthylazine-desethyl
Bifenazate	Dichlorvos	Fenthion-sulfoxide	Methiocarb	Propamocarb	Terbutryn
Bifenthrin	Dicrotophos	Fenuron	Methiocarb-sulfone	Propaquizafop	Tetraconazole
Bitertanol	Diethofencarb	Fipronili_POS	Methiocarb-sulfoxide	Propargite	Thiabendazole
Boscalid	Difenoconazole	Flazasulfuron	Methomyl	Propazine	Thiacloprid
Bromacil	Difenoxuron	Flonicamid	Methoxyfenozide	Propiconazole	Thiamethoxam
Bromuconazole	Diflubenzuron	Fluacrypyrim	Metobromuron	Propoxur	Thiobencarb
BTS_44595	Dimethoate	Fluazifop	Metolachlor	Propyzamide	Thiodicarb
BTS_44596	Dimethomorph	Flufenacet	Metolcarb	Proquinazid	Thiophanate-methyl
BTS-40348	Dimethylvinphos, Z-	Flufenoxuron	Metrafenone	Prosulfocarb	Tolfenpyrad
Bupirimate	Diniconazole	Fluometuron	Monocrotophos	Prothioconazole	Triadimefon
Buprofezin	Diuron	Fluopicolide	Monolinuron	Pymetrozine	Triadimenol
Butoxycarboxim	Dodine	Fluopyram	Monuron	Pyraclostrobin	Triallate
Carbaryl	Edifenphos	Flusilazole	Myclobutanil	Pyrethrini	Triazophos
Carbendazim	Emamectin B1a	Fluxapyroxad	Neburon	Pyrethrinii	Trichlorfon
Carbofuran	Epoxiconazole	Formetanate	Nitenpyram	Pyridaben	Triclocarban
Carbofuran, 3OH-	Ethiofencarb	Fosthiazate	Novaluron	Pyridalyl	Tricyclazole
Chlorantraniliprole	Ethion	Haloxyfop	Omethoate	Pyridaphenthion	Trifloxystrobin
Chlorbromuron	Ethiprole	Hexaconazole	Oxadiargyl	Pyridate	Triflumizole
Chlorfenvinphos, B-	Ethirimol	Hexaflumuron	Oxadixyl	Pyrimethanil	Triflumuron
Chlorfluazuron	Ethoprophos	Hexythiazox	Oxamyl	Pyriofenone	Triticonazole
Chloridazon	Etofenprox	Imazalil	Oxasulfuron	Pyriproxyfen	Tritosulfuron
Chlorotoluron	Etoxazole	Imidacloprid	Oxfendazole	Quinalphos	XMC
Chloroxuron	Famoxadone	Indoxacarb	Paclobutrazol	Quinoclamine	Zoxamide

Increasing the scope

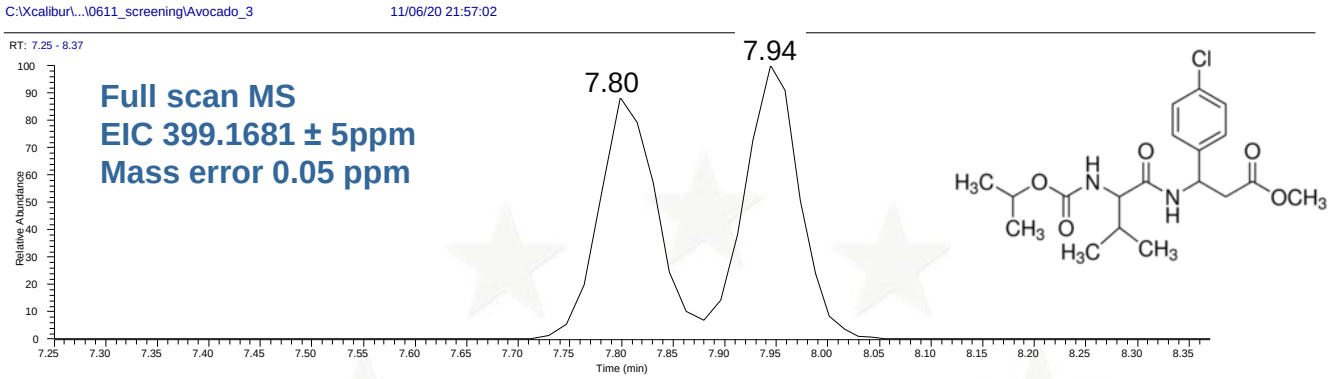


Acquistion modes:

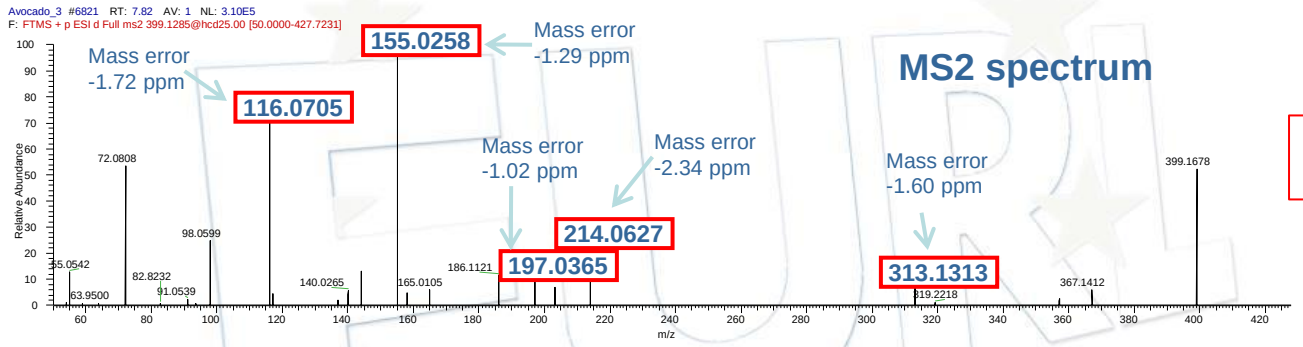
QE Focus (FS/AIF), Orbitrap Exploris 240 MS (FS/AIF/tMS2), Orbitrap Exploris 240 MS (FS/AIF/tMS2/ Data Dependent)

Database 1500 compounds

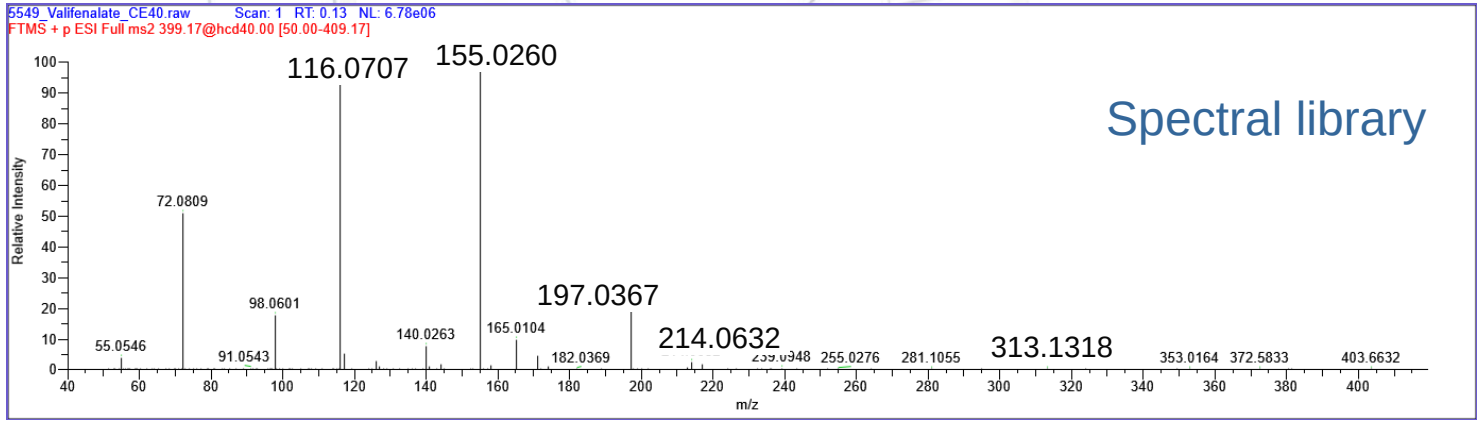
1-(4-Chlorophenyl)piperazine (p-(
1-Aminocyclohexanecarboxylic /
1-Methyl-3-Phenylpiperazine
1-Methylamino-1-(3,4-Methylene
10-Hydroxycarbazepine
11-Hydroxy-Delta-9-Thc
11-nor-9-Carboxy-Delta-9-THC
11-nor-9-Carboxy-Delta-9-THC-[
11-nor-9-Carboxy-Delta-9-THC-[
11-nor-9-Carboxy-Delta-9-THC_|
15-Acetyldeoxynivalenol_M+CH
15-Acetyldeoxynivalenol_M+HC
15-Acetyldeoxynivalenol_M+Na
15-Acetyldeoxynivalenol_M+NH
15-Acetyldeoxynivalenol_M-H
2,6-Dichlorobenzamide
2-Acetamidophenol
2-Hydroxypropoxycarbazone
2-Methyl-4,6-Dinitrophenol
2-NP-AHD
2-NP-AMOZ
2-NP-AMOZ-D5
2-NP-AOZ
2-NP-AOZ-D4
2-NP-SEM
2-Phenylcyclopropylamine
20-beta-Dihydrocortisol
20-beta-Dihydroprednisolone
21-Desacetyl Deflazacort
3,4,5-Trimethacarb
3,4-DMMC
3-Acetamidophenol
3-Acetyldeoxynivalenol_M+CH3
3-Acetyldeoxynivalenol_M+HC(
3-Acetyldeoxynivalenol_M-H
3-Amino-2-Oxazolidinone (AOZ
3-Hydroxystanozolol
3-Indoleacetic Acid
3-Methoxytyramine
3-Methyl-2-Quinoxalinecarboxyli
4-Acetamidoantipyrine
4-Aminoantipyrine
4-Aminobiphenyl
4-Aminophenol
4-EMC
5-Hydroxy Omeprazole
6-beta-Hydrocortisol
6-Methylthiopurine
6-Monoacetylmorphine
6-Phenyl-2-Thiouracil
6-Thioguanine
6beta-OH-21-Desacetyl Deflazac
6beta-OH-Budesonide
7-(2,3-Dihydroxypropyl)Theophy
7-Aminoflunitrazepam
7-Aminonitrazepam
Abamectin
Abamectin B1a
Acamprosate
Acebutolol
Acepromazine
Aceprometazine
Acetalozamide
Acetaminophen
Acetaminophen-D4
Acetamiprid-metabolite-6-chlor
Acetamiprid-metabolite-IM-1-4
Acetamiprid-metabolite-IM-2-1
Acetochlor
Acibenzolar-S-methyl
Acifluorfen
Allidochlor
Allopurinol
Alloxydim
Alminoprofen
Alpha-Ergocryptine
Alpha-Ergocryptine_M-H
Alpha-Ergocryptinine
Alpha-Ergocryptinine_M
Alpha-Hydroxy-Midazola
Alpha-Methylfentanyl
Alpha-Zearalanol
Alprazolam
Alprenolol
Alternariol
Alternariol_M-H
Alternariolmethylether
Alternariolmethylether_I
Altrenogest
Ametryn
Amfepramone
Amicarbazone
Amineptine
Aminocarb
Aminocyclopyrachlor
Aminopyralid
Aminopyrine
Amisulbrom
Amisulpride
Amitriptyline
Amodiaquine
Amoxapine
Amoxicillin
Amoxicilline
Amphetamine
Ampicillin
Amprenavir
Amrinone
Anabasine
Ancymidol
Anhydroecgonine
Anhydroecgonine Methy
Anilazine
Anisotropine Methylbro
Antimycin-A
Antipyrine
Apomorphine
Aprindine
Articaine
Aspon
Astemizole
Asulam
Atazanavir
Atenolol
Atorvastatin
Atracurium
Atraton
Atrazine-D5
Atrazine-Desethyl
Atropine
Azaconazole
Azadirachtin
Azafenidin
Azamethiphos
Azaperol
Azaperone
Azatadine
Azathioprine
Azimsulfuron
Azinphos-methyl-oxon
Azinphos-methyl-oxon_I
Aziprotryne
Benzobicyclon
Benzocaine
Benzofenap
Benzophenone
Benzoximate
Benzoylprop-eth
Benzphetamine
Benzthiazuron
Benzydamine
Benzyladenine
Benzylfentanyl
Bepridil
Beta-Zearalano
Betamethasone
Betamethasone
Betamethasone
Betanechol
Betaxolol
Bezafibrate
Bialaphos
Bioresmethrin
Biperiden
Bis(2-Ethylhexyl
Bisacodyl
Bisoprolol
Bispyribac
Boldenone
Brodifacoum
Bromadiolone
Bromazepam
Bromfenvinpho
Bromfenvinpho
Bromobutide
Bromoxynil
Bromperidol
Brompheniramii
Brompyrazon
Bufencarb
Bufexamac
Buflomedil
Bufotenine
Bumetanide
Buphedrine
Buphedrone
Bupivacaine
Bupropion
Buspirone
Butachlor
Butafenacil
Butafenacil_M+
Butocarboxim
Butorphanol
Butralin
Butroxydim
Buturon
Butylate
Butylbenzylphth
Butylone
Cadusafos
Cafeine
Cafenstrole
Cannabidiol
Cannabinol
Carbadox
Carbamazepine
Carbamazepine
Carbetamide
Carbimazole
Carbinoxamine
Carbofuran, 3OH
Carbofuran-3-K
Chloramben
Chloramphenic
Chloramphenic
Chloranocryl
Chlordiazepoxi
Chlordimeform
Chlorethoxyfos
Chlorimuron-et
Chlormequat C
Chlormezanon
Chlorotetracyc
Chlorothiazide
Chlorphenirami
Chlorphoxim
Chlorproethazi
Chlorpromazin
Chlorpromazin
Chlorpropamid
Chlorpropham
Chlorprothixen
Chlorpyrifos-m
Chlorpyrifos-ox
Chlorsulfuron
Chlortalidone
Chlortetracyclir
Chlorthiamid
Chlorthiophos
Chlortoluron
Ciclesonide
Cilazapril
Cimaterol
Cimbuterol
Cimetidine
Cinchonine
Cinidon-ethyl
Cinnarizine
Cinosulfuron
Ciprofloxacin
Cis-Mefentanyl
Citalopram
Citreoviridin
Citreoviridin_M
Citreoviridin_M
Citrinin
Citrinin_M-H
Clanobutin
Clemastine
Clenbuterol
Clenpenterol
Clenproperol
Clethodim
Clethodim-sulf
Clethodim-sulf
Clethodim-sulf
Clidinium
Clindamycin
Clobazam
Clobetasol Prc
Clobetasone B
Clobutinol
Clodinafop-pro
Clofencet
Clofibrate
Clofilium Tosyl
Clomethiazole
Clomipramine
Clonazepam
Clonidine
Cloprop
Clopyralid
Cloquintocet-m
Cyanazine
Cyanophos
Cyclanilide
Cycloate
Cyclobenzaprine
Cycloheximide
Cyclopiazonic-Aci
Cyclopiazonic-Aci
Cyclosporine A
Cyclosulfamuron
Cycloxydim
Cycluron
Cymarin
Cymoxanil
Cymoxanil_M-C3H
Cypermethrin
Cyphenothrin
Cyprazine
Cyproheptadine
Cyprosulfamide
Cysteine
Cythioate
Cytisine
D-Trans-Allethrin
Daimuron
Dalapon
Daminozide
Danazol
Danofloxacin
Dapsone
Darunavir
Dazomet
Deacetyl Diltiazem
Decoquinate
DEF
Deiquat
Demeton
Demeton-O
Demeton-O-Methy
Demeton-S (Disulf
Demeton-S-sulfon
Demexiptiline
Deoxycorticosterc
Deoxynivalenol_M
Deoxynivalenol_M
Deoxynivalenol_M
Des-(2-Hydroxyeth
Desipramine
Desmedipham
Desmedipham_M+
Desmethyl Nefopa
Desmethylcitalopr
Desmethylclozapir
Desmethyldoxepin
Desmethylmirtazap
Desmetryn
Desonide
Desoximetasone
Desoxycarbadox
Desoxycortone
Despropionyl p-Flu
Detomidine
Dexamethasone
Dextromethorphan
Dextropropoxyphe
Diacetoxyscirpeno
Diacetoxyscirpeno
Diafenthiuron
Dialifor
Diallate
Diamidafos
Diflufenican
Diflufenzopyr
Digoxin
Dihydro Capsaic
Diltiazem
Dimefox
Dimefuron
Dimepiperate
Dimepiperate_M
Dimethachlor
Dimethametryn
Dimethenamid
Dimethirimol
Dimethoxybenzi
Dimethyl Phthal
Dimethylamylam
Dimethylcathino
Dimetilan
Dimetotiazine
Dimetridazole
Dimidium
Dimoxystrobin
Dinitramine
Dinoseb
Dinotefuran
Dinotefuran-me
Dinoterb
Dioxacarb
Dioxathion
Dioxathion_M-C
Diphenamid
Diphenylamine
Dipropetryn
Dipyridamole
Disopyramide
Disulfiram
Disulfoton Sulfc
Ditalimfos
Dithiopyr
DMST
DNOC
Dobutamine
Dodemorph
Domperidone
Dopamine
Doramectin_M+
Doramectin_M+
Dosulepin
Doxapram
Doxepin
Doxorubicin
Doxycycline
Doxylamine
Droperidol
Drospirenone
Duloxetine
Ebastine
Ecgonine
Ecgonine d3
EDDP
Edrophonium
Efavirenz
Emamectin Ben
EMDP
Emetine
Emtricibatine
Enalaprilat
Enrofloxacin
Ephedrine
Epinephrine
Epitestosterone
Etaconazol
Etamiphylline
Ethaboxam
Ethacrynic Ac
Ethametsulfur
Ethidimuron
Ethiofencarb S
Ethiolate
Ethion-monox
Ethofumesate
Ethoxyquin
Ethoxysulfuro
Ethyl Loflazep
Ethyl Paraben
Ethylenethiour
Ethylmorphine
Ethylone
Etifoxine
Etobenzanid
Etodolac
Etomidate
Etoposide
Etoricoxib
Etrimfos
Famotidine
Famphur
Famphur-oxo
Famprofazon
Felbamate
Fenaminosulf
Fenamiphos-(
Fenbendazole
Fenbufen
Fenfuram
Fenofibrate
Fenoprop
Fenoterol
Fenoxanil
Fenoxaprop-e
Fenpiclonil
Fenspiride
Fensulfothion
Fentanyl
Fenthion-oxo
Fentrazamide
Fexofenadine
Finasteride
Firocoxib
Flamprop Isop
Flamprop-M-i
Flamprop-me
Flecainide
Flephedrone
Fleroxacin
Florasulam
Florfenicol
Florfenicol Ar
Florfenicol_M
Florfenicol_M
Florfenicol_M
Fluazifop-But
Fluazifop-P-b
Fluazinam
Fluazuron
Flubendiamide
Flubenzimine
Flucarbazone
Fluconazole
Fludrocortiso
Flufenpyr-ethy
Flumazenil
Fluroxypyr_M-H
Flurprimidol
Flurtamone
Fluspirilene
Flusulfamide
Fluthiacet-meth
Fluticasone
Flutolanil
Flutriafol
Fluvalinate, T-
Fluvoxamine
Fonofos
Foramsulfuron
Forchlorfenuror
Formesafen
Formoterol
Fuberidazole
Furalaxyl
Furaltadone
Furathiocarb
Furazolidone
Furilazole
Furilazole_M-C
Furmecyclox
Fusarenon-X
Fusarenon-X_M
Fusarenon-X_M
Fusarenon-X_M
Gabapentin
Galantamine
gamma-Aminob
Gelsemine
Gibberellic Acid
Glafenine
Glibornuride
Glimepiride
Glutamic Acid
Glyburide
Glycopyrrolate
Griseofulvin
Guaifenesin
Guanabenz
Guanfacine
Halcinonide
Halofenozide
Halofenozide_M
Haloperidol
Haloperidol-D4
Halosulfuron-m
Haloxyfop-2-Et
Haloxyfop-meth
Harmine
Heptaminol
Heptenophos
Heroin
Hexaflumuron
Hexazinone
Hexestrol
Hippuric Acid
Homocysteine
HT2-Toxin
HT2-Toxin_M+(
HT2-Toxin_M+
Hydramethylnor
Hydrocortisone
Hydrocortisone
Hydrolyzed-Fur
Hydroxyfentanyl
Hydroxyitracona
Hydroxyzine
Hymexazol
Ioxynil
Ipconazole
Ipratropium
Iprobenfos
Iproniazid
Ipronidazole
Ipronidazole-
Irebsartan
Isazofos
Isocarbamid
Isocarboxazid
Isofenphos
Isofenphos-o
Isofenphos_I
Isomethiozin
Isoniazide
Isopropalin
Isopropamide
Isoproturon-[
Isopyrazam
Isothipendyl
Isouron
Isoxaben
Isoxadifen-et
Isoxathion
Isoxicam
Isoxsuprine
Itraconazole
Ivermectin
Ivermectin B1
Jervine
Kadethrin
Kanamycin
Karbutilate
Kavain
Ketamine
Ketoconazol
Ketoprofen
Ketorolac
Ketotifen
Kojic-Acid
L-(-)-Noreph
L-Histidine
L-Isoleucine
L-Methionine
L-Methionine
L-PFBS
L-PFDS
L-PFHxS
L-PFOSK
L-Thyronine
L-Tyrosine
Labetalol
Lacidipine
Lacosamide
Lactofen
Lamotrigine
LAMPA
Lansoprazole
Lasalocid
Levomeprom
Levorphanol
Lidocaine
Lincomycin
Linezolid
Lomefloxacir
Loprazolam
Loratadine
Lorazepam
Lormetazepa
Lornoxicam
Medazepam
Medroxyproges
Mefenacet
Mefenpyr-diethy
Mefloquine
Mefluidide
Megestrol Acet
Melatonin
Meleagrin
Meleagrin_M-H
Meloxicam
Melphalan
Mepenzolate
Meperidine
Mephedrone
Mephospholan
Mepivacaine
Meprednisone
Meprobamate
Mepronil
Mescaline
Mesosulfuron-r
Mesotrione
Mesterolone
Metaflumizone
Metanephrine
Metazachlor
Metformin
Methabenzthiaz
Methacrifos
Methacrifos_M
Methandienone
Methaqualone
Methazolamide
Methcathinone
Methedrone
Methenolone
Methfuroxam
Methohexital
Methoprotryne
Methotrexate
Methotrimepraz
Methoxetamine
Methoxsalen
Methoxyamphe
Methoxymethar
Methylephedrin
Methylone
Methylphenidat
Methylpredniso
Methyltestoster
Methysticin
Metoclopramid
Metofluthrin
Metolazone
Metominostrob
Metoprolol
Metosulam
Metoxuron
Metribuzin
Metronidazole
Metronidazole-
Metsulfuron-me
Mevinphos
Mevinphos-Cis
Mexacarbate
Mexiletine
Mianserine
Midazolam
Mifepristone
Miglitol
Mycophenolic-Ac
Mycophenolic-Ac
Mycophenolic-Ac
N,N-Dimethyltrypt
N-Butylscopolam
N-Desmethyl Mep
N-Desmethylclob
N-Desmethylfluni
N-Desmethyltrimi
N-Desmethylvenl
N-EtFOSAA
N-Ethylbuphedror
N-MeFOSAA
N-Methylscopola
Nabumetone
Nadolol
Nafcillin
Nafronyl Oxalate
Nalbuphine
Naled
Nalidixic Acid
Nalorphine
Naloxone
Naltrexone
Nandrolone Deca
Naphthaleneacet
Naphyrone
Napropamide
Naproxene
Naptalam
Narasin_M+Na
Narasin_M+NH4
Narasin_M-H
Nebivolol
Nefazodone
Neosolaniol_M+(
Neosolaniol_M+I
Neostigmine
Neriifolin
Netilmicin
Nevirapine
Nicarbazin
Nicardipine
Niclosamide
Nicosulfuron
Nicotine
Nifedipine
Nifenazone
Niflumic Acid
Nifuroxazide
Nikethamide
Nimesulide Reduc
Nimodipine
Nithiazine
Nitralin
Nitrazepam
Nitrendipine
Nitrofurazone
Nivalenol_M+CH
Nivalenol_M+HC
Nizatidine
Nomifensine
Nor-LSD
Norbenzoylecgon
Norbormide
Norbuprenorphine
Norcocaine
Nordazepam
Norephedrine
Norepinephrine
Norethandrolone
Ohmefentanyl
Oleandrin
omega-Hydroxynorfen
Omeprazole Sulphone
Ondansetron
Opipramol
Orbencarb
Orbifloxacin
Ormetoprim
Orphenadrine
ortho-Chlorophenylpip
Oryzalin
Ouabain
Oxabetrinil
Oxacillin
Oxadiazon
Oxamyl-oxime
Oxatomide
Oxaziclomefone
Oxcarbazepine
Oxine-Copper
Oxitropium
Oxolinic Acid
Oxprenolol
Oxycarboxin
Oxyclozanide
Oxycodone
Oxydemeton Methyl
Oxyfluorfen
Oxymorphone
Oxyphenbutazone
Oxyphenonium
Oxytetracycline
Paclitaxel
Papaverine
Parathion
Parathion-methyl-oxo
Parathion-oxon
Paraxanthine
Paroxetine
Patulin
Paxilline
Paxilline_M+CH3OO
Paxilline_M+HCOO
Paxilline_M-H
Pebulate
Pefloxacin
Penbutolol
Penfluridol
Penfluron
Penicillic-Acid
Penicillic-Acid_M-H
Penicillin-G
Penicillin-V
Penoxsulam
Pentamidine
Pentanochlor
Pentedrone
Pentylone
Perazine
Perphenazine
PFBA
PFDA
PFDoA
PFHpA
PFHxA
PFHxDA
PFNA
PFOA
PFODA
PFPeA
Phosphamidon
Phthalic Acid, Bis-(
Phthalic Acid, Bis-(
Phthalic Acid, Bis-(
Phthalic Acid, Bis-(
Phthalic Acid,Bis-N
Physostigmine
Picaridin
Picloram
Picloram_M-H
Picolinafen
Picoxystrobin
Pilocarpine
Pimozide
Pindolol
Pindone
Pinoxaden
Pioglitazone
Pipamperone
Pipemidic Acid
Pipenzolate
Piperalin
Piperonyl-butoxide
Piperophos
Pipotiazine
Piracetam
Pirbuterol
Pirimiphos-ethyl
Piroxicam
Posaconazole
Pramipexole
Prazepam
Prazepam-D5
Prazosin
Prednisone
Pregabalin
Pretilachlor
Pridinol
Prifinium
Prilocaine
Primaquine
Primidone
Primisulfuron-met
Probenazole
Probenecid
Procainamide
Prochlorperazine
Procyazine
Procyclidine
Prodiamine
Prohexadione
Prolintane
Promethazine
Prometon
Propachlor
Propafenone
Propanil
Propantheline
Propaphos
Propentofylline
Propericiazine
Propetamphos
Propham
Propham_M-C3H
Propionyl Promazi
Propisochlor
Propizepine
Propoxycaine
Propoxycarbazone
Propoxyphene
Propylene Thioure
Pyriftalid
Pyrilamine
Pyrimethamin
Pyrimidifen
Pyrinuron
Pyrithiobac
Pyroquilon
Pyroxasulfone
Pyroxsulam
Quinclorac
Quinidine
Quinine
Quinupramine
Quizalofop-M
R(-)-Apocode
R-Chloroquine
Rabenzazole
Ractopamine
Rafoxanide
Raltegravir
Ramipril
Ranitidine
Remifentanyl
Repaglinide
Rescinnamine
Resmethrin
Retrorsine
Ribavirin
Ricinine
Rifabutin
Rimsulfuron
Risperidone
Rofecoxib
Romifidine
Ronidazole
Ropivacaine
Roquefortine-
Roquefortine-
Rosiglitazone
Roxithromycir
Rufinamide
S-(-)-Dropropi
S-Metolachlo
Saflufenacil
Salbutamol
Salmeterol
Salvinorin A
Saquinavir
Sarafloxacin
Schradan
Scopolamine
Sebuthylazine
Sebuthylazine-
Secbumeton
Sedaxane
Senecionine
Sertraline
Sethoxydim
Siduron
Sildenafil Citra
Simeconazole
Simetone
Simetryn
Solanidine
Solanine
Sotalol
Sparfloxacin
Sparteine
Spinetoram 1
Spinetoram 2
Spinosad A
Sulfamethoxazole
Sulfamethoxypyrida
Sulfamonomethoxi
Sulfanitran
Sulfaphenazole
Sulfapyridine
Sulfaquinoxaline
Sulfasalazine
Sulfathiazole
Sulfentrazone
Sulfentrazone_M+N
Sulfisomidine
Sulfisoxazole
Sulfometuron-meth
Sulfosulfuron
Sulfotep
Sulindac Sulfide
Sulprofos
Sumatriptan
SWEP
T-2-Toxin
T-2-Toxin_M+Na
T-2-Toxin_M+NH4
Tacrine
TCMTB
Tebupirimfos
Tebutam
Tebuthiuron
Temazepam
Tembotrione
Temephos
Tentoxin
Tentoxin_M+CH3O
Tentoxin_M+HCOC
Tentoxin_M+NH4
Tentoxin_M-H
Tenuazonic-Acid
Tenuazonic-Acid_N
TEPP
Tepraloxydim
Terbacil
Terbinafine
Terbucarb
Terbufos
Terbufos-oxon-sulf
Terbufos-sulfone
Terbufos_M-C4H7
Terbumeton
Terbutaline
Terfenadine
Testosterone
Testosterone 17-En
Testosterone 17-Isc
Testosterone 17-Pr
Testosterone 17-Un
Testosterone Acet
Testosterone Benz
Testosterone Cypic
Testosterone Deca
Testosterone Prop
Tetrachlorvinphos
Tetracycline
Tetramethrin
Tetramisole
Tetrazepam
TFMPP
THC
THC-COOH
Thenylchlor
Theobromine
Thiabendazole,5OH
Timolol
Tinidazole
Tiocarbazil
Tiotropium
Tixocortol Pivalate
Tobramycin
Tofisopam
Tolbutamide
Tolbutamide_M-H
Tolmetin
Tolylfluanid
Tolylfluanid_M-CCl2FS
Torsemide
Tralkoxydim
Tramadol
Tranexamic Acid
Trazodone
Trenbolone
Tri-Isobutyl Phosphate
Triamcinolone Acetonid
Triamcinolone Hexacetc
Triamterene
Triasulfuron
Triazamate
Triazolam
Triazoxide
Tribenuron-methyl
Tributyl Phosphate
Trichlamide
Trichloronat
Triclabendazole
Triclopyr
Tridemorph
Trietazine
Trifloxysulfuron
Trifluoperazine
Trifluperidol
Triflupromazine
Triflusulfuron-methyl
Triforine
Triforine_M-CH2NO
Trihexyphenidyl
Trimetazidine
Trimethacarb, 2,3,5-
Trimethoprim
Trimethoxyamphetamine
Trimipramine
Trinexapac-ethyl
Tripelennamine
Tropatepine
Tropicamide
Tylosin
Uniconazole
Uradipil
Valdecoxib
Valethamate
Valifenalate
Valproamide
Valsartan
Vamidothion
Vamidothion-sulfone
Vardenafil
Venlafaxine
Verapamil
Vernolate
Verrucarol
Viloxazine
Vincristine
Voriconazole
Warfarin
Xipamide



Valifenalate in avocado (2 peaks)



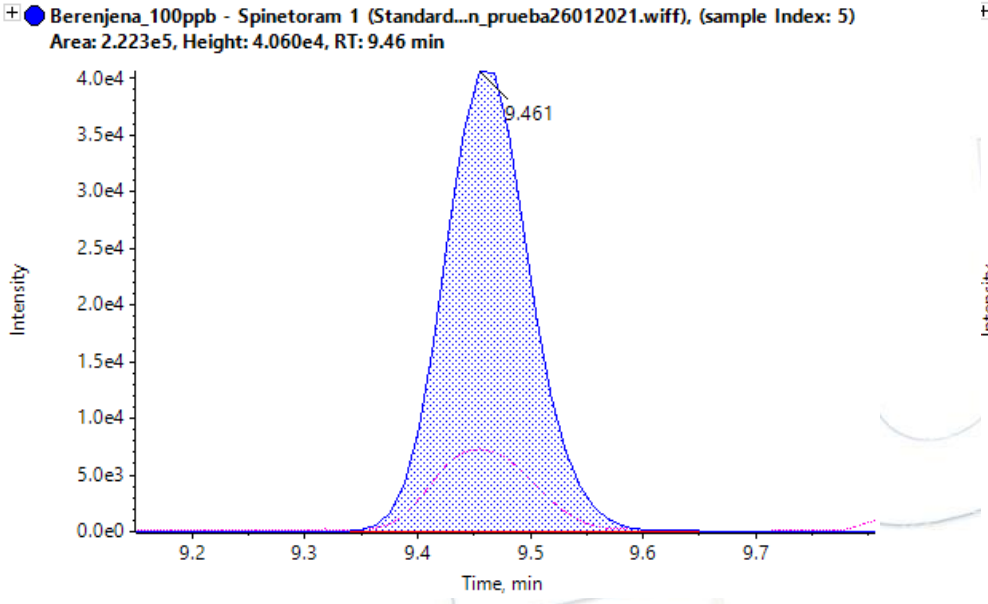
Fragment ion present in the database



False Positives

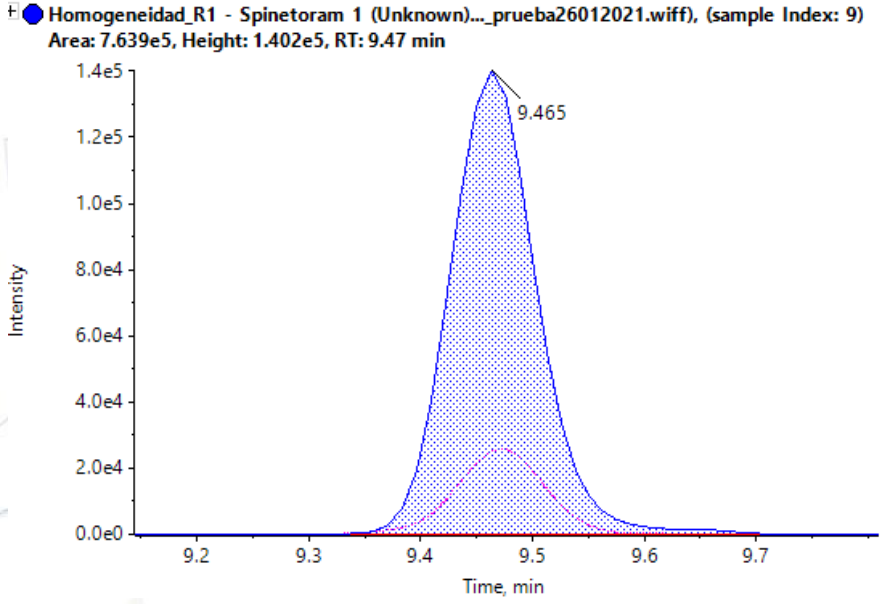
Spinetoram J
LC-MS/MS

Standard 0.1 mg/kg
(aubergine blank matrix)



SRM 1: 748.3>142.1
SRM 2: 748.3>98.1
Ion ratio: 0.2125

FV23 Sample



SRM 1: 748.3>142.1
SRM 2: 748.3>98.1
Ion ratio: 0.1922

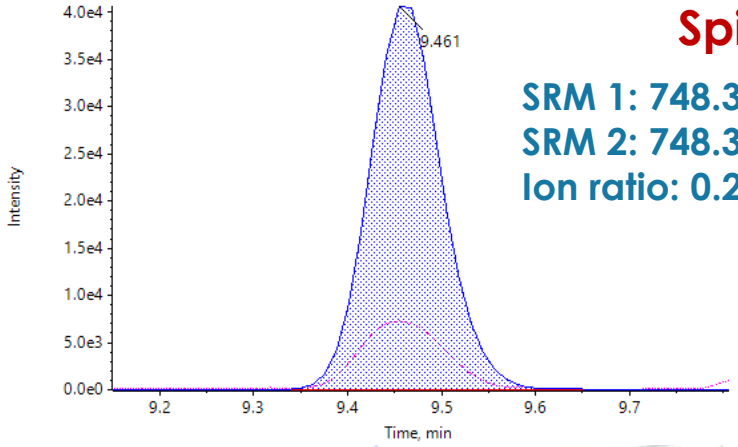
False Positives

Spinetoram J
LC-MS/MS

Standard 0.1 mg/kg
(aubergine blank matrix)

FV23 Sample

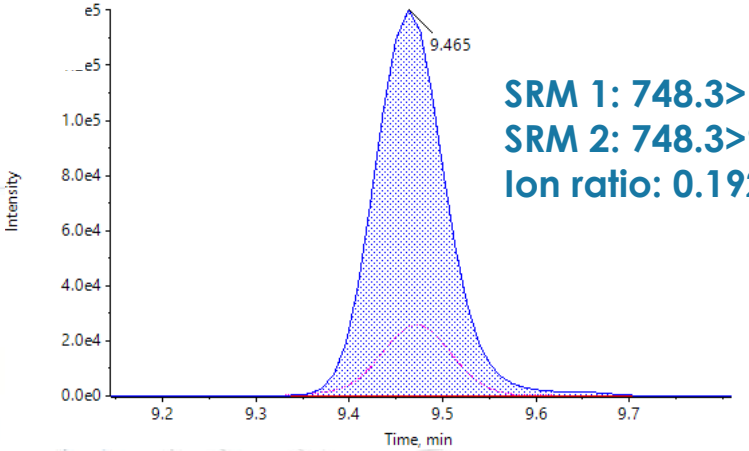
Berenjena_100ppb - Spinetoram 1 (Standard...n_prueba26012021.wiff), (sample Index: 5)
Area: 2.223e5, Height: 4.060e4, RT: 9.46 min



Spinetoram

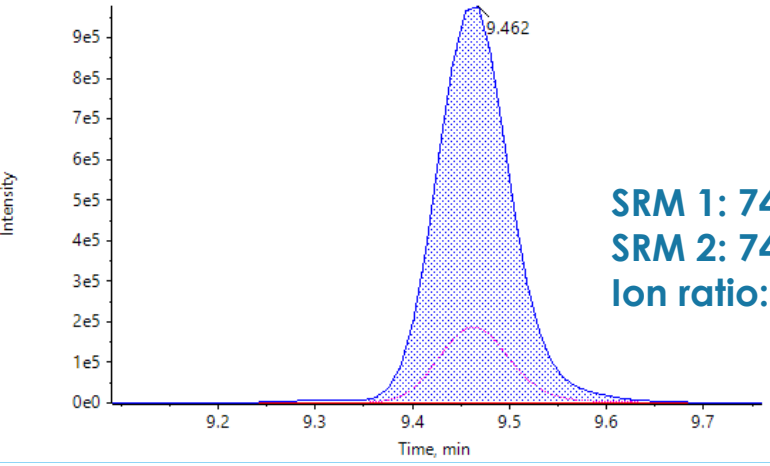
SRM 1: 748.3>142.1
SRM 2: 748.3>98.1
Ion ratio: 0.2125

Homogeneidad_R1 - Spinetoram 1 (Unknown)..._prueba26012021.wiff), (sample Index: 9)
Area: 7.639e5, Height: 1.402e5, RT: 9.47 min



SRM 1: 748.3>142.1
SRM 2: 748.3>98.1
Ion ratio: 0.1922

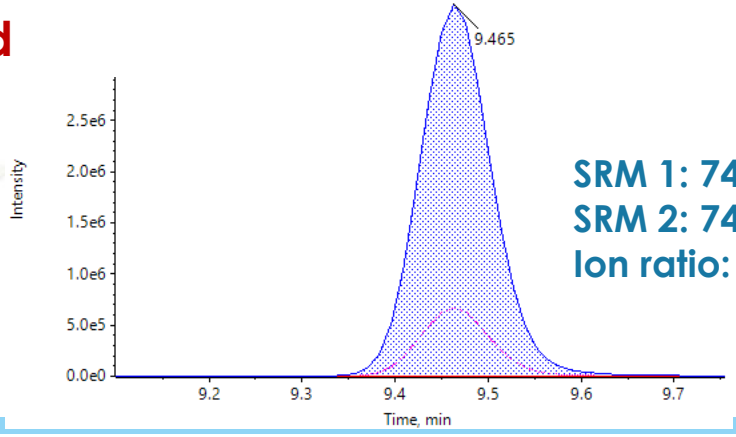
Berenjena_100ppb - Spinosyn D 1 (Standard..._prueba26012021.wiff), (sample Index: 5)
Area: 5.387e6, Height: 9.766e5, RT: 9.46 min



Spinosad

SRM 1: 746.2>142.0
SRM 2: 746.2>98.2
Ion ratio: 0.1915

Homogeneidad_R1 - Spinosyn D 1 (Unknown)...prueba26012021.wiff), (sample Index: 9)
Area: 1.988e7, Height: 3.634e6, RT: 9.47 min

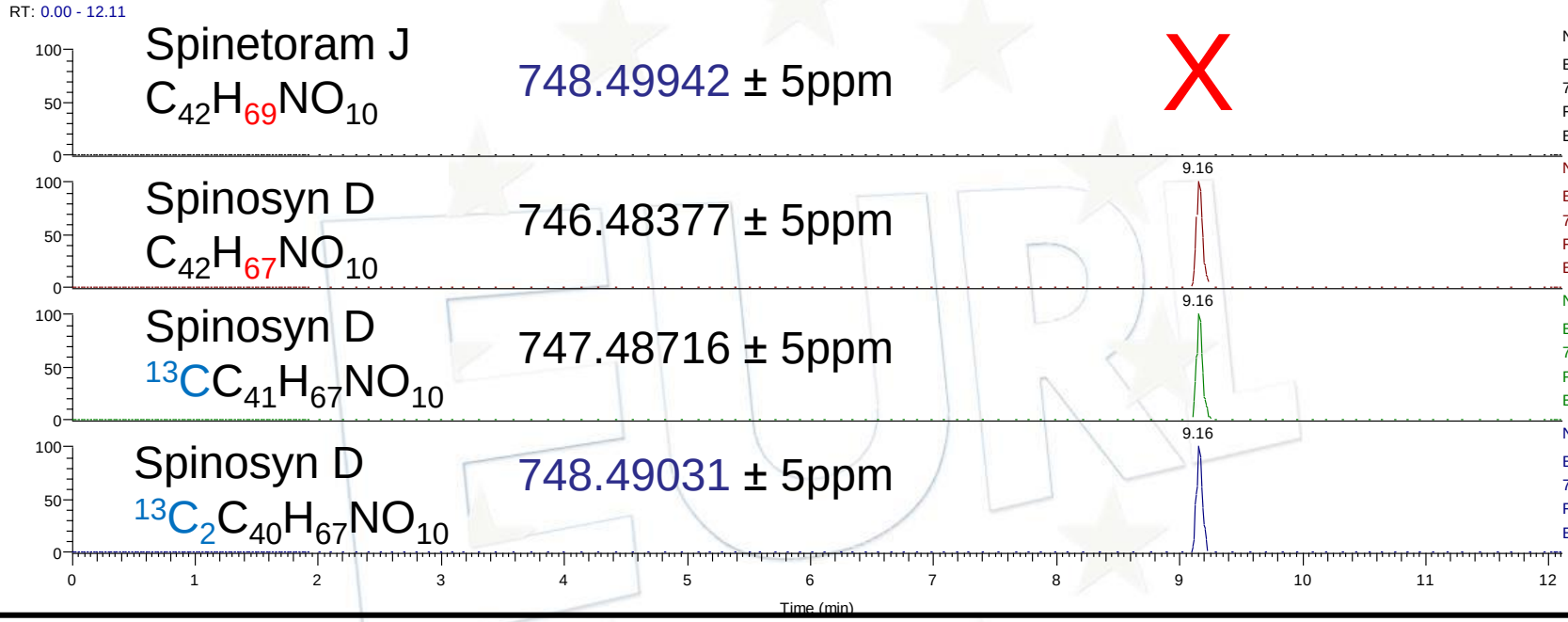


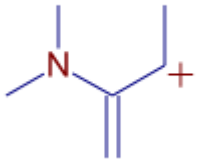
SRM 1: 746.2>142.0
SRM 2: 746.2>98.2
Ion ratio: 0.1813

False Positives

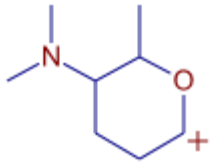
FV23 Sample

Spinetoram J
LC-MS HRMS





m/z 98.09643



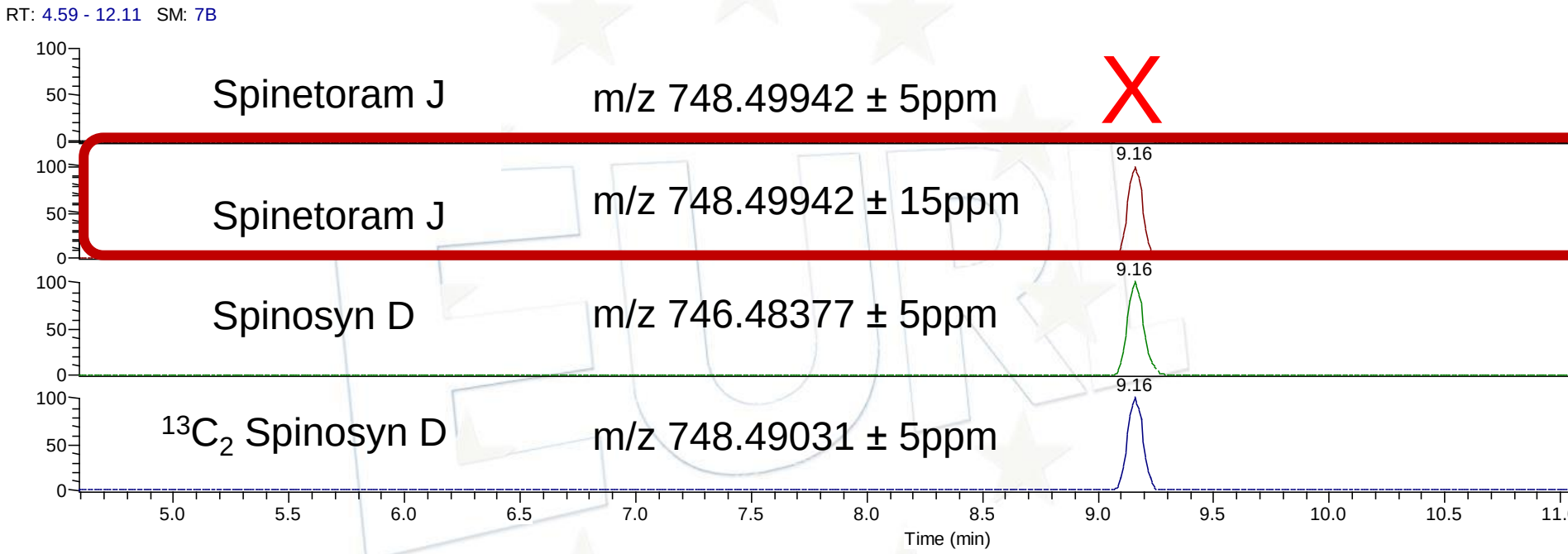
m/z 142.12264

Common fragment ions of spinosyn A, spinosyn D, spinetoram J, and spinetoram L

False Positives

Spinetoram J
LC-MS HRMS

FV23 Sample



Spinetoram J m/z 748.49942

$^{13}C_2$ Spinosyn D m/z 748.49031

Difference

-12.2 ppm

SAMPLE	MATRIX	TARGET/QUANTITATIVE	SCREENING
001	Kiwi		
002	Kiwi		
003	Kiwi		
004	Kiwi	Phosmet	
005	Kiwi		
006	Kiwi		
007	Kiwi		
008	Kiwi		Forchlorfenuron
009	Kiwi	Boscalid	Forchlorfenuron
010	Onion		Beauvericin; Penicillic-Acid
011	Onion		
012	Onion		
013	Onion		
014	Onion		Beauvericin
015	Onion		Beauvericin_M+NH4; Penicillic-Acid
016	Onion		
017	Onion		
018	Onion		
019	Onion		
020	Onion		
021	Onion		
022	Onion		Beauvericin
023	Onion	Target/Quantitative	
024	Onion		
025	Onion		Beauvericin
026	Orange	Imazalil	
027	Orange	Acetamiprid; Fenpyroximate; Pyrimethanil	Acetamiprid-metabolite-IM-2-1
028	Orange	Pyrimethanil; Thiabendazole;Imazalil	
029	Orange	Acetamiprid; Pyrimethanil; Propiconazole; Imazalil	
030	Orange	Imazalil	
031	Orange	Imidacloprid; Pyriproxyfen	Imidacloprid,desnitro; Imidacloprid,desnitro-olefin
032	Orange	Pyriproxyfen; Imidacloprid	Imidacloprid,desnitro; Imidacloprid,urea
033	Orange	Acetamiprid; Imazalil	
034	Orange	Acetamiprid; Pyriproxyfen	Acetamiprid-metabolite-IM-2-1
035	Orange	Hexythiazox; Pyriproxyfen; Imazalil	
036	Orange	Thiabendazole; Propiconazole; Imazalil	
037	Orange	Acetamiprid; Pyrimethanil; Imazalil	
038	Orange	Acetamiprid	
039	Orange		
040	Orange	Acetamiprid; Fenpyroximate	
041	Orange		
042	Orange	Acetamiprid; Etofenprox; Phosmet; Imazalil	
043	Orange	Acetamiprid; Imazalil	
044	Orange	Thiabendazole; Pyrimethanil; Imazalil	Imidacloprid,desnitro; Thiabendazole,5OH
045	Orange	Pyriproxyfen; Imazalil	
046	Orange		
047	Orange		Imidacloprid,desnitro
048	Pineapple		Beauvericin_M+NH4
049	Raisins	Famoxadone; Fluxapyroxad; Indoxacarb; Mandipropamid; Metalaxyl; Methoxyfenozide; Metrafenone; Penconazole; Proguinazid; Pyrimethanil; Sulfoxaflor; Tebuconazole; Zoxamide	
050	Strawberry	Boscalid; Fluopyram	

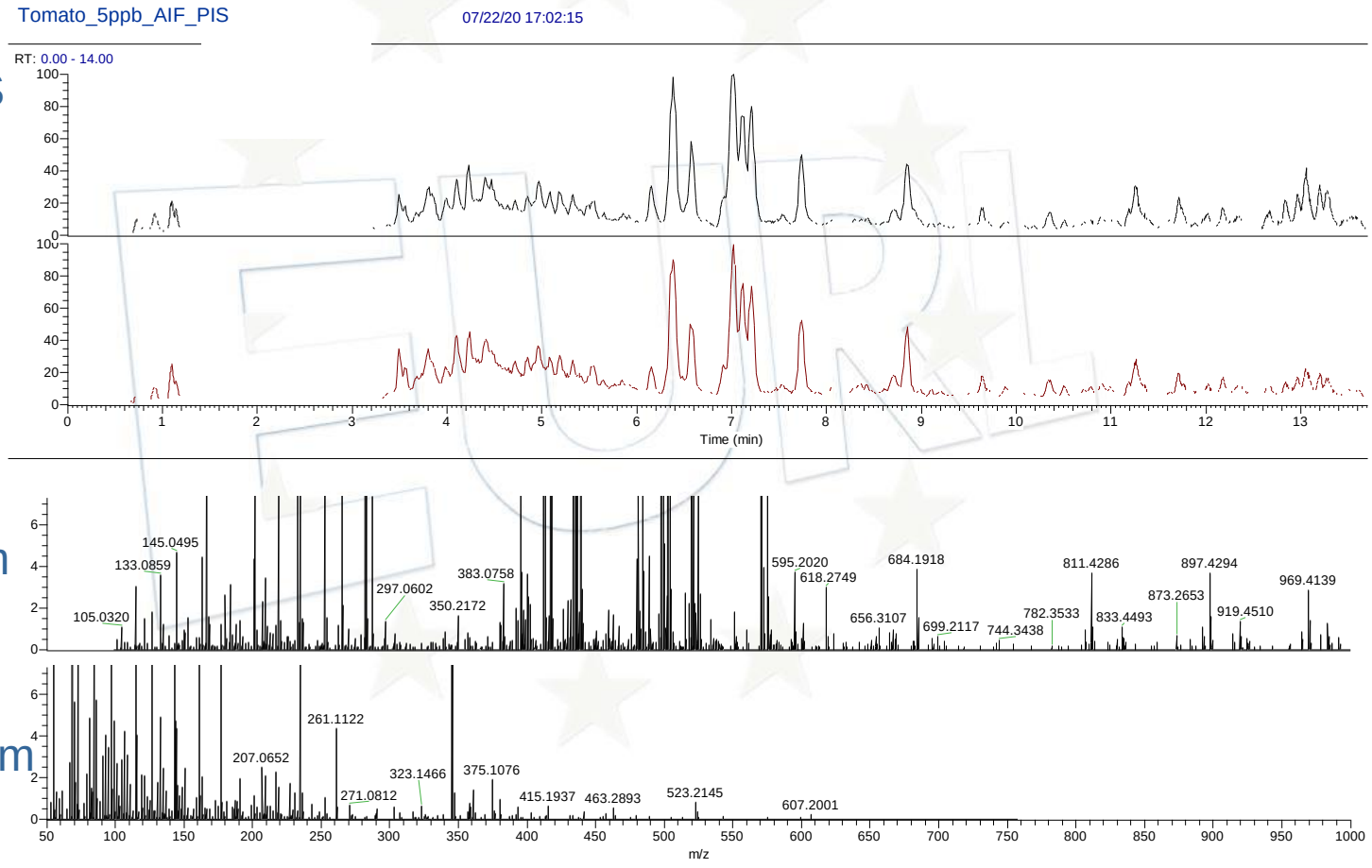
Screening (non regulated compounds)

Full scan MS TIC

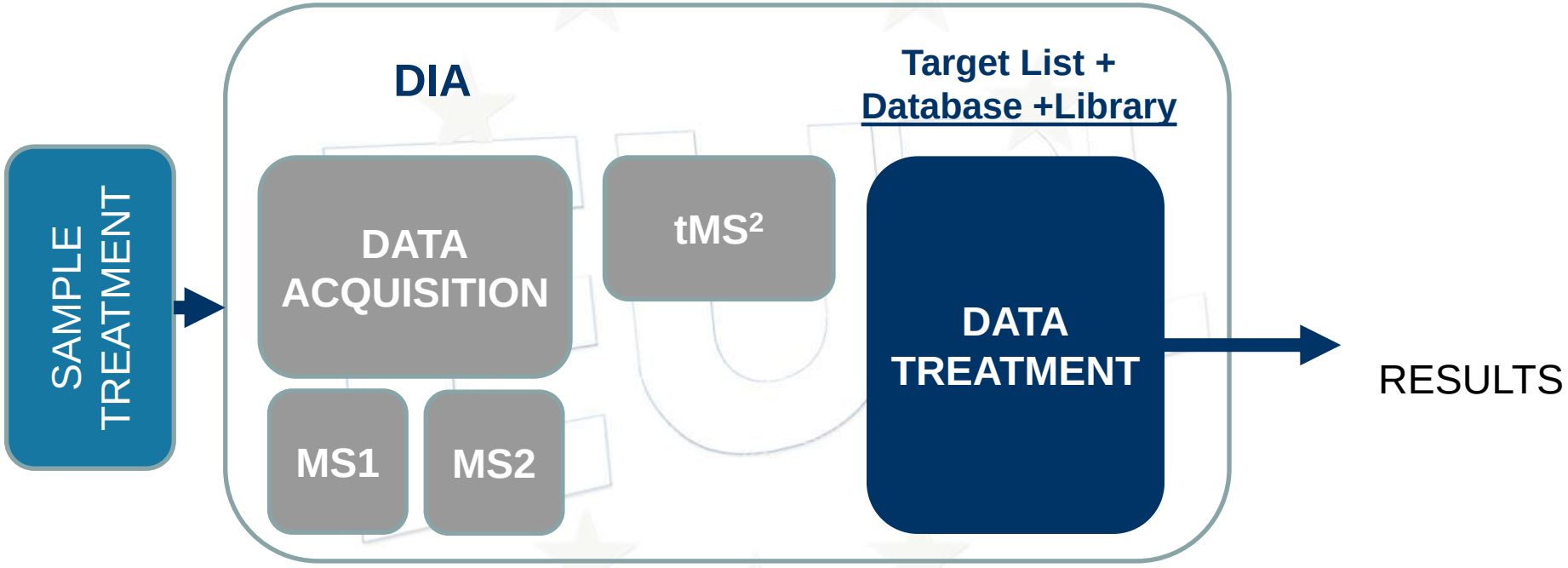
AIF MS2 TIC

MS spectrum

MS2 spectrum



Screening using a Target List & Database



Precursor ion (mass tolerance 5 ppm) - 580 hits

Precursor ion (mass tolerance 5 ppm) + 1 fragment ion (5 ppm) + isotopic pattern 6 hits

Compounds

1 EFS_HRAM_Compound_Database

	Measured A	Selected	MZ	RT	IP	FI	LS	Flag	Compound Name
	Aa	Aa							Aa
1	4.1262E07	☑	●		●	●		●	Eplerenone
2	2.1196E07	☑	●		●	●		●	Carbamazepine
3	2.0971E07	☑	●		●	●		●	Norepinephrine
4	1.9936E07	☑	●		●	●		●	Azoxystrobin
5	1.6037E07	☑	●		●	●		●	Isocarboxazide
6	5.5493E06	☑	●		●	●		●	Imidacloprid

Precursor ion (mass tolerance 5 ppm) + 1 fragment ion (5 ppm) + isotopic pattern 6 hits

Compounds

1 EFS_HRAM_Compound_Database

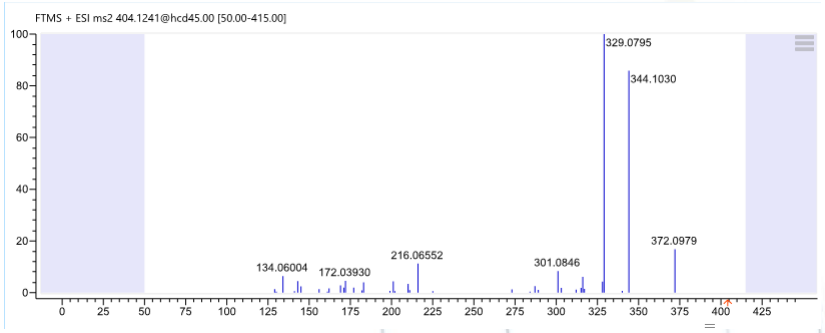
	Measured A	Selected	MZ	RT	IP	FI	LS	Flag	Compound Name	Match Result Name	Formula	Adduct
	Aa	Aa							Aa	Aa	Aa	Aa
1	4.1259E07	☑	●		●	●		●	Eplerenone	Eplerenone@RT 8.11	C24H30O6	M+H
2	2.1202E07	☑	●		●	●		●	**Carbamazepine**	**Carbamazepine@RT 5.79**	**C15H12N2O**	**M+H**
3	2.0971E07	☑	●		●	●		●	Norepinephrine	Norepinephrine@RT 1.15	C8H11NO3	M+H
4	1.9968E07	☑	●		●	●		●	Azoxystrobin	Azoxystrobin@RT 6.97	C22H17N3O5	M+H
5	1.6037E07	☑	●		●	●		●	Isocarboxazide	Isocarboxazide@RT 3.78	C12H13N3O2	M+H
6	5.5493E06	☑	●		●	●		●	Imidacloprid	Imidacloprid@RT 4.18	C9H10ClN5O2	M+H

mzCloud™

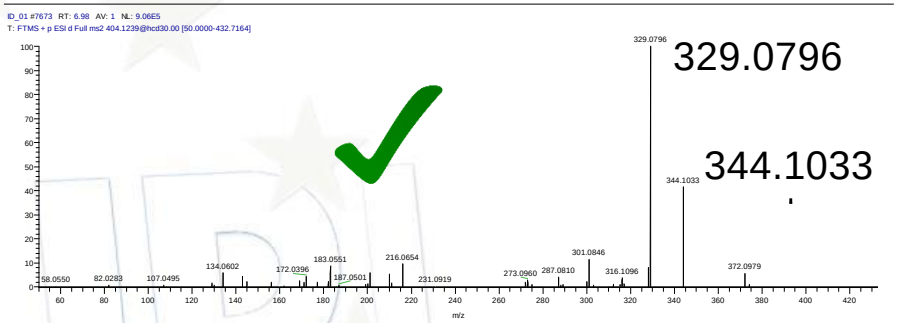
MS2 spectrum

Azoxystrobin

Library

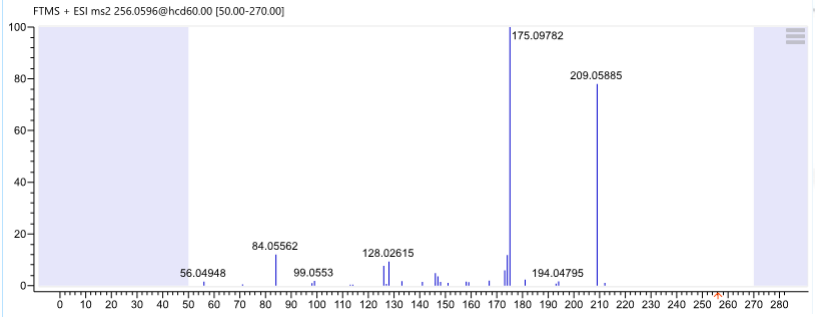


Sample

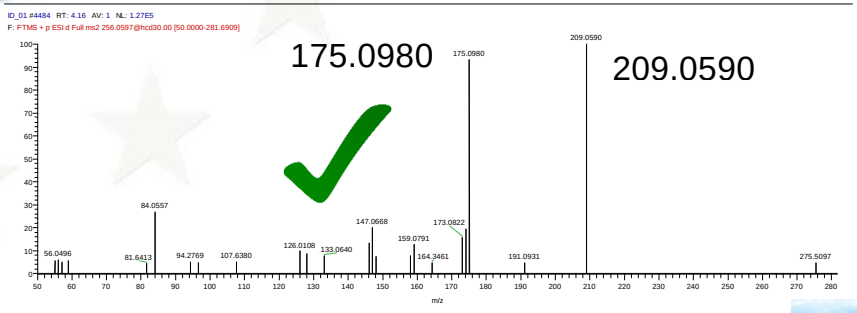


Imidacloprid

Library



Sample

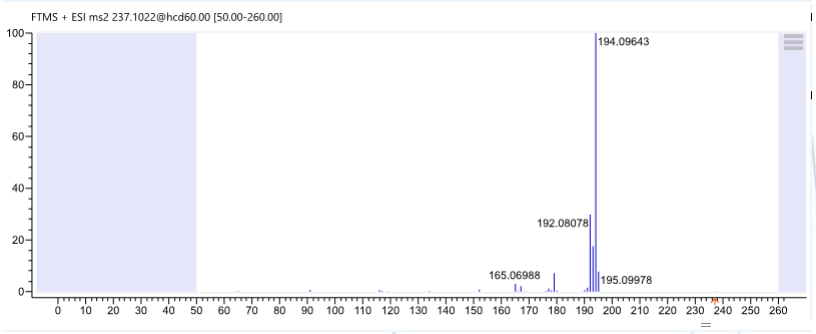


mzCloud™

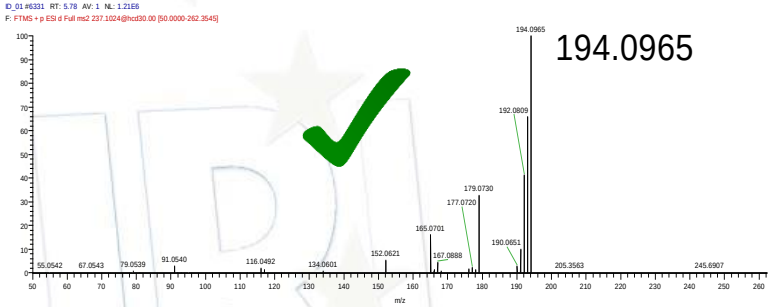
MS2 spectrum

Carbamazepine

Library

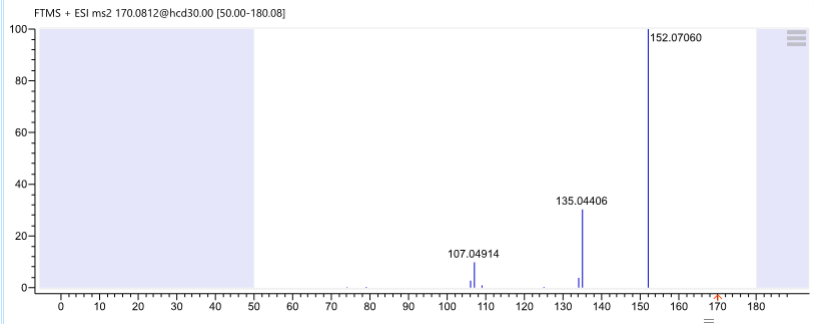


Sample

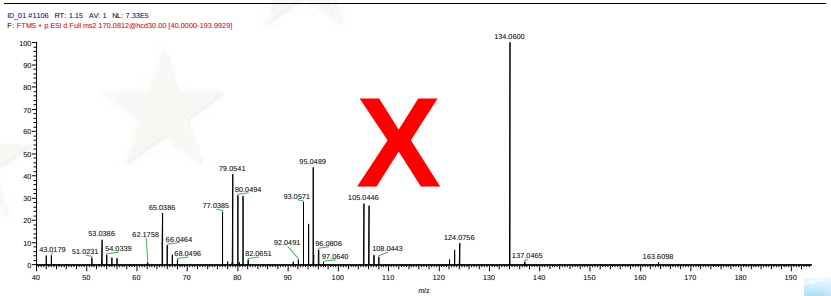


Norepinefrine

Library



Sample



Screening

Screening with TraceFinder (local data bases and libraries)

Samples
Screening
ID_01

Compounds

	Measured Ar	Selected	MZ	RT	IP	FI	LS	Flag	Compound Name	Match Result Name	Formula	Adduct	Confirmed	m/z (Expected)	m/z (Apex)
96	7.5947E04	☑							Buspirone	Buspirone@RT 7.99	C21H31N5O2	M+H	0 out of 2	386.2550	386.2563
97	5.5176E04	☑							Butocarboxim	Butocarboxim@RT 1.05	C7H14N2O2S	M+Na	0 out of 2	213.0668	213.0659
98	3.5435E04	☑							Butoxycarboxim	Butoxycarboxim@RT 7.49	C7H14N2O4S	M+H	0 out of 2	223.0747	223.0752
99	4.4501E04	☑							Butralin	Butralin@RT 3.26	C14H21N3O4	M+H	0 out of 2	296.1605	296.1594
100	5.4848E05	☑							Buturon	Buturon@RT 7.73	C12H13ClN2O	M+H	0 out of 2	237.0789	237.0795
101	5.5018E05	☑							Butylbenzylphthalate	Butylbenzylphthalate@RT 9.22	C19H20O4	M+H	1 out of 2	313.1434	313.1437
102	2.9523E05	☑							Butylone	Butylone@RT 1.05	C12H15NO3	M+H	0 out of 2	222.1125	222.1123
103	1.0334E06	☑							Cafeine	Cafeine@RT 3.83	C8H10N4O2	M+H	1 out of 2	195.0876	195.0876
104	8.1785E04	☑							Cannabidiol	Cannabidiol@RT 8.27	C21H30O2	M+H	0 out of 2	315.2319	315.2325
105	2.1202E07	☑							Carbamazepine	Carbamazepine@RT 5.79	C15H12N2O	M+H	2 out of 2	237.1022	237.1024
106	2.2058E04	☑							Carbaryl	Carbaryl@RT 1.12	C12H11NO2	M-C2H2NC	0 out of 2	145.0648	145.0647
107	2.3680E06	☑							Carbendazim	Carbendazim@RT 1.04	C9H9N3O2	M+H	1 out of 2	192.0768	192.0767
108	3.0157E05	☑							Carbetamide	Carbetamide@RT 3.53	C12H16N2O3	M+H	1 out of 2	237.1234	237.1234
109	2.9523E05	☑							Carbofuran	Carbofuran@RT 1.05	C12H15NO3	M+H	0 out of 2	222.1125	222.1123
110	1.7086E05	☑							Carbofuran, 3OH-	Carbofuran, 3OH-@RT 4.3	C12H15NO4	M+H	0 out of 2	238.1074	238.1073
111	3.0490E04	☑							Carbofuran-3-Keto	Carbofuran-3-Keto@RT 4.42	C12H13NO4	M+H	0 out of 2	236.0917	236.0907
112	7.8044E04	☑							Carbosulfan	Carbosulfan@RT 5.46	C20H32N2O3S	M+H	0 out of 2	381.2206	381.2196
113	3.7574E06	☑							Carboxin	Carboxin@RT 5.79	C12H13NO2S	M+H	1 out of 2	236.0740	236.0741

Chromatogram
M+H
ID_01 Carbamazepine NL: 6.13E6 m/z: 237.1011 - 237.1034
F: FTMS + p Full ms [100.0000-1000.0000]
RT: 5.79
AA: 21201890.36
AH: 6129627.50
237.1022
mass error 0.74 ppm
Relative Intensity
RT(min)
Carbamazepine

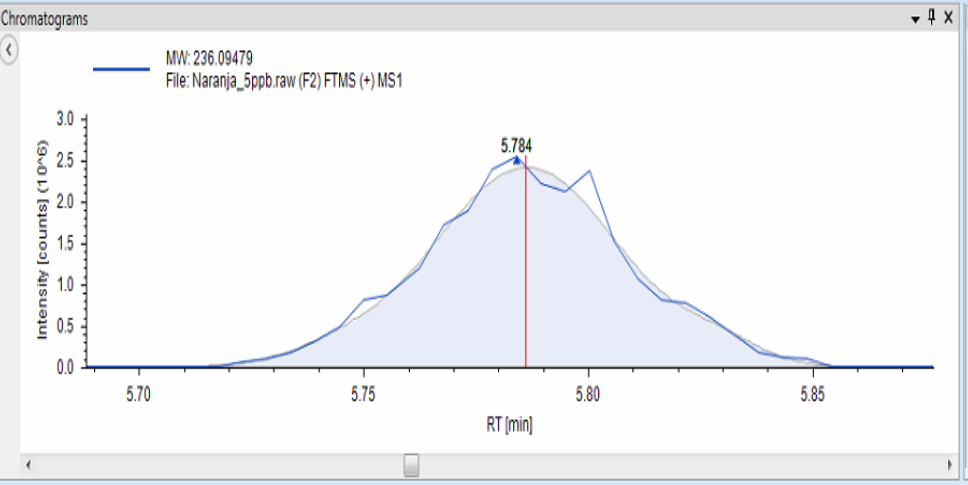
Spectrum
Spectrum | Isotopes 100% (3 of 4) | Fragments (1 of 2)
All Fragments
#1: 220.07529
#2: 194.09612
Minimum # of fragments needed: 1
ID_01 #: 6342 RT: 5.79
F: FTMS + p ESI d Full ms2 237.1024@hcd30.00 [50.0000-
detected
MS2 fragments
Intensity
m/z
#2: 194.09612
Data base
MS2 fragments

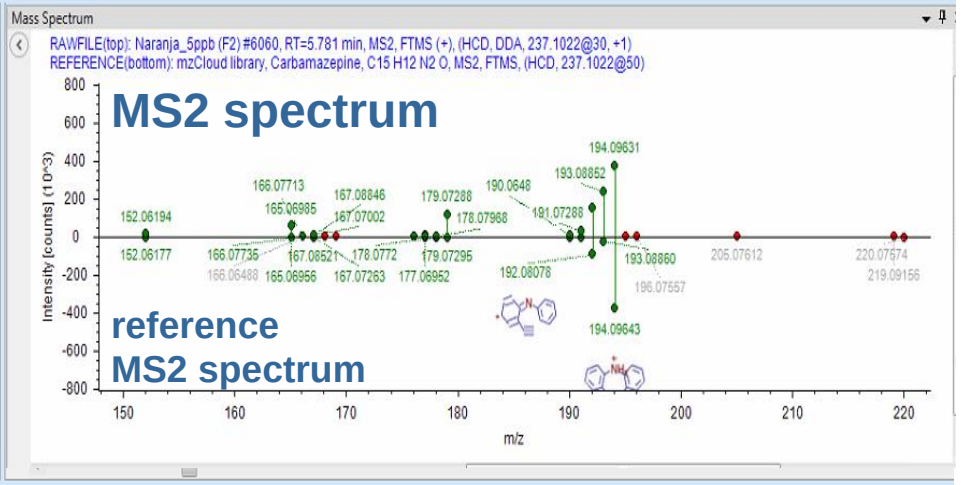
Fragment #2: 194.0961mass error 1.62 ppm

EPRW 2022 BOLOGNA

Screening

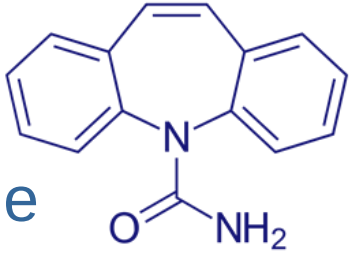
Screening with Compound Discoverer (mzCloud™, Chemspider™, etc.)





Compounds | Compounds per File | Merged Features | Features | mzCloud Results | ChemSpider Results | Mass List Search Results | Input Files | Specialized Traces

	Checked	Name	Formula	Annotation Sc	Molecular Weight	RT [min]	Area (Max.)	Mass Defect					# ChemSpider Results	# mzCloud Results	mzCloud Best Match	Mass List Matches	mzCloud Best Sim. Match	MS2	Group Areas
2519		Carbamazepine	C15 H12 N2 O		236.09479	5.786	8032719	0.749	0.685	0.831	0.831	0.953	142	5	79.5				8.03e6



Carbamazepine

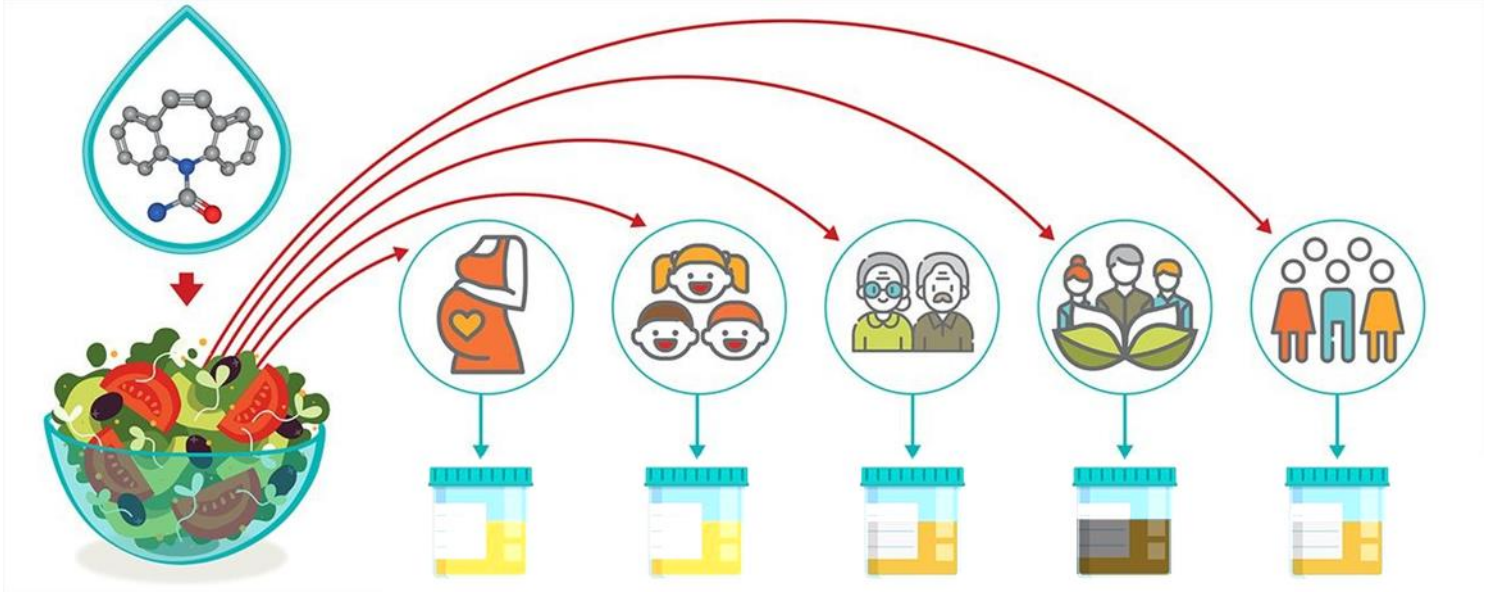
Environment International

Volume 143, October 2020, 105951

ELSEVIER

Involuntary human exposure to carbamazepine: A cross-sectional study of correlates across the lifespan and dietary spectrum

Michael Schapira [a], Orly Manor [a], Naama Golan [b], Dorit Kalo [c], Vered Mordehay [b], Noam Kirshenbaum [b], Rebecca Goldsmith [a, d], Benny Chefetz [b] [1] ✉, Ora Paltiel [a] [1] ✉

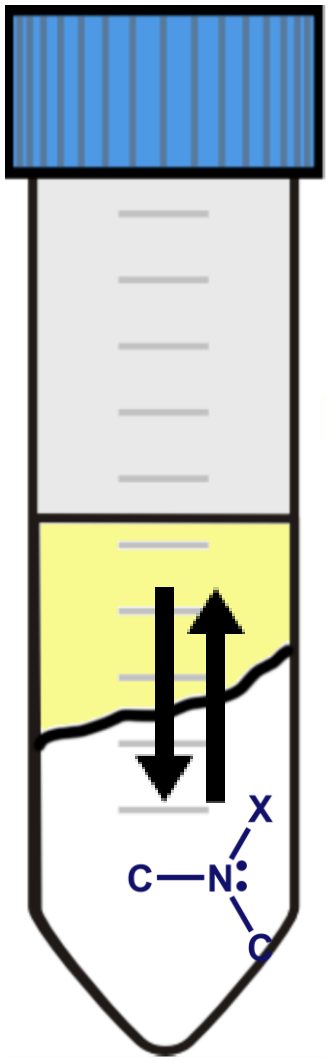


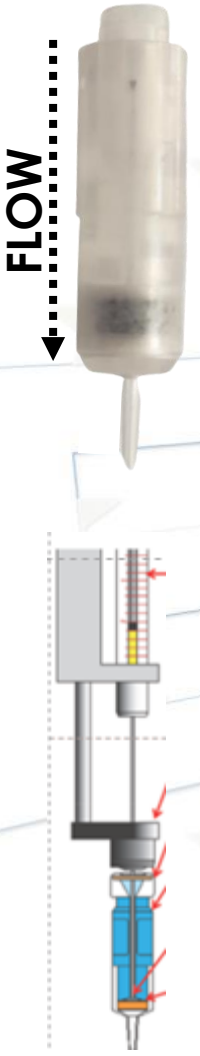
NEW TECHNOLOGIES

Automation

THEORETICAL IMPLEMENTATION

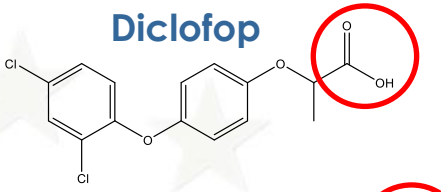
PRACTICAL IMPLEMENTATION



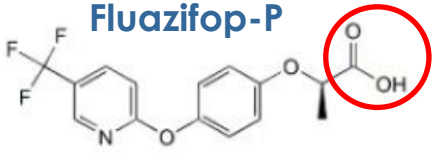


$MgSO_4$
CarbonX
C18
PSA

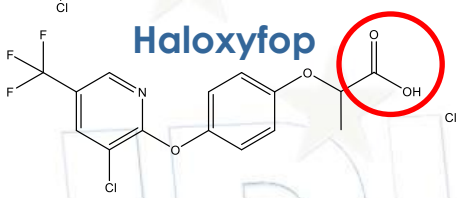
Diclofop



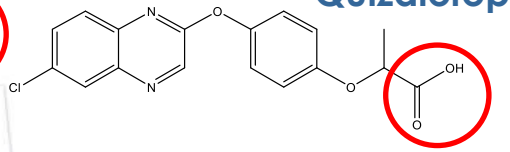
Fluazifop-P



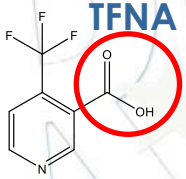
Haloxyfop



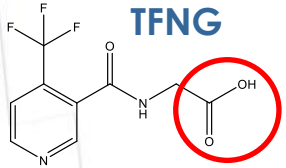
Quizalofop

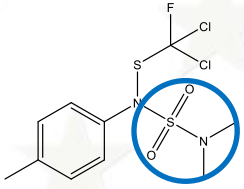


TFNA

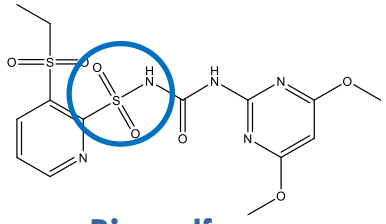


TFNG





Tolylfluanid



Rimsulfuron

EXTRACTION STEP

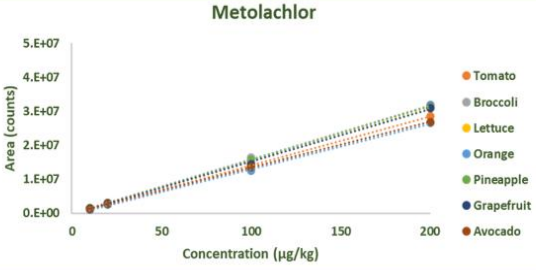
Citrate QuEChERS

CLEAN-UP STEP

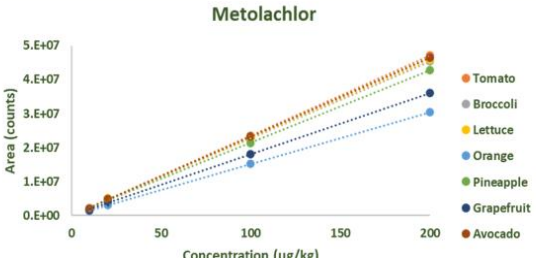
MgSO4
PSA
C18
CarbonX

MgSO4
PSA

AUTOMATED µSPE

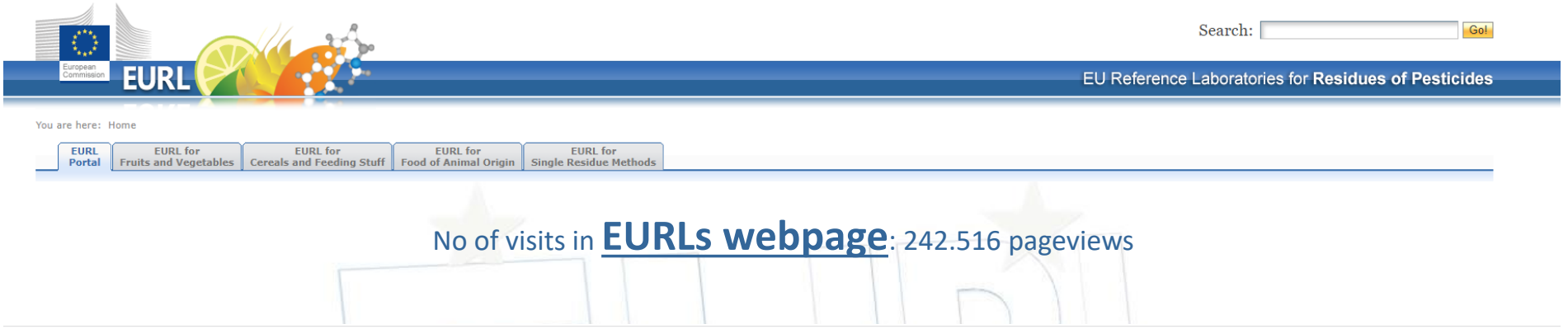


dSPE

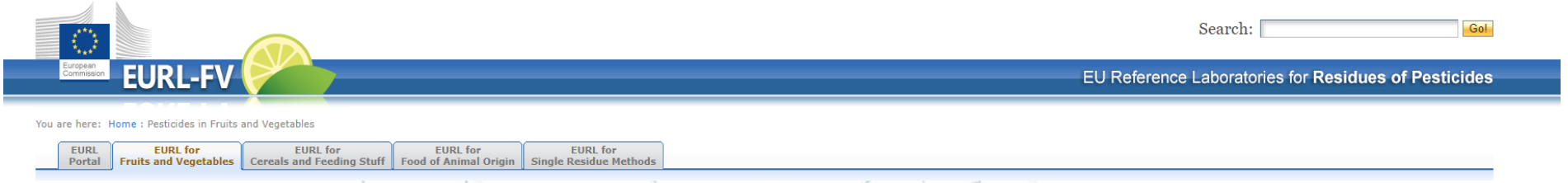



New
Technologies
Knowledge
And
skills

No of visits per year



No of visits in **EURLs webpage**: 242.516 pageviews



No of visits in **EURL-FV specific webpages**: 43285 visits

13886 Main EURL-FV webpage
6434 EURL-FV23
5382 EU Procedures
3398 List of methods FV
2882 Workshops
2782 Last publications
1825 EURL-SM13
…

e-Platform

Dear colleagues,

EURL-FV provides a series of formative tutorials related to the difficulties, new MRM approaches, etc.... that can be found in the routine work in the laboratory:

» **EURL-FV (2021-T1) Solutions for addressing specific LC-MS problematic pesticide residues in Multiresidue Methods.**

» **EURL-FV (2021-T2) Solutions for addressing specific LC-MS problematic pesticide residues in Multiresidue Methods. Part II.**

» **EURL-FV (2021-T3) Measurement Uncertainty (MU) in the AQC EU-SANTE Document. Part I.**

» **EURL-FV (2022-T4). Spinosad quantitation strategies.**

If you wish to obtain a certificate of the trainings received in these tutorials, you should register and also fill in correc ent questionnaire of the content of the tutorials (if you answers are not correct you can fill in the assessment again).

EURL-FV Cha YouTube

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- Panel
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- Listas
- Estadísticas
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- Subtítulos
- Derechos de autor

Vídeo	Visibilidad	Restricciones	Fecha ↓	Visualizaciones	Comentarios	Me gusta (vs. No me gusta)
Correct spinosad quantitation strategies Añadir descripción	Público	Creado para niños	12 may 2022 Publicado	142	0	–
EURL Tutorial 1 Uncertainty SANTE AValverde CFerrer Añadir descripción	Oculto	Creado para niños	5 ago 2021 Subido	461	0	100,0 % 8 Me gusta
202105 LC Specific issues II In this tutorial, you will find some examples of specific problems encountered with different pesticides when analysed by LC-MS/MS.	Oculto	Creado para niños	18 jun 2021 Subido	321	0	100,0 % 6 Me gusta
202104 LC Specific issues EURL-FV (2021-T1) Solutions for addressing specific LC-MS problematic pesticide residues in Multiresidue Methods.	Oculto	Creado para niños	3 may 2021 Subido	858	0	100,0 % 6 Me gusta

EPRW 2022 BOLOGNA

Thank You
for Your Attention

EURL EUROPEAN UNION REFERENCE LABORATORY

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