



UNIVERSITÀ  
DEGLI STUDI  
DI PADOVA

**Targeted and non-targeted analysis of organic  
compounds by high resolution mass spectrometry.**

Marco Roverso<sup>a</sup>, Sara Bogialli<sup>a</sup>, Roberta Seraglia<sup>b</sup>, Paolo Pastore<sup>a</sup>

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UHPLC-HRMS/MS  
(ESI-Orbitrap RP 140,000 FWHM)



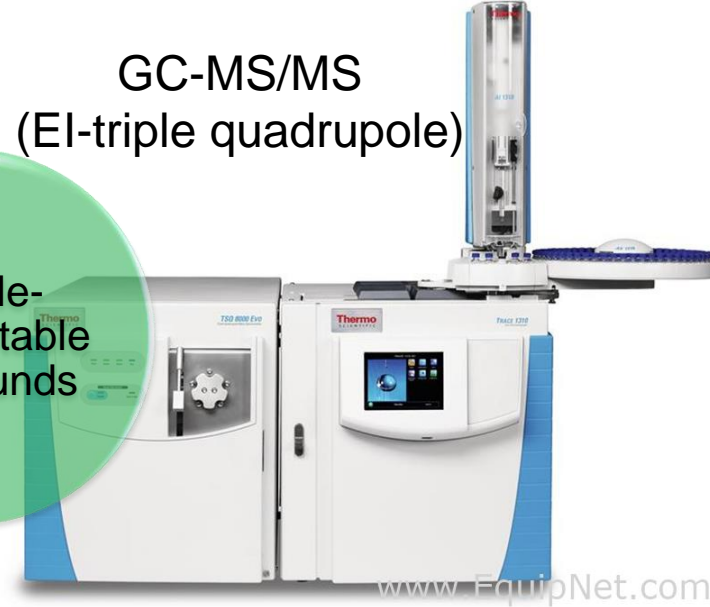
Medium polar- non volatile-thermolabile compounds

Chemical characterization

Volatile-thermostable compounds

Elements analysis-speciations  
HPLC-ICP-MS

GC-MS/MS  
(EI-triple quadrupole)



www.EquipNet.com



Regular Article

Nanoaggregates in aqueous solution: Probing the co-reduction reaction with Pt-N active

Giulio Fracasso<sup>a</sup>, Paola Elena Nicolato<sup>c</sup>, Pasquale Vincenzo Amendola<sup>b</sup>, Riccardo Brandiele, Denis Badocco, Paolo...

<sup>a</sup> Department of Medicine, Immunology and Microbiology, University of Padua, Italy

<sup>b</sup> Department of Chemistry, University of Padua, Italy  
<sup>c</sup> CNR - ICMATE, Padova, Italy

Contents lists available at ScienceDirect

### Nanoparticle Synthesis

## Room-Temperature Crystallization of CuS Nanostructures for Photothermal Applications through a Nanoreactor Approach

Giulia Morgese,<sup>[a]</sup> Paolo Dolcet,<sup>\*[a,b]</sup> Alessandro Feis,<sup>[c]</sup> Cristina Gellini,<sup>[c]</sup> Stefano Gialanella,<sup>[d]</sup> Adolfo Speghini,<sup>[e]</sup> Denis Badocco,<sup>[a]</sup> Paolo Pastore,<sup>[a]</sup> Maurizio Casarin,<sup>[a]</sup> and Silvia Gross<sup>\*[a,b]</sup>

### Metallomics

PAPER

View Article Online  
View Journal | View Issue



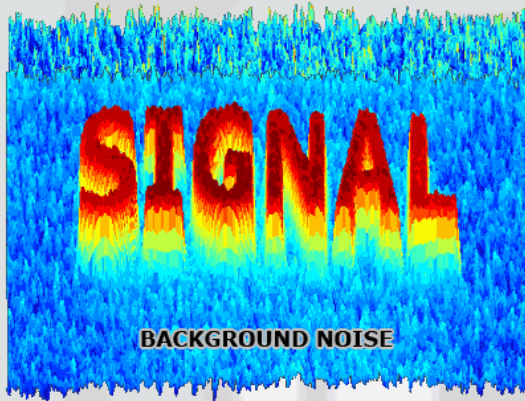
Cite this: *Metallomics*, 2015, 7, 1146

### The metallome of the human placenta in gestational diabetes mellitus†

Marco Roverso,<sup>ab</sup> Chiara Berté,<sup>a</sup> Valerio Di Marco,<sup>\*a</sup> Annunziata Lapolla,<sup>b</sup> Denis Badocco,<sup>a</sup> Paolo Pastore,<sup>a</sup> Silvia Visentin<sup>c</sup> and Erich Cosmi<sup>c</sup>



Ancient proverb:  
On a Dark night you can see more stars



*“Mass spectrometry is the art of measuring atoms and molecules to determine their molecular weight. Such mass or weight information is sometimes sufficient, frequently necessary, and always useful in determining the identity of a species”*

John B. Fenn, Nobel\_2002



Photo from the Nobel Foundation archive.  
John B. Fenn  
Prize share: 1/4



Photo from the Nobel Foundation archive.  
Koichi Tanaka  
Prize share: 1/4



Photo from the Nobel Foundation archive.  
Kurt Wüthrich  
Prize share: 1/2

## What We Do....

Development of new qualitative and quantitative analytical method based on chromatography coupled with mass spectrometry

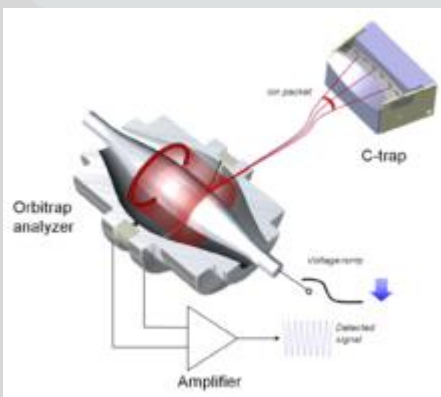
### Chromatography- High resolution Mass Spectrometry

# Resolution and accuracy

$$\text{Resolving power ( R )} = m/\Delta m$$

Compound with MW=200 ,  $\Delta m=0.014$  > R=14000

How many  
compounds?  
**resolution**  
correct identification?  
**accuracy**

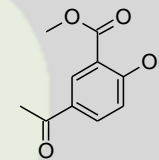
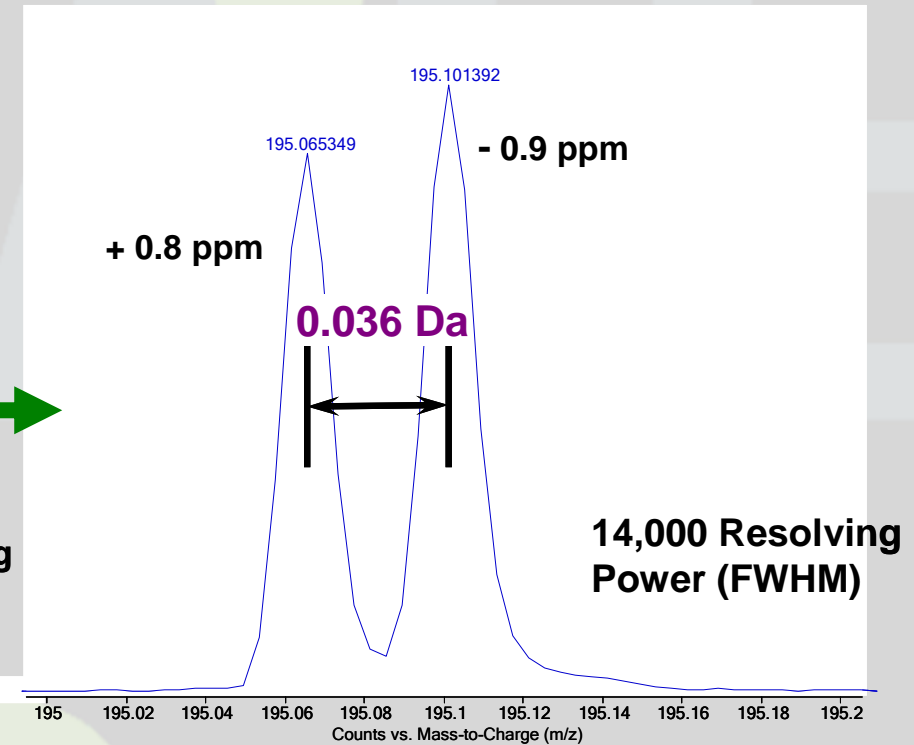
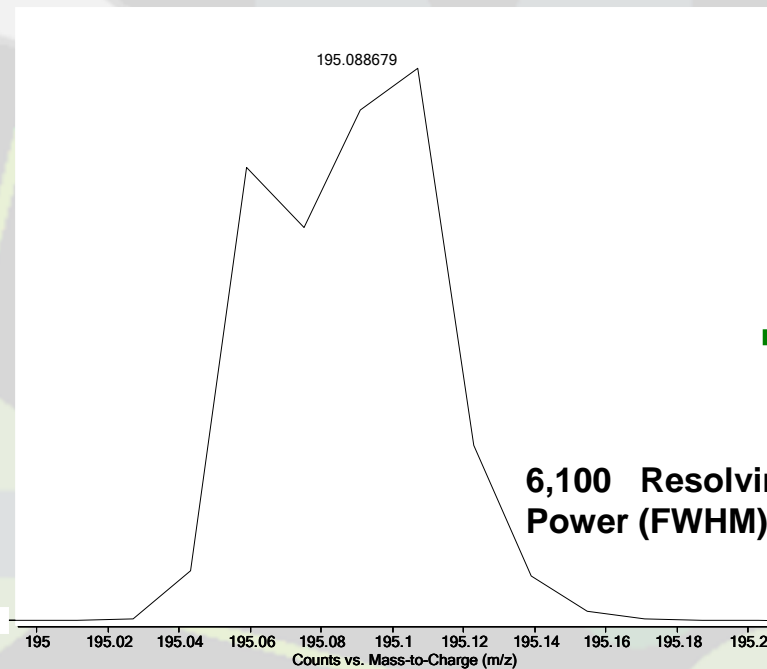
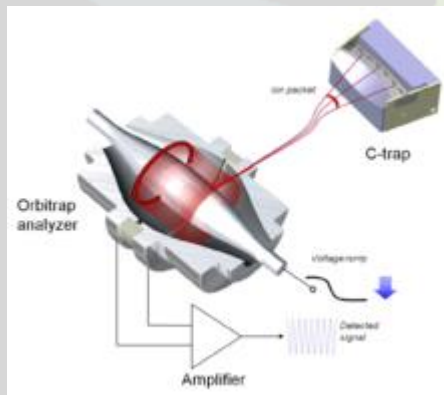


# Resolution and accuracy

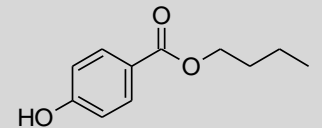
$$\text{Resolving power (R)} = m/\Delta m$$

Compound with MW=200,  $\Delta m=0.014$  > R=14000

How many  
compounds?  
**resolution**  
correct identification?  
**accuracy**



Methyl 5-acetylsalicylate  
[M+H]<sup>+</sup> = m/z 195.06519



Butyl paraben  
[M+H]<sup>+</sup> = m/z 195.10157

# Who and what Have we to face out?

“There are **known knowns** These are things we know that we know

“There are **known unknowns**. That is to say, there are things that we know we don't know.

But there are also **unknown unknowns**. There are things we don't know we don't know.”

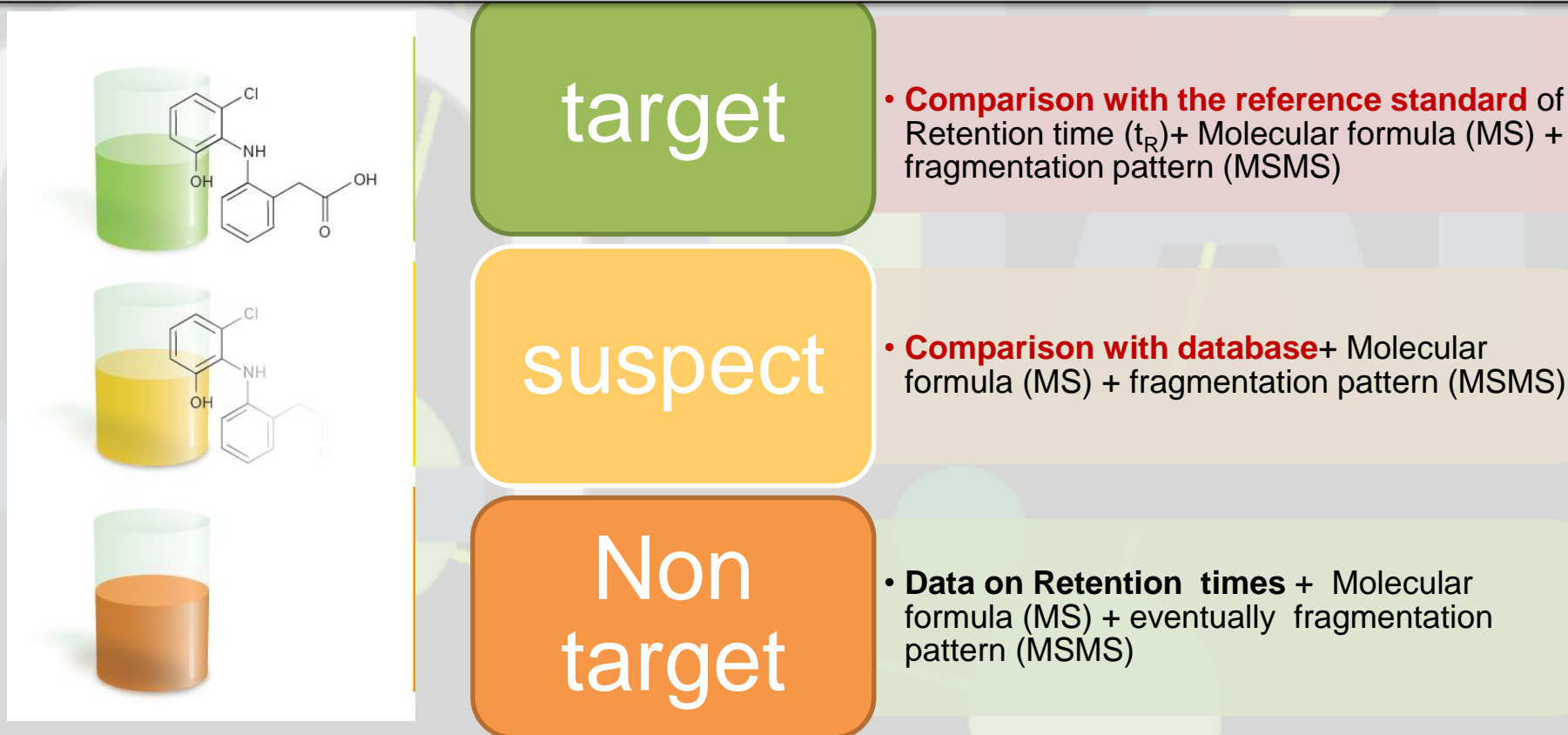
*Donald Rumsfeld, Ex Secretary of Defense, USA*



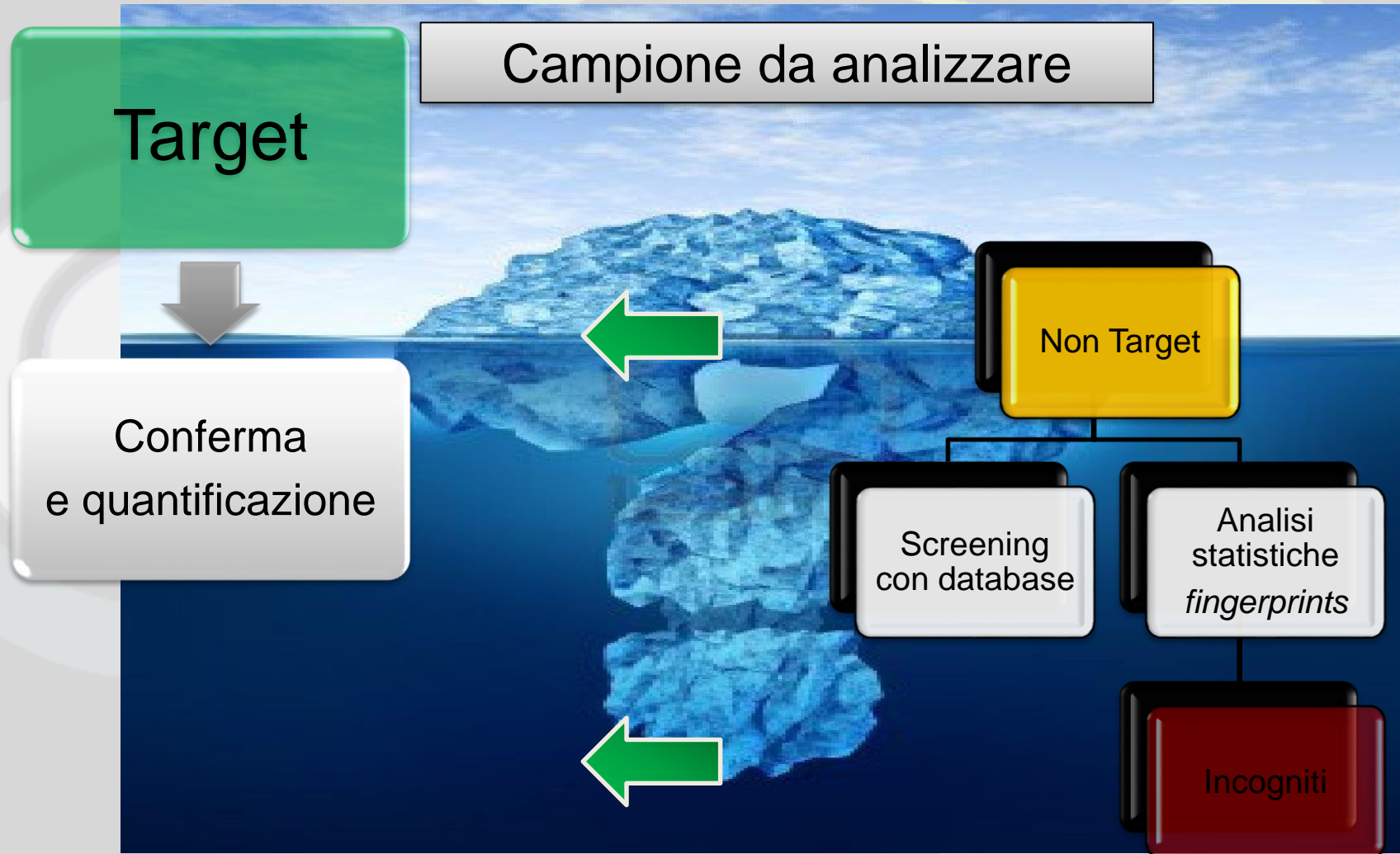
- Ci sono «informazioni» conosciute che sappiamo di sapere. **“Target”**
- Ci sono «informazioni» sconosciute che sappiamo di non sapere. **“UnTargeted”**
- Ma ci sono anche «informazioni» a noi sconosciute che non sappiamo di non sapere. **“UnKnown”**

# The language of the HRMS methods Harmonization

All analyses without a pure standard start as non-target and could remain unknown



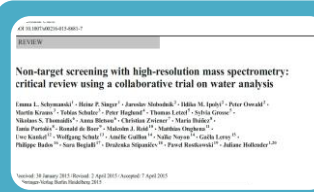
# Analisi Target e Non-Target





## Emerging contaminants

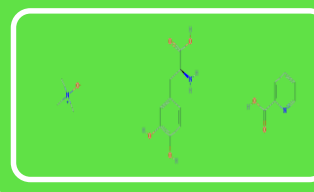
- Endocrine disruptors (EDs)
- Illicit drugs
- Pharmaceuticals
- Flame retardants
- Plasticisers
- Food additives
- Personal Care Products
- Perfluorinated compounds
- Disinfection by-products
- Transformation products
- Algal toxins
- etc...



Target & non-target analysis



Characterization of organic compounds  
(organometallic, cultural heritage)



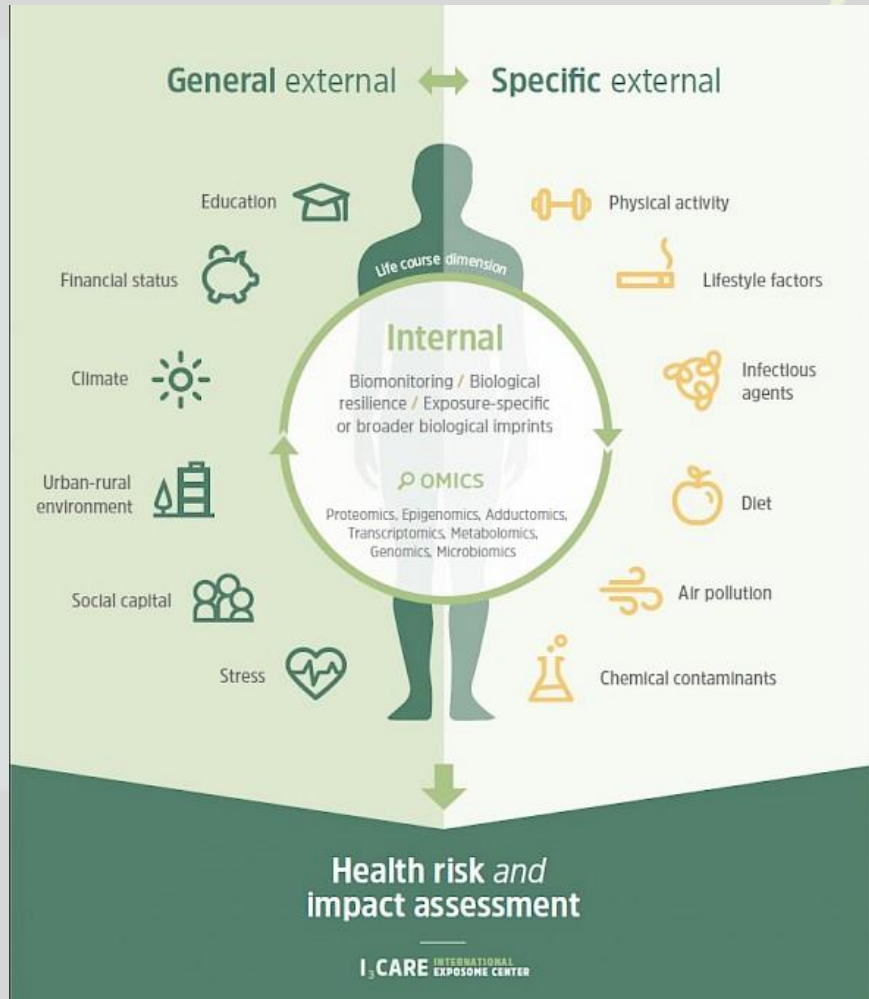
Metabolomic  
Clinical markers (Alzheimer, Parkinson, Diabetes)



Biomarkers in food



Contaminants (Biomarkers) in environment



Chemical contaminants in environment:

- Pesticides, Erbicides
- Industrial residues
- Endocrine disruptors (e.g plastificant)
- Pharmaceuticals
- Personal care products
- Cleaning products
- ....
- Metabolites

EXPOSOME

Bioactive compounds  
produced by extremophiles  
plants

hydroxyflavone	239.0714	<i>Z.punc.</i> , prop.	(Agliero et al., 2010; Vera et al., 2011; Jimenez et al., 2014)
7-hydroxy-8-methoxyflavone	269.0819	<i>Z.punc.</i> , prop.	(Agliero et al., 2010; Vera et al., 2011; Jimenez et al., 2014)
7,4'-dihydroxy-5-methoxyflavone	285.0768	prop.	(Agliero et al., 2010)

## 1. From literature

- MS identification in full scan analysis of suspect for *Z. punctata*.

Multi-step workflow:

1. (pse)
2. diagn
3. chara
4. molec

Journal of Functional Foods 33 (2017) 423–432

Contents lists available at ScienceDirect

Journal of Functional Foods

journal homepage: [www.elsevier.com/locate/jfff](http://www.elsevier.com/locate/jfff)

ELSEVIER

Use of a LC-DAD-QTOF system for the characterization of the phenolic profile of the argentinean plant *Zuccagnia punctata* and of the related propolis: New biomarkers

Elisiana Rita Solorzano<sup>a</sup>, Claudio Bortolini<sup>a</sup>, Sara Bogiatti<sup>a,\*</sup>, Iole Maria Di Gangi<sup>a</sup>, Gabriella Favaro<sup>a</sup>, Luis Maldonado<sup>b</sup>, Paolo Pastore<sup>a</sup>

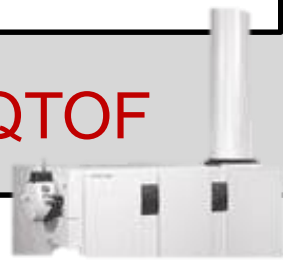
<sup>a</sup>Department of Chemical Sciences, University of Padua, Via Marzolo, 1, 35131 Padua, Italy  
<sup>b</sup>Estación Experimental Agropecuaria Famaillá, Instituto Nacional de Tecnología Agropecuaria, Ruta provincial 301, km 32, Famaillá, Tucumán, Argentina

CrossMark

## LC-DAD

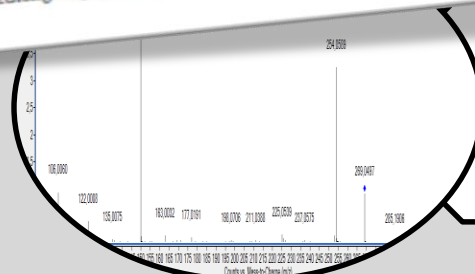
Identification of the largest peaks with UV spectra.

## LC-ESI-QTOF



## 3. LC-HR- tandem MS

- AutoMS fragmentation scan of the previously selected MS precursor ions



Bioactive compounds produced by extremophiles plants

## 1. Raw formula

Accurate mass

DBE

$$C - \frac{H}{2} - \frac{X}{2} + \frac{N}{2} + 1$$

## 2. Structural formula

DBE

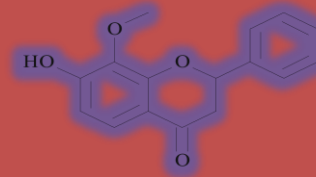
Fragmentation  
pattern

## 3. Isomeric variant

UV spectra  
(if present)

Chromatographic  
behaviour

Biological  
mechanism

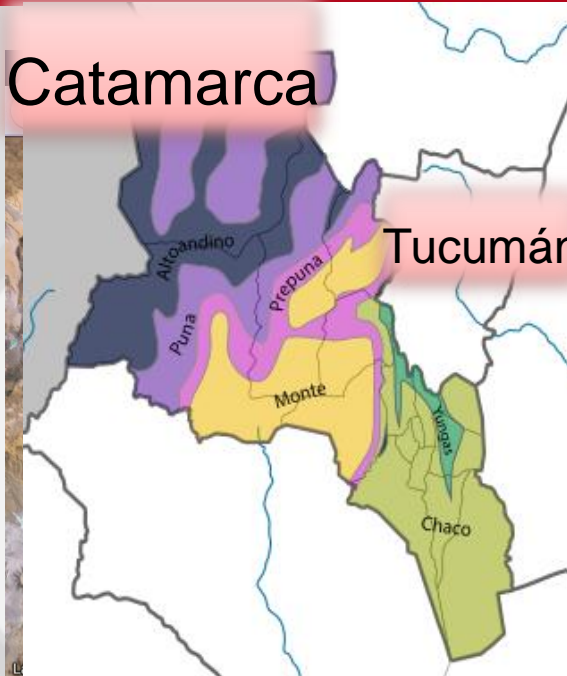


# Propolis analysis\_results

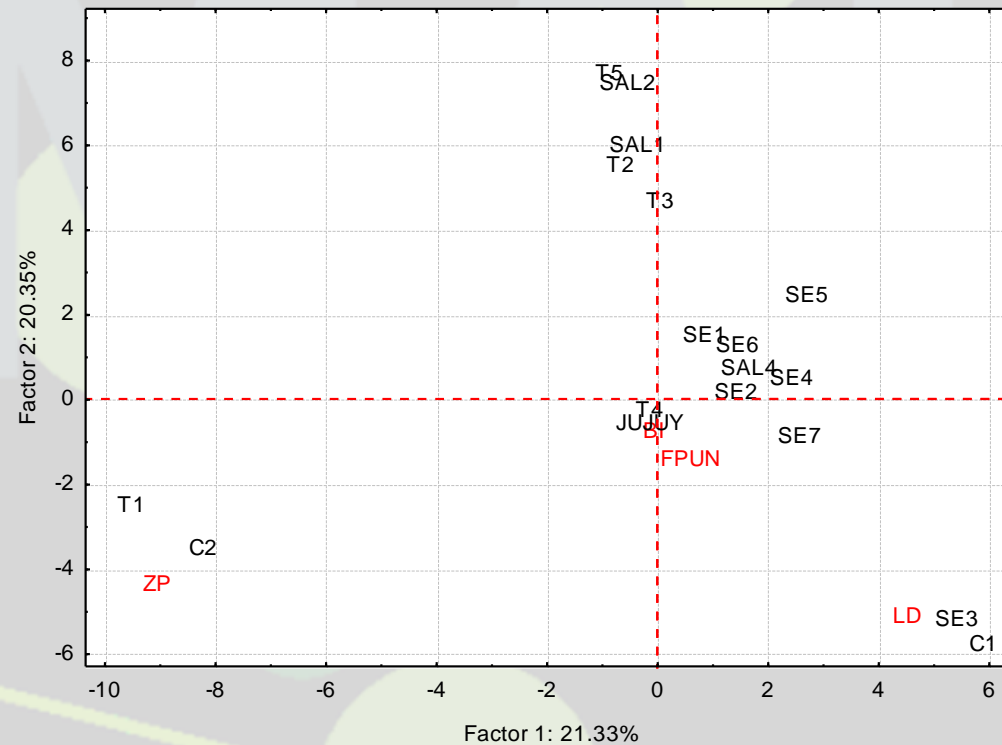
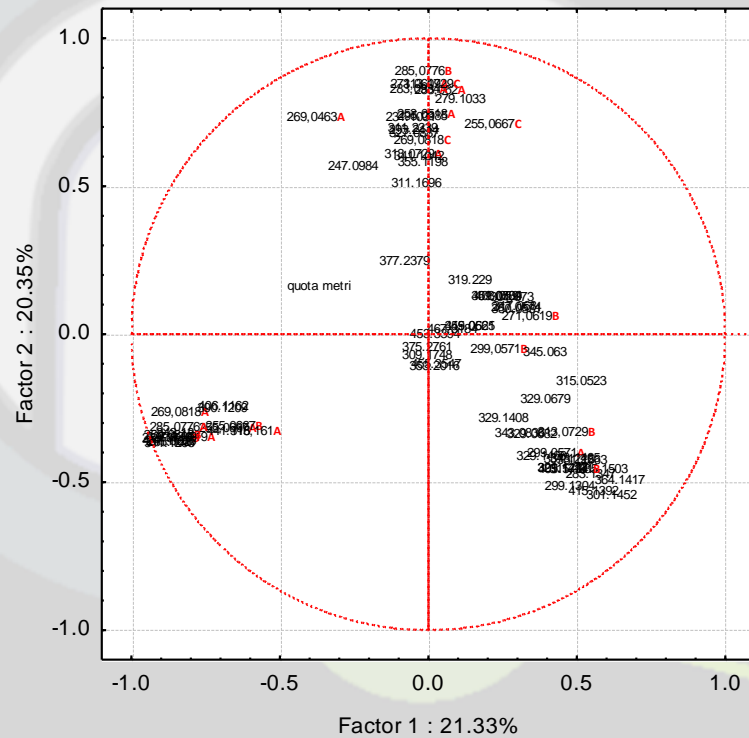
Compounds	Reports	% relative area				
		Z.p-E	T1-E	T2-E	C1-E	C2-E
<b>Chalcones and Dihydrochalcones</b>						
1 s	2',4'-dihydroxychalcone	Z.punc., prop.	95.3	104.3		59.7
2 t	2',4'-dihydroxy-3'-methoxychalcone	Z.punc., prop.	34.5	13.4		2.0
3 s	2',4',4'-trihydroxy-6'-methoxychalcone	prop.	10.0	2.1		9.1
<b>Flavanones</b>						
1* t	7-hydroxyflavanone	Z.punc., prop.	57.9	24.9		24.8
2* s	7-hydroxy-8-methoxyflavanone	Z.punc., prop.	22.3	34.1		8.9
3* s	7,4'-dihydroxy-5-methoxyflavanone	prop.	2.0	15.7		1.3
10 s	pinocembrin (5, 7-dihydroxyflavanone)	Z.punc., prop.	2.3	13.9		7.1
<b>Flavones</b>						
14 s	3,7-dihydroxy-8-methoxyflavone	Z.punc., prop.	6.3	4.2		4.5
15 s	rhamnocitrin (3,5,4'-trihydroxy-7-methoxyflavone)	Z.punc., prop.	2.3	3.7	5.1	2.3
20 t	galangin (3,5,7-trihydroxyflavone)	Z.punc., prop.	22.5	36.7	61.4	12.7
25 t	chrysin (5,7- dihydroxyflavone)	prop.	3.7	77.7	34.8	7.0
26 s	3,7-dihydroxyflavone	Z.punc.	5.3	5.6		5.3
<b>Acids and esters</b>						
28 s	1,1-dimethylallyl caffeic acid	prop.		11.9	36.9	8.4
32 s	1-methyl-3-(4'-hydroxyphenyl)-propyl caffeic acid ester	Z.punc.	21.9	35.0	0.4	24.2
33 s	1-methyl-3-(3',4'-dihydroxyphenyl)-propyl caffeic acid ester	Z.punc.	36.8	76.0		51.1
<b>Proposed non target compounds</b>						
34 nt	7,8-dihydroxyflavanone		8.6	10.3		7.4
35 nt	3,7-dihydroxyflavanone		5.2	5.0		3.5
36 nt	pinobanksin-5-methyl eter (3,7-dihydroxy-5-methoxyflavanone)		3.6	20.4	14.7	5.9
37 nt	3,7,8-trihydroxydihydroflavanone		6.3	27.7	96.3	3.8
38 nt	4'-hydroxy-2'-methoxydihydrochalcone		100.0	68.5		53.3
39 nt	2',4'-dihydroxydihydrochalcone		23.6	23.3		14.5
40 nt	4'-terbutyloxyphenyl p-coumaric acid ester		0.9	0.6		0.5
41 nt	1-methyl-3-(4'-hydroxyphenyl)-propyl p-coumaric acid ester		22.8	25.3		18.2
42 nt	geranyl caffeate		9.4	25.8	1.3	20.7
43 nt	1-methyl-3-(3',4'-di hydroxyphenyl)-propyl ferulic acid ester		3.4	8.9		4.8
44 nt	2-methyl-3-(3'-hydroxy-4'-methoxyphenyl)-propyl caffeic acid ester		4.9	3.8		2.3

# Z.p. phytogeographical region

Catamarca



## An alternative bottom-up approach based on PCA analysis

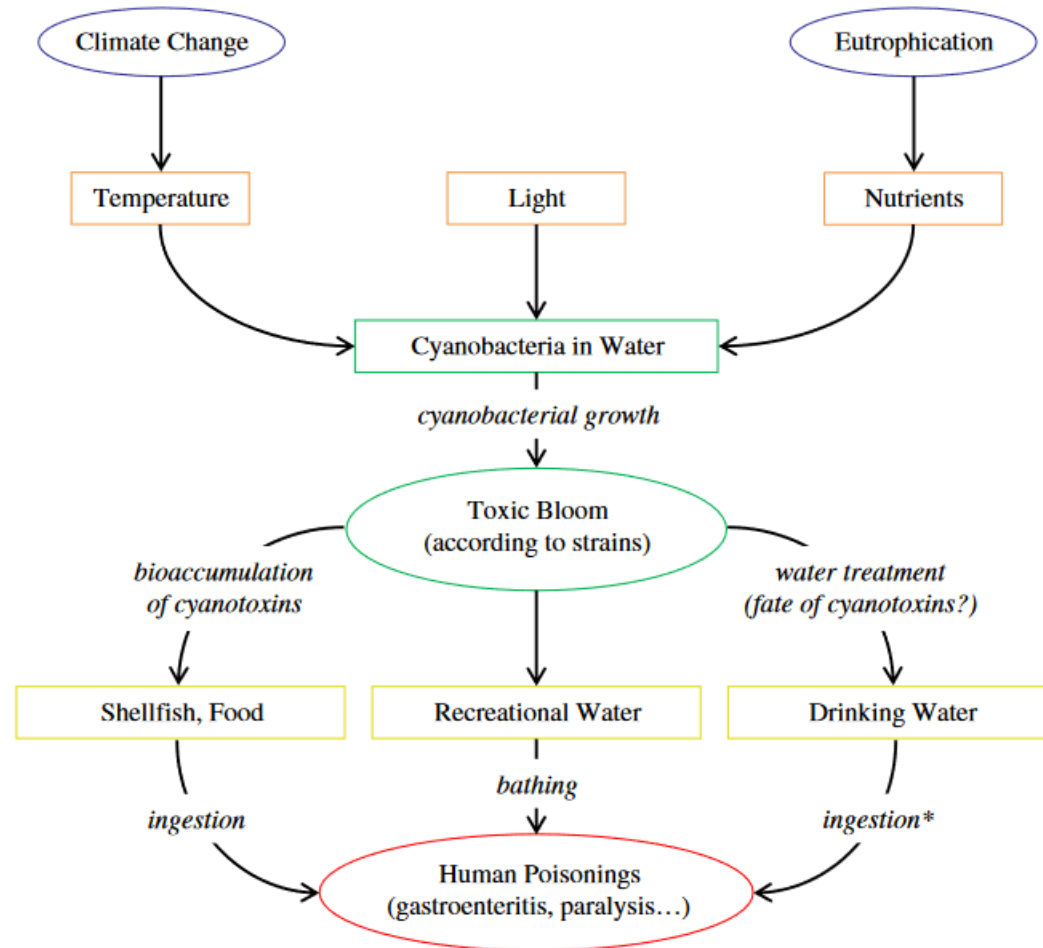


A preliminary elaboration gives a clear indication of some sources and drives the MS data analysis





# Cyanotoxins in water

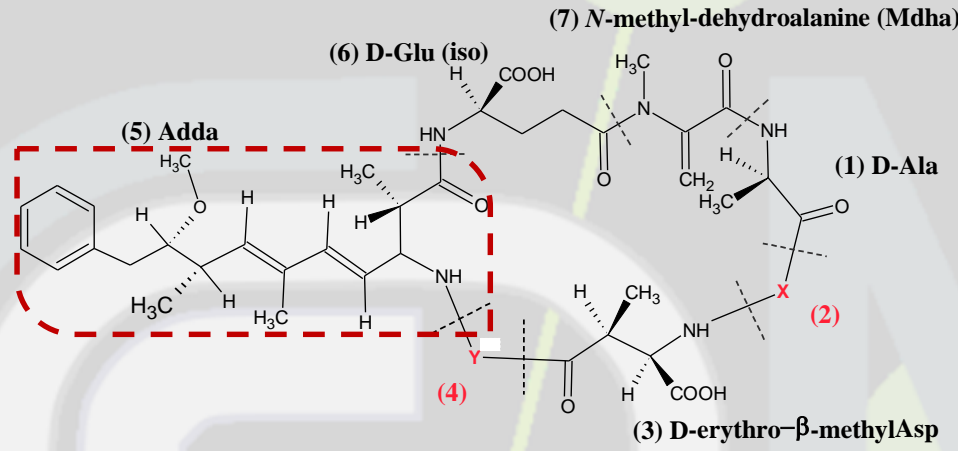


\* 80% of human exposure to cyanotoxins (WHO, 1998)

Fig. 1. Origin of toxic cyanobacterial blooms and human exposure.



# Cyanotoxins\_cyclic peptides Microcystins (MCs)



**Adda:**  
(2S,3S,8S,9S)-  
3-amino-9-methoxy-2,6,8-trimethyl-10-  
phenyldeca-4,6-dienoic acid

TABLE 2. Primary Microcystin Analogues With Variations in Amino Acids 2 (X) and 4 (Y)

Analogue	Structure
Microcystin-AR	cyclo (-D-Ala-L-Ala-D-MeAsp-L-Arg-Adda-D-Glu-Mdha-)
Microcystin-FR	cyclo (-D-Ala-L-Phe-D-MeAsp-L-Arg-Adda-D-Glu-Mdha-)
Microcystin-HilR	cyclo (-D-Ala-L-Hil-D-MeAsp-L-Arg-Adda-D-Glu-Mdha-)
Microcystin-HtyR	cyclo (-D-Ala-L-Hty-D-MeAsp-L-Arg-Adda-D-Glu-Mdha-)
Microcystin-LA	cyclo (-D-Ala-L-Leu-D-MeAsp-L-Ala-Adda-D-Glu-Mdha-)
Microcystin-LABA	cyclo (-D-Ala-L-Leu-D-MeAsp-L-Aba-Adda-D-Glu-Mdha-)
Microcystin-LF	cyclo (-D-Ala-L-Leu-D-MeAsp-L-Phe-Adda-D-Glu-Mdha-)
Microcystin-LL	cyclo (-D-Ala-L-Leu-D-MeAsp-L-Leu-Adda-D-Glu-Mdha-)
Microcystin-LM	cyclo (-D-Ala-L-Leu-D-MeAsp-L-Met-Adda-D-Glu-Mdha-)
Microcystin-LR	cyclo (-D-Ala-L-Leu-D-MeAsp-L-Arg-Adda-D-Glu-Mdha-)
Microcystin-LV	cyclo (-D-Ala-L-Leu-D-MeAsp-L-Val-Adda-D-Glu-Mdha-)
Microcystin-LW	cyclo (-D-Ala-L-Leu-D-MeAsp-L-Trp-Adda-D-Glu-Mdha-)
Microcystin-LY	cyclo (-D-Ala-L-Leu-D-MeAsp-L-Tyr-Adda-D-Glu-Mdha-)
Microcystin-M(O)R	cyclo (-D-Ala-L-Met(O)-D-MeAsp-L-Arg-Adda-D-Glu-Mdha-)
Microcystin-RA	cyclo (-D-Ala-L-Arg-D-MeAsp-L-Ala-Adda-D-Glu-Mdha-)
Microcystin-RR	cyclo (-D-Ala-L-Arg-D-MeAsp-L-Arg-Adda-D-Glu-Mdha-)
Microcystin-WR	cyclo (-D-Ala-L-Try-D-MeAsp-L-Arg-Adda-D-Glu-Mdha-)
Microcystin-YA	cyclo (-D-Ala-L-Tyr-D-MeAsp-L-Ala-Adda-D-Glu-Mdha-)
Microcystin-YM(O)	cyclo (-D-Ala-L-Tyr-D-MeAsp-L-Met(O)-Adda-D-Glu-Mdha-)
Microcystin-YR	cyclo (-D-Ala-L-Tyr-D-MeAsp-L-Arg-Adda-D-Glu-Mdha-)
Microcystin-(H4)YR	cyclo (-D-Ala-L-(H4)Tyr-D-MeAsp-L-Arg-Adda-D-Glu-Mdha-)

WHO provisional limit for drinking water  
1 µg/L expressed as MC-LR equivalents

Uncertainty factor 1000

Intended with ELISA assay

More than 120 known variants,  
12 certified standards available

# LC-MS for «early warning system»

“National group for management of cyanobacteria risks in water intended for human consumption”

New parameter in D.Lgs. 21/10

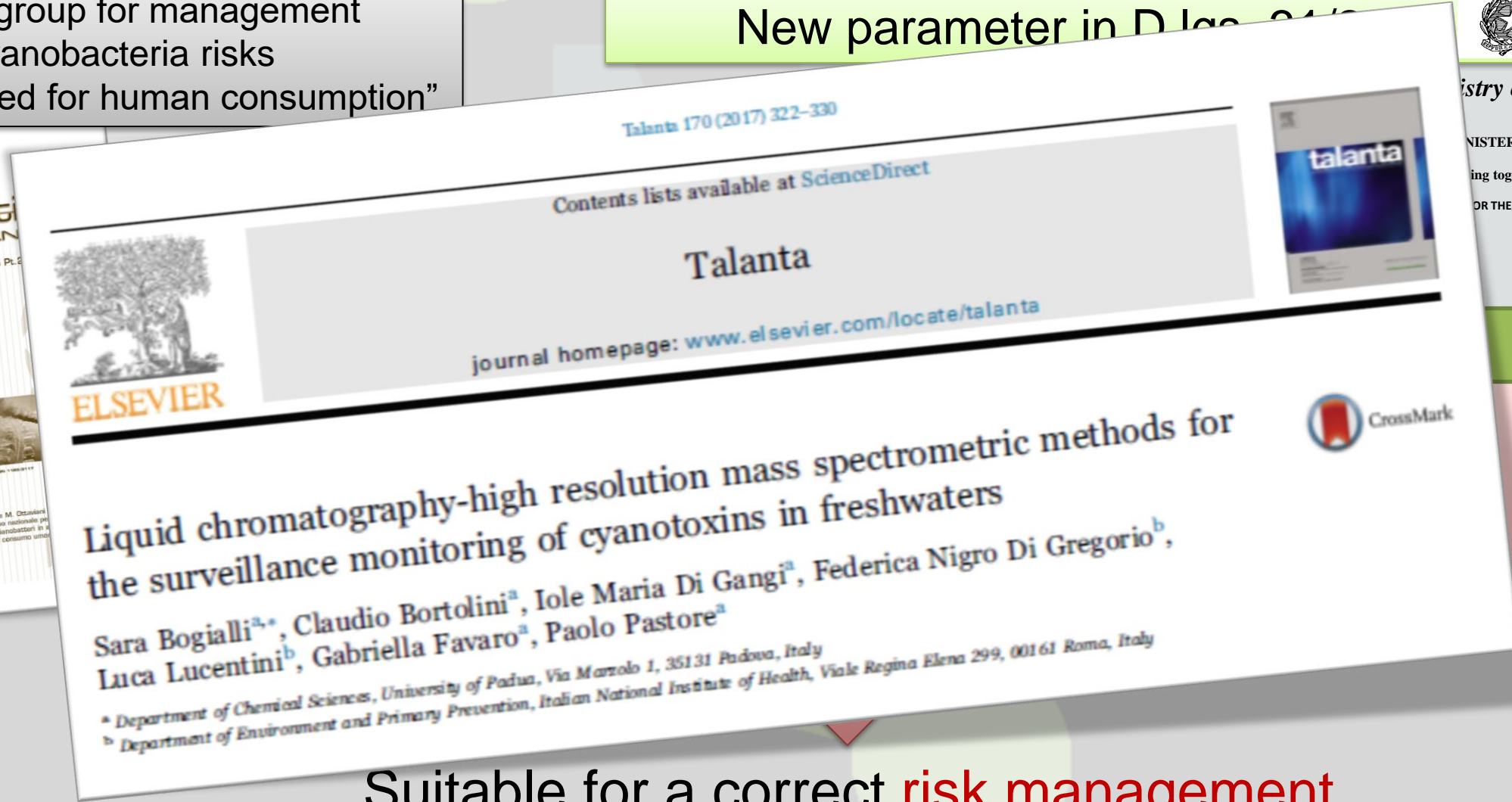
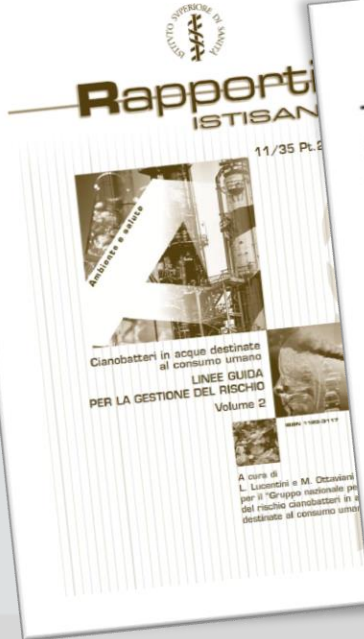


Ministry of Health

MINISTER FOR HEALTH

Working together with

Ministry of the Environment, Land and Sea



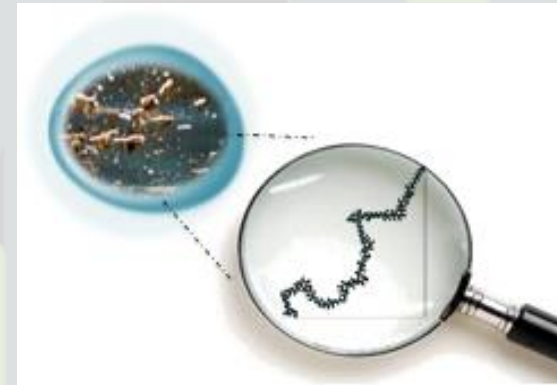
Suitable for a correct risk management

## DISC-UNIPD: Characterization of species-dependent toxicity

Sampling of blooms or in-lab cells growths



Extraction of toxins:  
intra and extracellular content



TARGETED analysis

UNTARGETED analysis

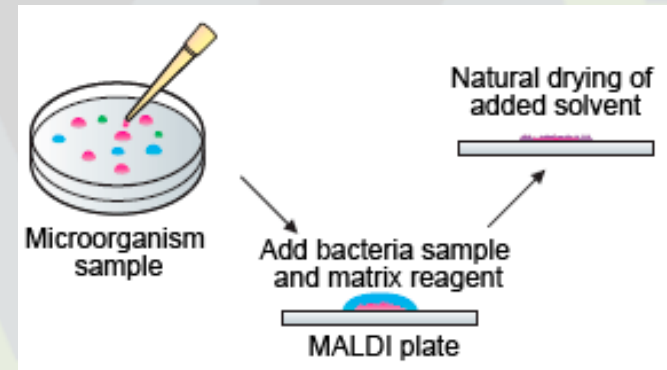
Quantification  
of KNOWN toxins

Characterization of  
UNKNOWN toxins

DATABASE



## ICMATE-CNR: Characterization of cyanobacteria species



Protein profile  
(hopefully species-dependent)

DATABASE



## Analytical method and protocols for Data analysis

Talanta 194 (2019) 233–242

Contents lists available at ScienceDirect

Talanta

journal homepage: [www.elsevier.com/locate/talanta](http://www.elsevier.com/locate/talanta)



A new method for the determination of primary and secondary terrestrial and marine biomarkers in ice cores using liquid chromatography high-resolution mass spectrometry

Amy C.F. King<sup>a,b,\*</sup>, Chiara Giorio<sup>b,\*,\*</sup>, Eric Wolff<sup>c</sup>, Elizabeth Thomas<sup>a</sup>, Ornella Karroca<sup>b,d</sup>, Marco Roverso<sup>e</sup>, Margit Schwikowski<sup>f</sup>, Andrea Tapparo<sup>e</sup>, Andrea Gambaro<sup>d</sup>, Markus Kalberer<sup>b</sup>

analytical  
chemistry

Cite This: *Anal. Chem.* 2019, 91, 5051–5057

pubs.acs.org/ac

### Direct Injection Liquid Chromatography High-Resolution Mass Spectrometry for Determination of Primary and Secondary Terrestrial and Marine Biomarkers in Ice Cores

Amy C. F. King<sup>\*,†,‡</sup>, Chiara Giorio<sup>\*,‡,§</sup>, Eric Wolff<sup>||</sup>, Elizabeth Thomas<sup>†</sup>, Marco Roverso<sup>§</sup>, Margit Schwikowski<sup>‡</sup>, Andrea Tapparo<sup>§</sup>, Sara Bogialli<sup>§</sup>, and Markus Kalberer<sup>‡,¶</sup>



Cite This: *ACS Sens.* 2018, 3, 1291–1298

pubs.acs.org/acssensors

### Electrochemosensor for Trace Analysis of Perfluorooctanesulfonate in Water Based on a Molecularly Imprinted Poly(*o*-phenylenediamine) Polymer

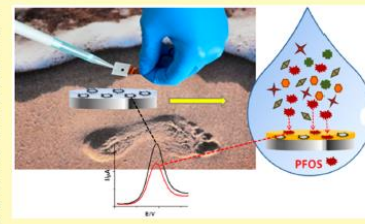
Najmeh Karimian<sup>†</sup>, Angela M. Stortini<sup>†</sup>, Ligia M. Moretto<sup>†</sup>, Claudio Costantino<sup>†</sup>, Sara Bogialli<sup>‡,§</sup>, and Paolo Ugo<sup>\*,†,§</sup>

<sup>†</sup>Department of Molecular Sciences and Nanosystems, University Ca' Foscari of Venice, via Torino 155, 30172 Venezia Mestre, Italy

<sup>‡</sup>Department of Chemical Sciences, University of Padova, via F. Marzolo 1, 35131 Padova, Italy

Supporting Information

**ABSTRACT:** This work is aimed at developing an electrochemical sensor for the sensitive and selective detection of trace levels of perfluorooctanesulfonate (PFOS) in water. Contamination of waters by perfluorinated alkyl substances (PFAS) is a problem of global concern due to their suspected toxicity and ability to bioaccumulate. PFOS is the perfluorinated compound of major concern, as it has the lowest suggested control concentrations. The sensor reported here is based on a gold electrode modified with a thin coating of a molecularly imprinted polymer (MIP), prepared by anodic electropolymerization of *o*-phenylenediamine (*o*-PD) in the presence of PFOS as the template. Activation of the sensor is achieved by template removal with suitable solvent mixture. Voltammetry, a quartz



Article



Atmospheric Environment 178 (2018) 129–139

Contents lists available at ScienceDirect

Atmospheric Environment

journal homepage: [www.elsevier.com/locate/atmosenv](http://www.elsevier.com/locate/atmosenv)

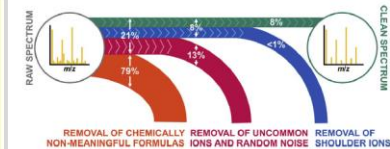


A new processing scheme for ultra-high resolution direct infusion mass spectrometry data

Arthur T. Zielinski<sup>a</sup>, Ivan Kourtchev<sup>a</sup>, Claudio Bortolini<sup>b</sup>, Stephen J. Fuller<sup>a</sup>, Chiara Giorio<sup>a</sup>, Olalekan A.M. Popoola<sup>a</sup>, Sara Bogialli<sup>b</sup>, Andrea Tapparo<sup>b</sup>, Roderic L. Jones<sup>a</sup>, Markus Kalberer<sup>a,\*</sup>

<sup>a</sup>Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, United Kingdom  
<sup>b</sup>Department of Chemical Sciences, University of Padova, via Marzolo 1, 35131 Padova, Italy

GRAPHICAL ABSTRACT



## Identification of binders in paintings



**GUM ARABIC**  
(natural polymers)  
polysaccharides



**ANIMAL GLUE**  
(proteins)



**ACRYLIC**  
(synthetic polymer)



**EGG YOLK**  
(proteins)



**LINSEED OIL**  
(lipids)



**MILK (caseins)**  
(proteins)



**BEESWAX**  
(lipids and waxes)

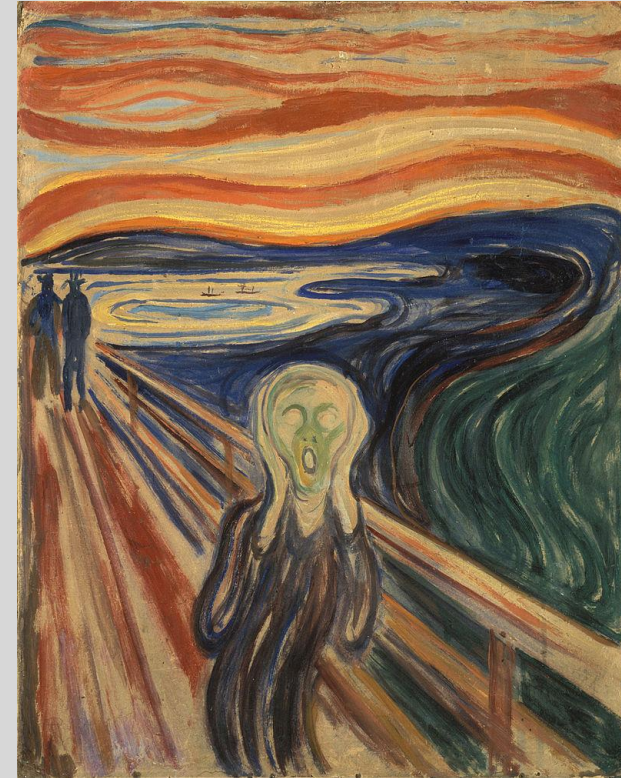
## Identification of binders in paintings

### **BINDERS:**

- Usually BIG molecules
- Very different (chemically)
- Usually present in mixture
- Pigments might chemically modify the binder (?)
- Low amount of sample



***Single MS-based analytical method  
for binders characterization***





## Untargeted Analysis of known binders and pigments

Binder (or mixture)

Binder (or mixture)

*Extraction  
(derivatization)*

*Matrix addition  
(enzymatic digestion)*



Statistical Analysis



DATABASE  
(and analytical method)

## Analysis of unknown samples



Sampling  
( $< 1$  mg)



MS analysis



**BINDER ID**  
(1-2 hours)



DATABASE



UNIVERSITÀ  
DEGLI STUDI  
DI PADOVA

# Collaboration\_Padua\_DISC

## Characterization of materials; food adulterants



Synthesis of organometals for catalysis and medical applications

ORGANOMETALLICS

Platinum(II) Complexes with Novel Diisocyanide Ligands: Catalysts in Alkyne Hydroarylation

Daniela Vicenzi,<sup>1</sup> Paolo Sgarbosa,<sup>1,2</sup> Andrea Biffis,<sup>1</sup> Cristina Tubaro,<sup>3,4</sup> Marino Basato,<sup>1</sup> Rino A. Mudele,<sup>1</sup> Arianna Lanna,<sup>1</sup> Fabrizio Nestola,<sup>1</sup> Sara Bogiatti,<sup>1</sup> Paolo Pastore,<sup>1</sup> and Alfonso Venzo<sup>1</sup>

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Supporting Information

Journal of Inorganic Biochemistry  
Journal of Inorganic Biochemistry  
Journal homepage: www.elsevier.com/locate/jinorgbio

Synthesis and biological assays on cancer cells of dinuclear gold (I) complexes with novel functionalised di(heterocyclic carbene) ligands

Marco Baron,<sup>1</sup> Stéphanie Bellemain-Lapomaz,<sup>1,2</sup> Cristina Tubaro,<sup>1,3,4</sup> Marino Basato,<sup>1</sup> Sara Bogiatti,<sup>1</sup> Alessandro Diolmella<sup>1</sup>

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Dalton Transactions  
PAPER  
Check for updates  
Cite this Dalton Trans., 2016, 47, 355

A square planar gold(III) bis-(1,1'-dimethyl-3,3'-methylene-diimidazol-2,2'-diylidene) trication as an efficient and selective receptor towards halogen anions: the cooperative effect of Au...X and X...HC interactions†

Marco Baron,<sup>1</sup> Anna Dall'Anese,<sup>1</sup> Cristina Tubaro,<sup>1,2</sup> Laura Orzan,<sup>1,3</sup> Valerio Di Marco,<sup>1</sup> Sara Bogiatti,<sup>1</sup> Claudia Graiff,<sup>1,4</sup> and Marino Basato<sup>1</sup>

Cultural Heritage

CHEMISTRY  
A EUROPEAN JOURNAL  
FULL PAPER  
DOI: 10.1002/chem.201300756

Degradation Products from Naturally Aged Paper Leaves of a 16th-Century-Printed Book: A Spectrochemical Study

Maddalena Bronzato,<sup>[a]</sup> Paolo Calvini,<sup>[b]</sup> Carlo Federici,<sup>[c]</sup> Sara Bogiatti,<sup>[a]</sup> Gabriella Favaro,<sup>[a]</sup> Moreno Meneghetti,<sup>[a]</sup> Miriam Mba,<sup>[a]</sup> Marina Brustolon,<sup>[a]</sup> and Alfonso Zoleo<sup>[a]</sup>

Research article  
Received 22 December 2015  
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Published online in Wiley Online Library  
wileyonlinelibrary.com DOI: 10.1002/jrs.4938

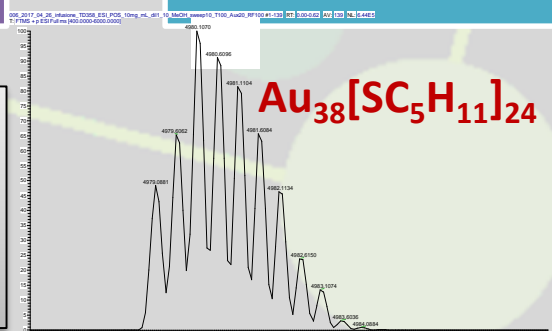
Composition and spectroscopic properties of historic Cr logwood

Silvia A. Centeno,<sup>a,\*</sup> Maddalena Bronzato,<sup>b</sup> Polonca Repret,<sup>c</sup> Alfonso Zoleo,<sup>b</sup> Alfonso Venzo,<sup>b</sup> Sara Bogiatti,<sup>b</sup> and Denis Badocco<sup>b</sup>

Food analysis

Sugars analysis  
With NMR & LC-MS

Nanomaterials



ACS NANO  
Gold Fusion: From  $Au_{25}(SR)_{18}$  to  $Au_{38}(SR)_{24}$ , the Most Unexpected Transformation of a Very Stable Nanocluster

Titano Dainese,<sup>1</sup> Sabrina Antonello,<sup>2</sup> Sara Bogiatti,<sup>1</sup> Wenwen Fei,<sup>1</sup> Alfonso Venzo,<sup>1</sup> and Flavio Maran<sup>1,2,3</sup>

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<sup>2</sup>Department of Chemistry, University of Connecticut, 55 North Eagleville Road, Storrs, Connecticut 06269, United States

Supporting Information

ABSTRACT: The study of the molecular cluster  $Au_{25}(SR)_{18}$ , has provided a wealth of fundamental insights into the properties of clusters protected by thiolated ligands (SL). This is also because this cluster has been particularly stable under a number of experimental conditions. Very unexpectedly, we found that paramagnetic  $Au_{25}(SR)_{18}$  undergoes a spontaneous bimolecular fusion to form another benchmark gold nanocluster,  $Au_{38}(SR)_{24}$ . We tested this reaction with a series of  $Au_n$  clusters. The fusion was confirmed and characterized by UV-vis absorption spectroscopy, ESI mass spectrometry, IR and <sup>13</sup>C NMR spectroscopy, and electrochemistry. NMR evidences the presence of four types of ligand and, for the same proton type, double signals caused by the diastereoisomerism arising from the chirality of the capping shell. This effect propagates

Co-reactants? No, thanks!

LC-HRMS



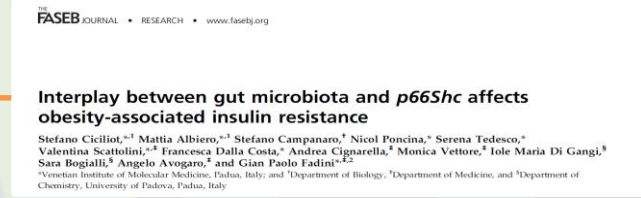
# Collaboration\_Padua\_University «Top-down» Metabolomic; biomarkers; environment



LC-HRMS

Dpt. of Medicine

Metabolomic on microbioma of diabetes



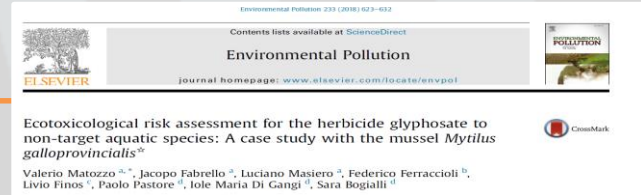
Dpt. Pharmaceutical Sciences

-Metabolomic on Microbioma  
Gastrointestinal disorder, Hepatite B  
-Pharmacokinetic



Dpt. of Biology

-Risk assessment on emerging contaminants  
(glyphosate, PFAs)  
-Marine Biology,  
Algal metabolites



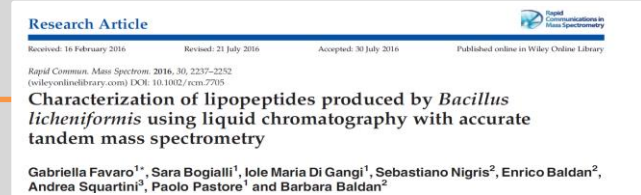
Dpt. of Land, Environment,  
Agriculture And Forestry

Pharmacokinetic of biocides

Regional project «INFUSE»  
Research activities for Spin-off  
Two patents

Dept. of Agronomy, Animals, Food,  
Natural Resources and Environment

Food contaminants (mycotoxins)  
Bacteria bioactive metabolites



# The analytical group

*... thanks for the attention.*

