

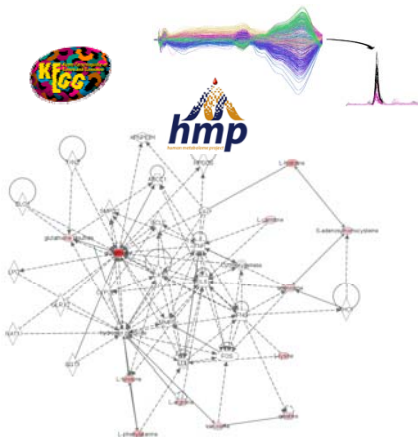


Foodomics: food science in the post-genomic era

Alejandro Cifuentes



Laboratory of Foodomics, CIAL
National Research Council of Spain (CSIC)
Madrid, Spain



CEICS Forum 2011, Tarragona

CURRENT CHALLENGES IN FOOD SCIENCE

**Production of new functional foods
(with scientifically proved claims)**

**Food safety, quality and traceability
(ideally as a whole) using omics
approaches**

**Develop, produce and monitor new
transgenics foods**

**Understand the effects of gene-food interaction on
human health (Nutrigenomics)**

**Explain the different answers from individuals to food:
personalized diet (Nutrigenetics)**



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New needs, new answers: Foodomics

Foodomics

We have defined **Foodomics** for the first time in a SCI journal as:
A discipline that studies the Food and Nutrition domains through the application of advanced omics technologies to improve consumer's well-being, health, and confidence.

(Cifuentes et al.; *J. Chromatogr. A* 1216 (2009) 7109;
Electrophoresis 31 (2010) 205;
Mass Spectrom. Rev. 2011, DOI 10.1002/mas).



Volume 1216, Issue 43, 23 October 2009 ISSN 0021-9673
ADVANCED SEPARATION METHODS IN FOOD ANALYSIS
Guest Ed.: A. Cifuentes

JOURNAL OF CHROMATOGRAPHY A
INCLUDING ELECTROPHORESIS, MASS SPECTROMETRY AND OTHER SEPARATION AND DETECTION METHODS

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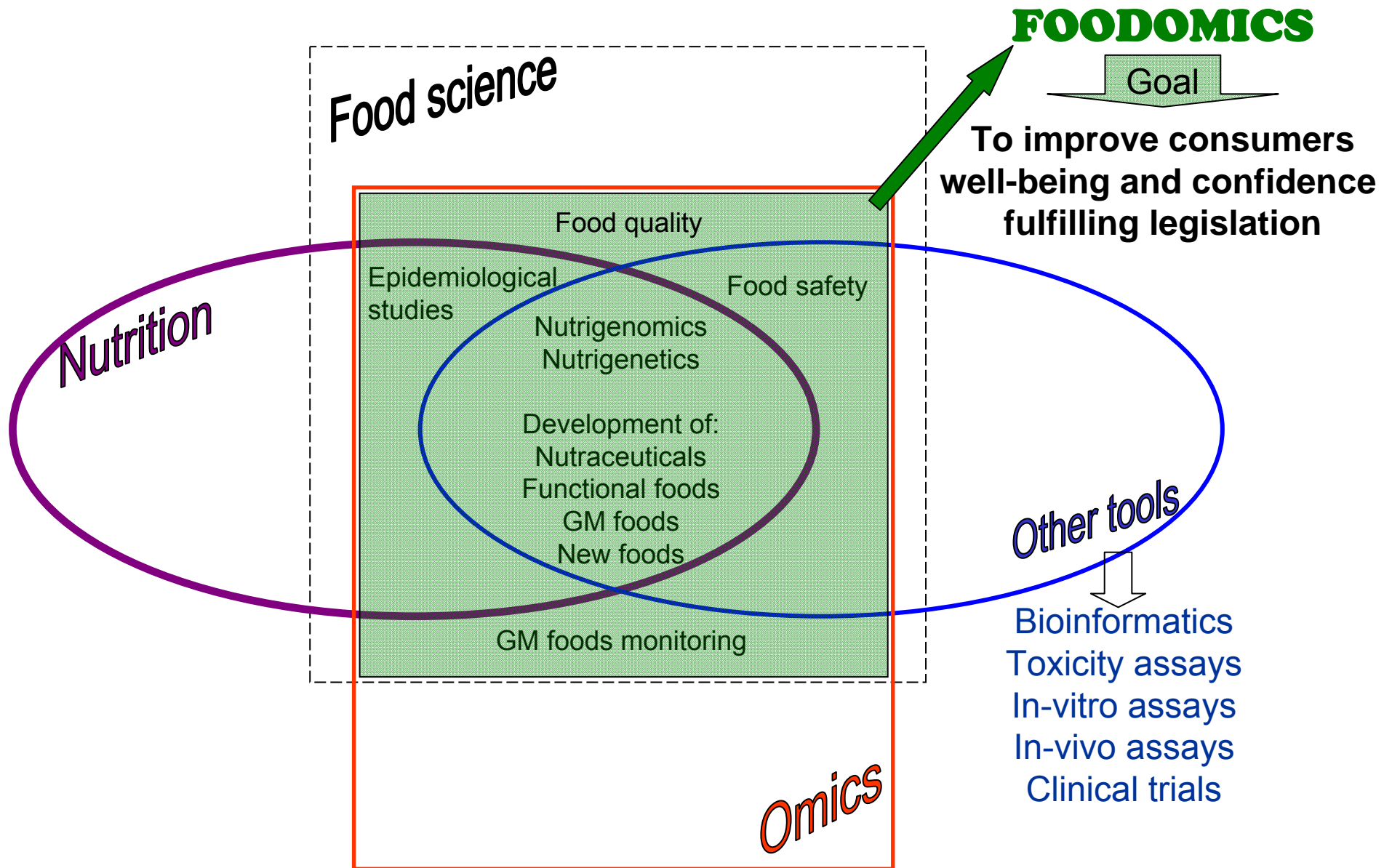
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The interest in Foodomics coincides with a clear shift in medicine and biosciences toward prevention of future diseases.



Foodomics: A new omics for a new food era



Foodomics papers from our group

-A. Cifuentes

“Food Analysis and Foodomics”

J. Chromatogr. A 1216 (2009) 7109-7110.

-M. Herrero, V. García-Cañas, C. Simo, A. Cifuentes

“Recent advances in the application of CE methods for food analysis and foodomics”

Electrophoresis 31 (2010) 205-228

-C. Simó, E. Domínguez-Vega, M.L. Marina, M.C. García, G. Dinelli, A. Cifuentes

“CE-TOF MS analysis of complex protein hydrolyzates from genetically modified soybeans. A tool for Foodomics”

Electrophoresis 31 (2010) 1175–1183

-M. Herrero, C. Simó, V. García-Cañas, E. Ibáñez, A. Cifuentes

“Foodomics: MS-based strategies in modern Food Science and Nutrition”

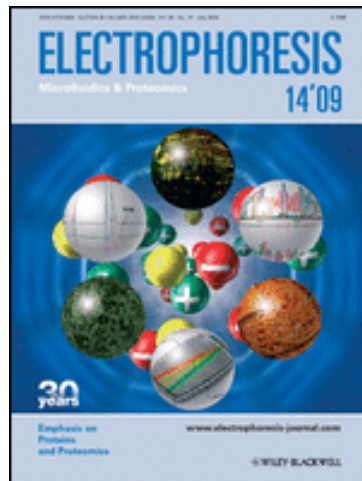
Mass Spectrom. Rev. 2011, DOI 10.1002/mas

ELECTROPHORESIS

(impact factor: 3.569)

Special issue on:

“Advanced Food Analysis and Foodomics”



Editor: *Alejandro Cifuentes*

a.cifuentes@csic.es

(to be published in summer 2012)



A book is now under preparation on:

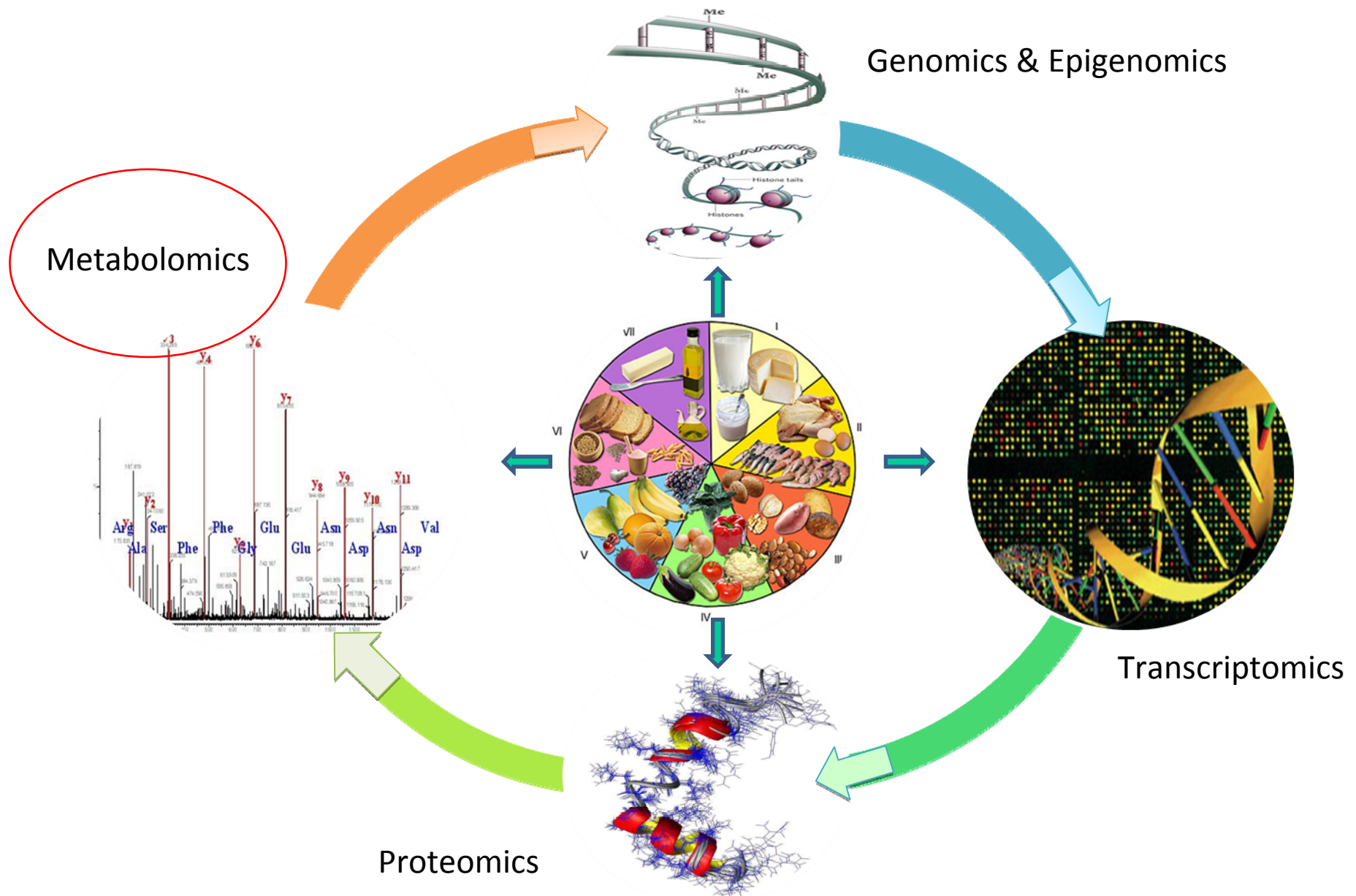
**“FOODOMICS:
ADVANCED MASS SPECTROMETRY IN
MODERN FOOD SCIENCE AND NUTRITION”**

Editor: *Alejandro Cifuentes*

a.cifuentes@csic.es

(to be published in autumn 2012)

Foodomics

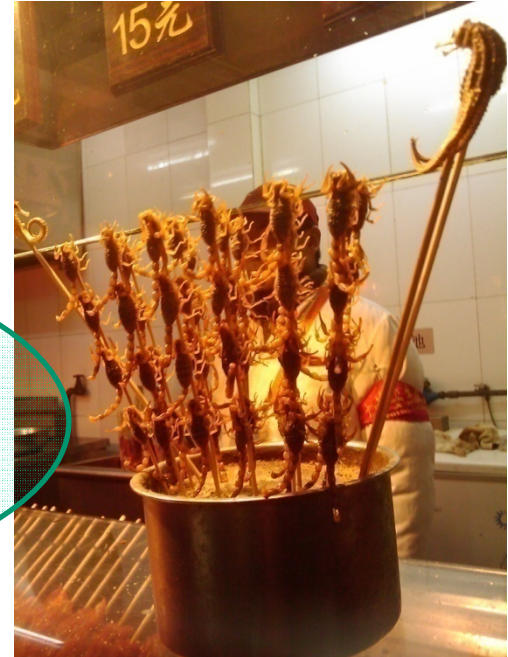


FOODOMICS: CURRENT CHALLENGES

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Transgenic maize (Bt corn)

A new CryIA(b) gene (encodes for a *Bacillus thuringiensis* protoxin) is inserted by recombinant DNA techniques into the maize genome.

The new protoxin acts as insecticide against lepidopters.

Transgenic soybean (RR soybean)

A new CP4 EPSPS gene from Agrobacterium (that encodes for a CP4 5-enolpyruvylshikimate-3-phosphate sintase, CP4-EPSPS) is inserted by recombinant DNA techniques into the soy genome.

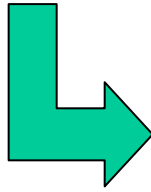
The new CP4-EPSPS enzyme allows to the GM plant to resist the effect of the herbicide glyphosate.

Can the new inserted genes give rise to other unintended effects?

The European Food Safety Agency (EFSA) recommends the development of profiling techniques to study these unexpected effects.



Second Generation GMOs



**THEIR SUCCESS WILL DEPEND (AMONG OTHER FACTORS)
ON PROVIDING STRONG SCIENTIFIC EVIDENCES ON:
-THEIR (HEALTH) BENEFITS FOR CONSUMERS
-THE EQUIVALENCE WITH THEIR NATURAL COUNTERPARTS
-NO ENVIRONMENTAL RISKS**

Macronutrients:

Proteins

Amino acid composition

Functionality, e.g. bread dough

Carbohydrates

Starch composition, inulin, monosaccharides

Vegetable oils

High-PUFA (e.g., oleic acid)

Micronutrients:

Vitamins, anti-oxidants (Golden rice)

Minerals (iron-fortified rice)

Miscellaneous:

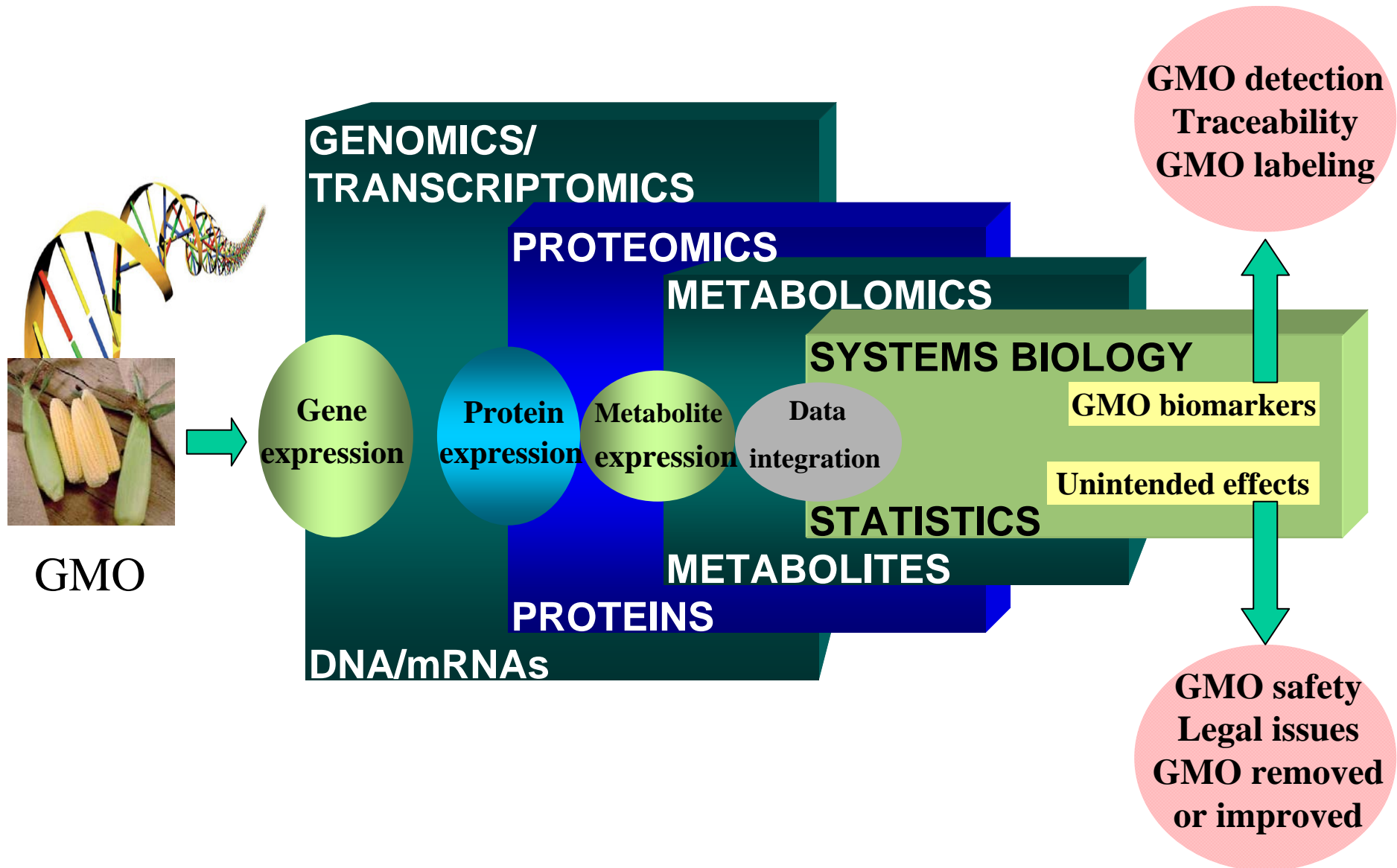
Hypoallergenic foods

Drought tolerance

Prolonged ripening



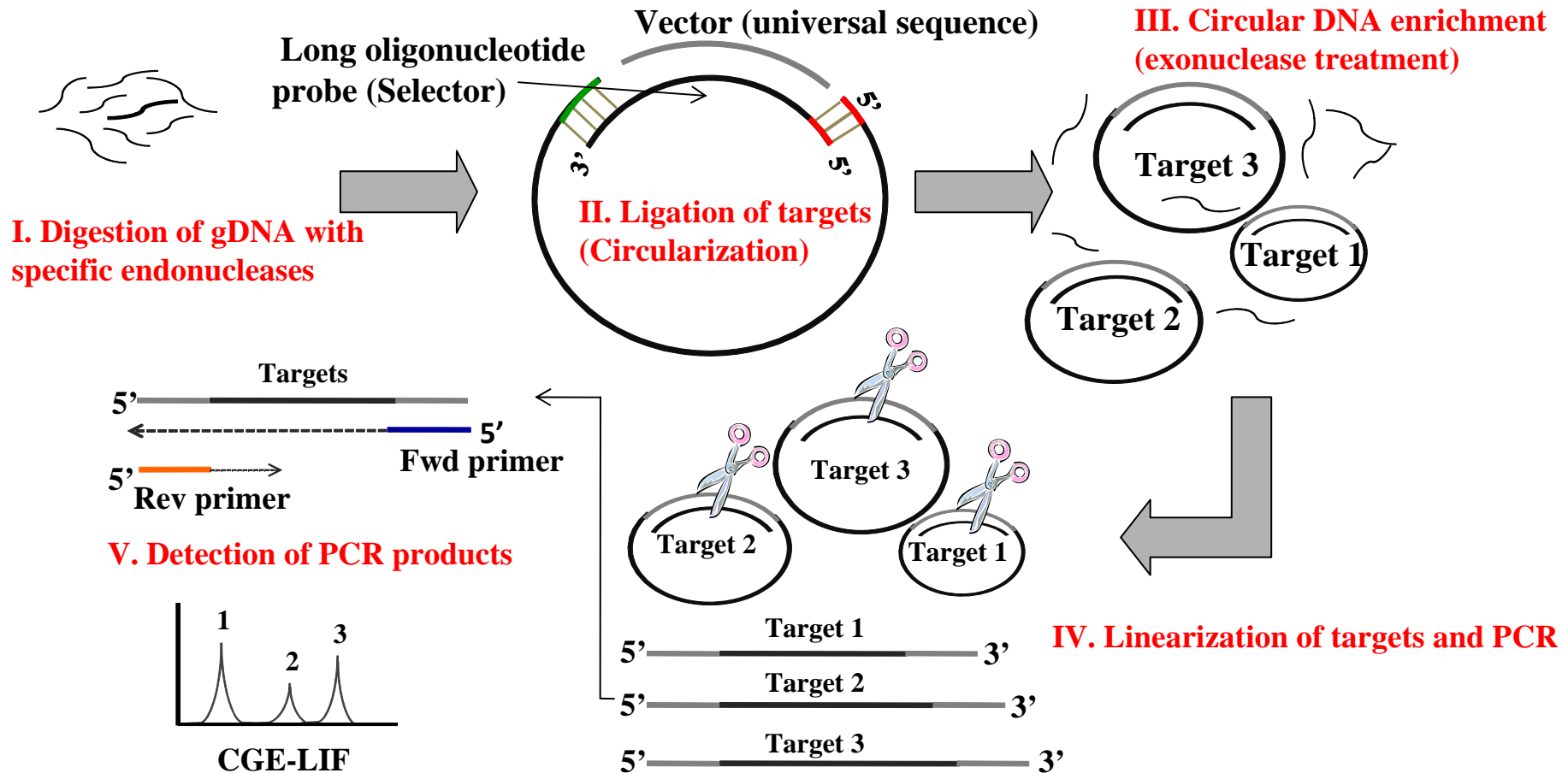
Ideal Foodomics platform for GMO analysis



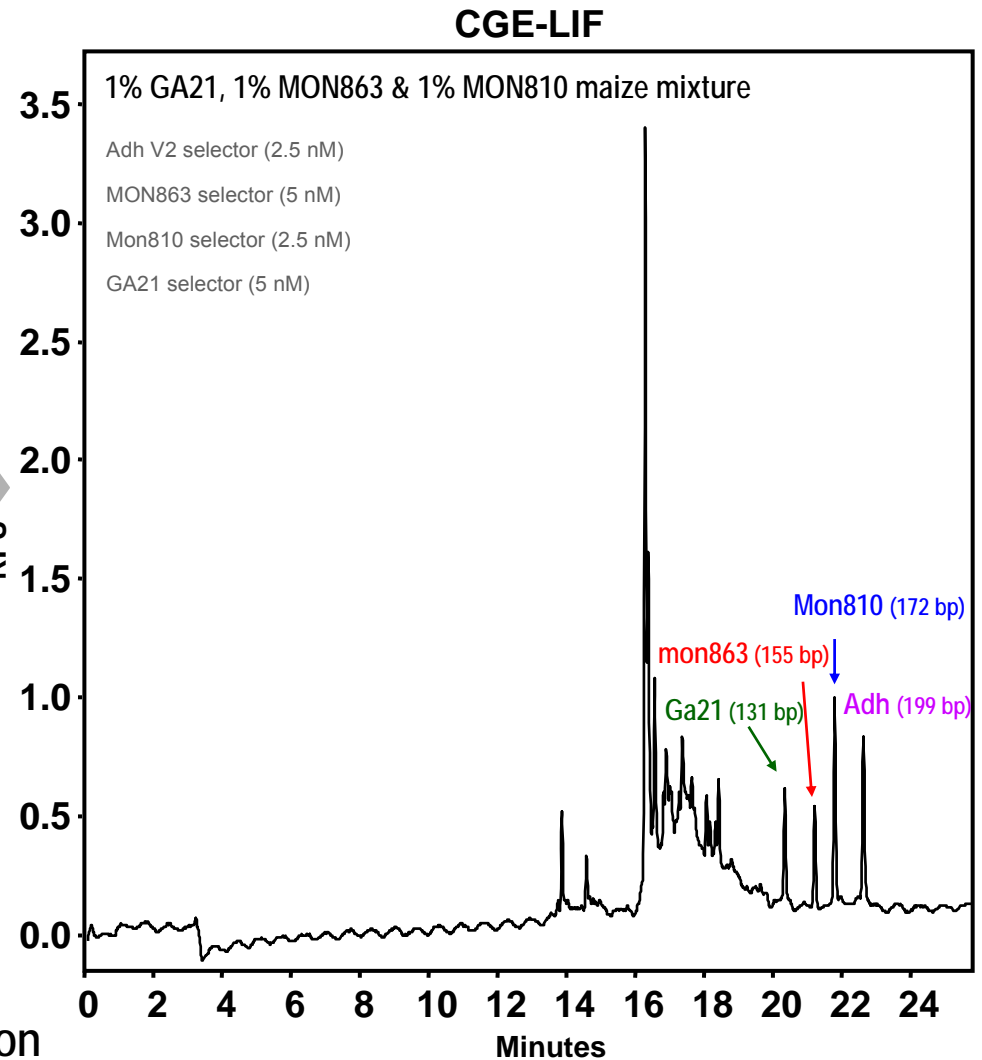
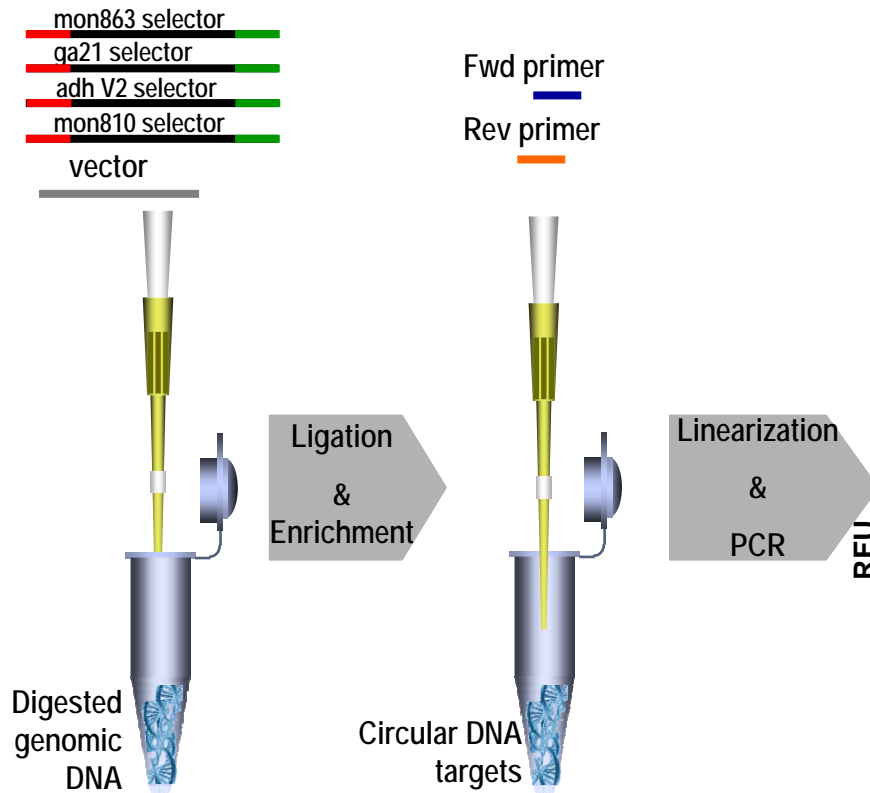
DNA analysis by CGE-LIF

Development of a novel analytical methodology, based on MLGA-**CGE-LIF**, to simultaneously detect multiple GMOs in a single reaction

Multiplex ligation dependent genome amplification (MLGA)



Simultaneous detection of multiple GMOs with MLGA-CGE-LIF



MLGA is very **flexible** since the incorporation of new additional selector probes to the ligation step requires minor adjustments of the selector concentration to detect all the DNA target with **LODs below 1%**

Calculated LODs (S/N=3)

0.2% GA21 maize

0.3% MON863 maize

0.1% MON810 maize

SHOTGUN PROTEOMICS by CE-TOF-MS: GM vs. wild soybean

SOYBEAN

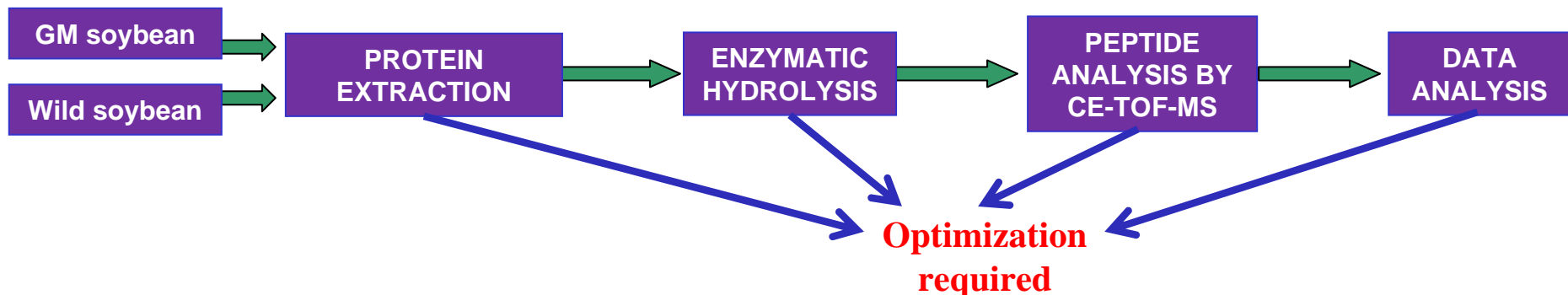
→ Protein content 40 %

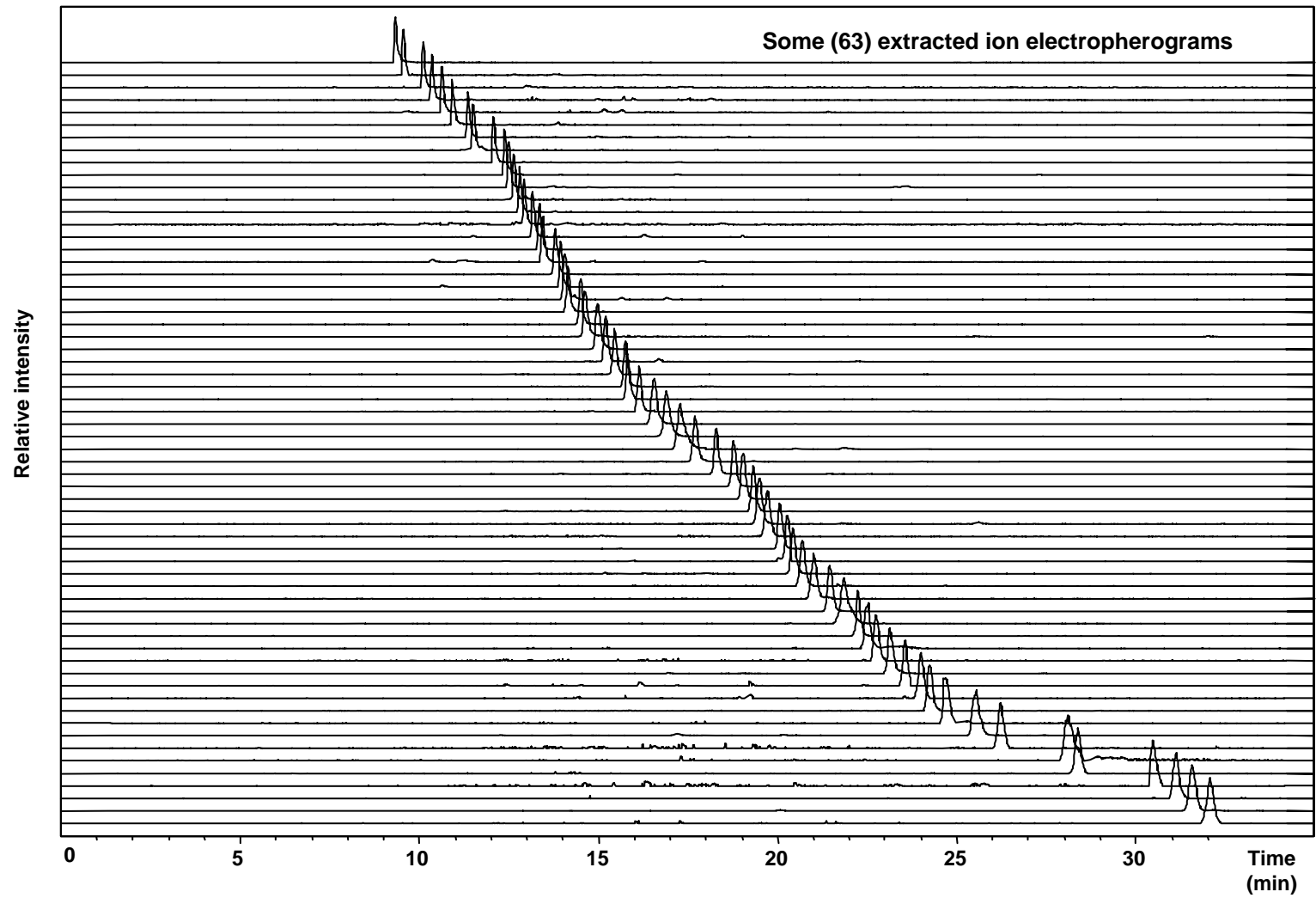
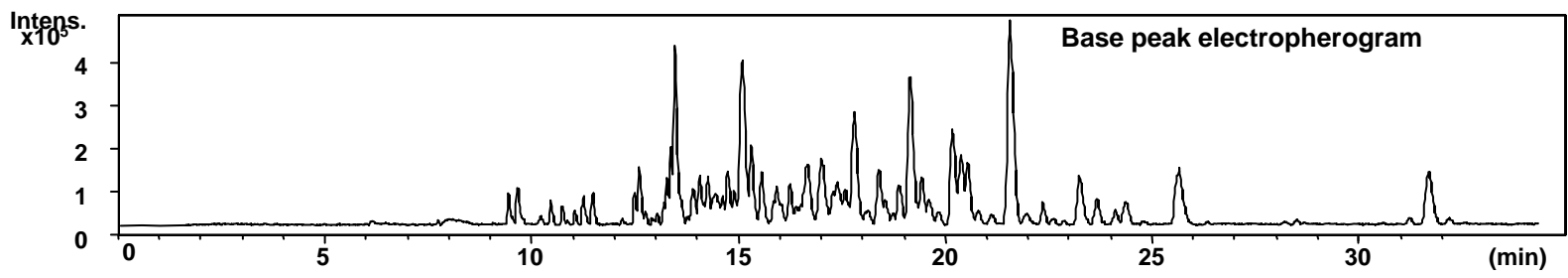
Well-known difficulties in protein separation:

- Different physico-chemical properties (*size, isoelectric point, hydrophobicity*) within a wide range of concentrations.
- Difficult to separate complex mixtures of proteins.
- Challenging identification of (large) proteins.

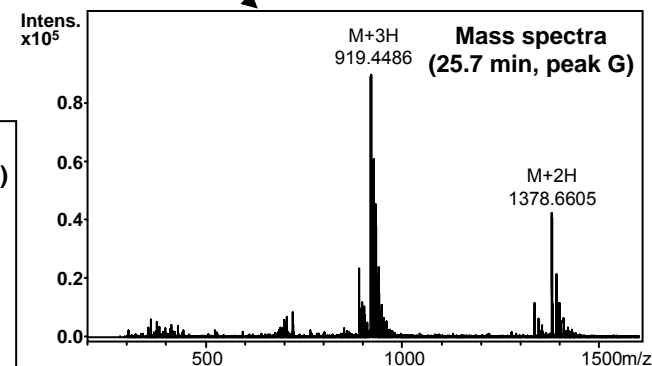
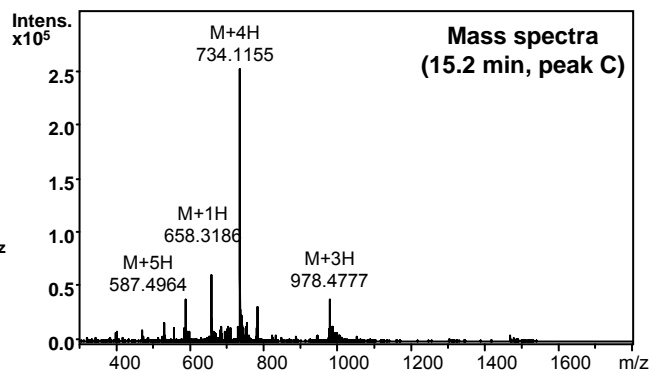
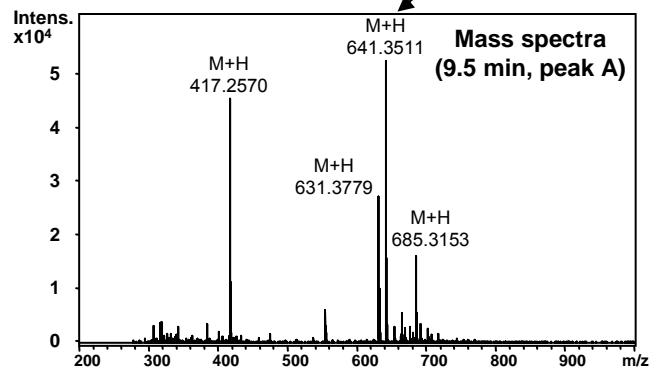
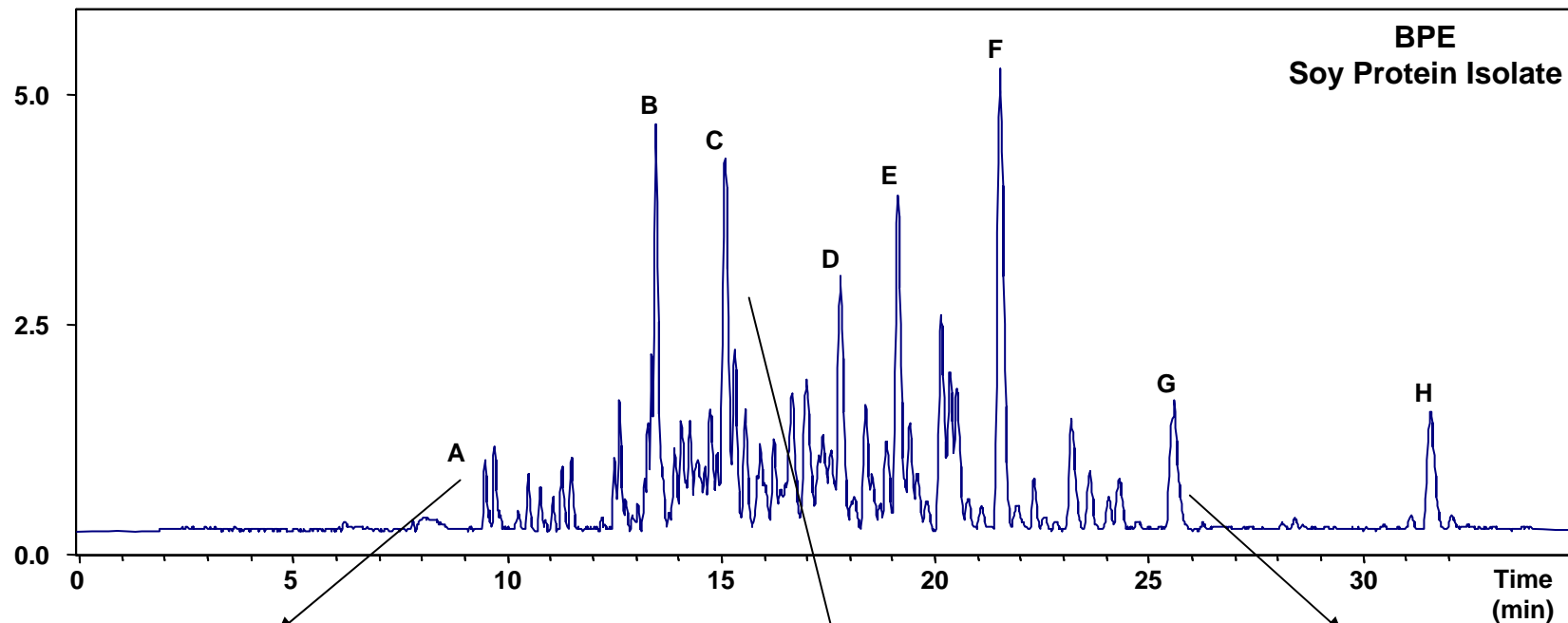
SHOTGUN PROTEOMICS by CE-TOF-MS

Analysis of peptides obtained after hydrolysis of complex protein mixtures





CE-TOF MS ANALYSIS UNDER SELECTED CONDITIONS



Complexity of the Peptidic Map



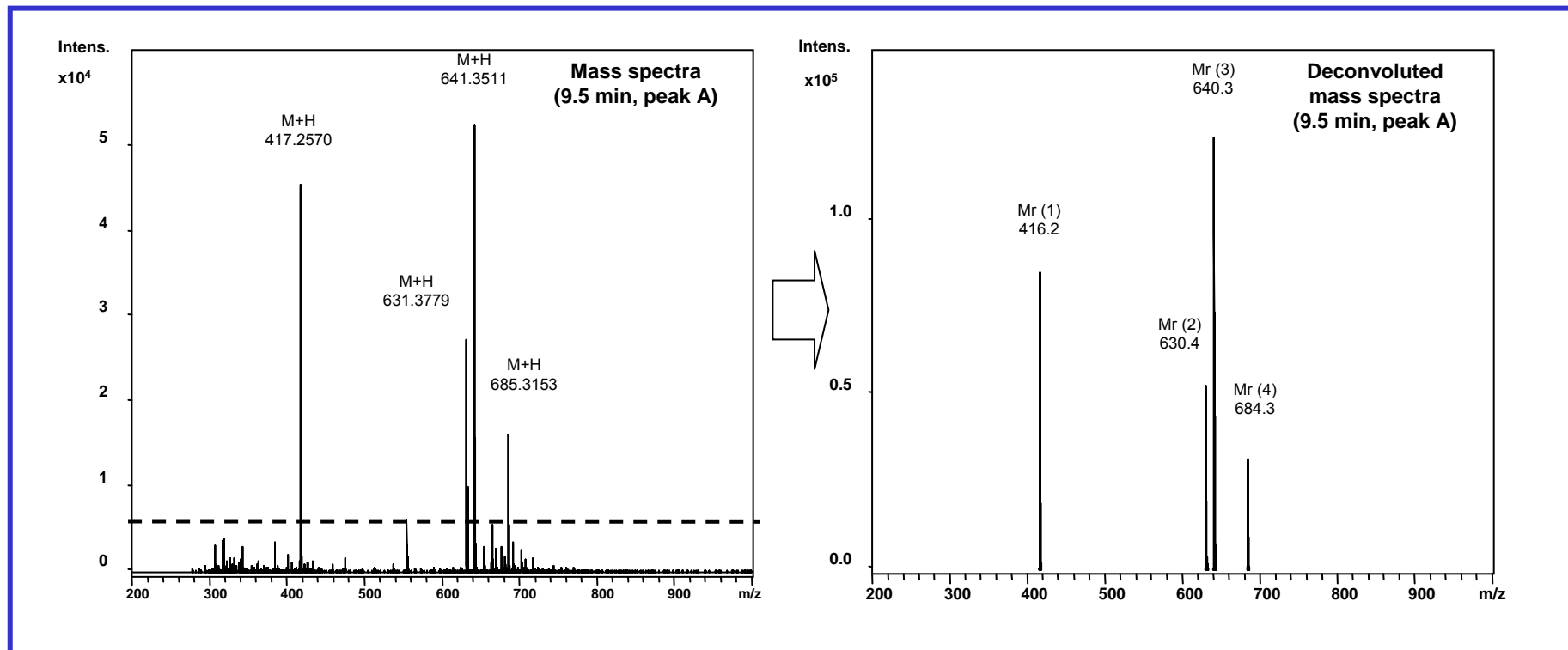
Automated interpretation

OPTIMIZATION OF AUTOMATED INTERPRETATION

Use of deconvolution tool → Study of the peptides obtained in 5 consecutive injections

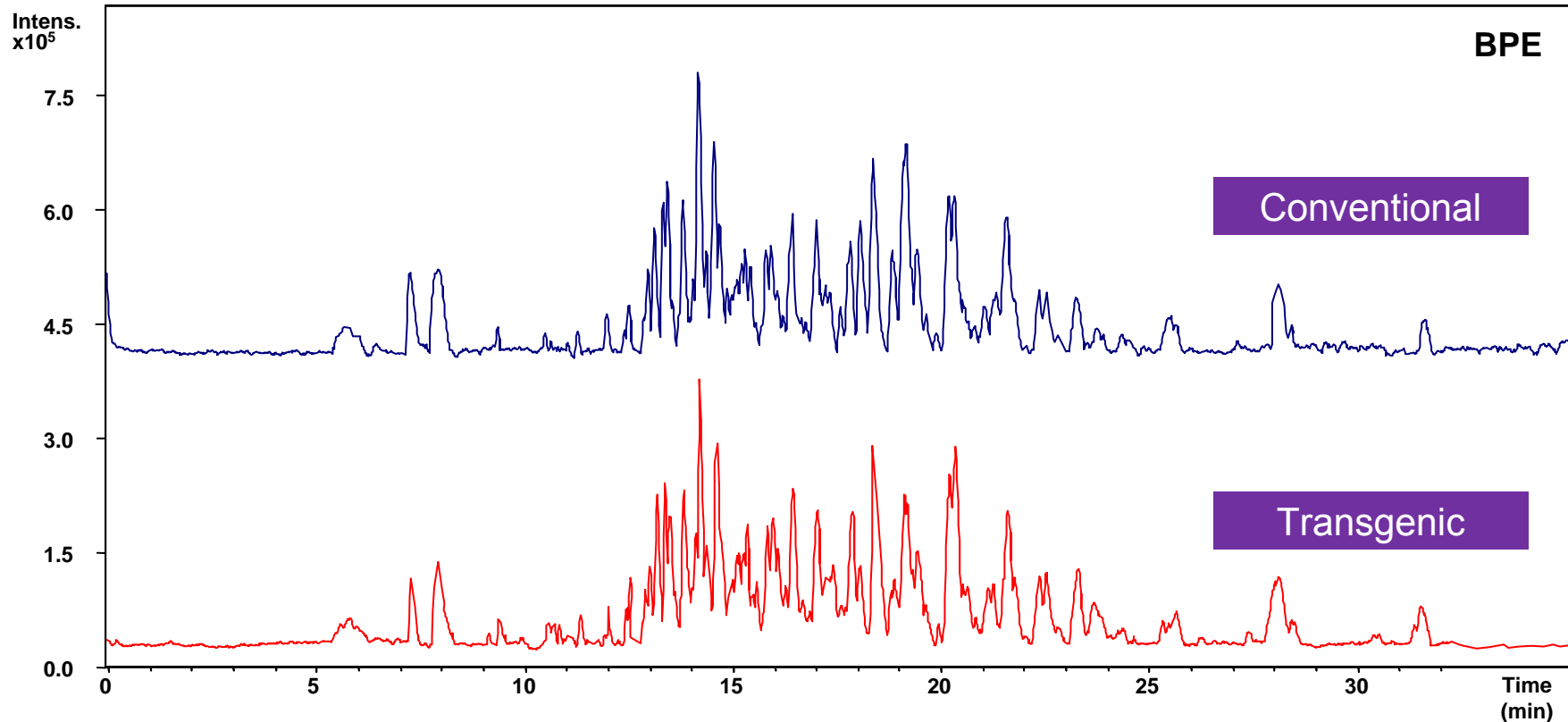
5 % Cutoff → The same peptides were not found in all the injections → ↑ cutoff in order to eliminate unstable signals

15 % Cutoff → The same peptides were found in all injections (simultaneous analysis of more than 150 peptides)



SHOTGUN PROTEOMICS by CE-TOF-MS:

GM vs. wild soybean

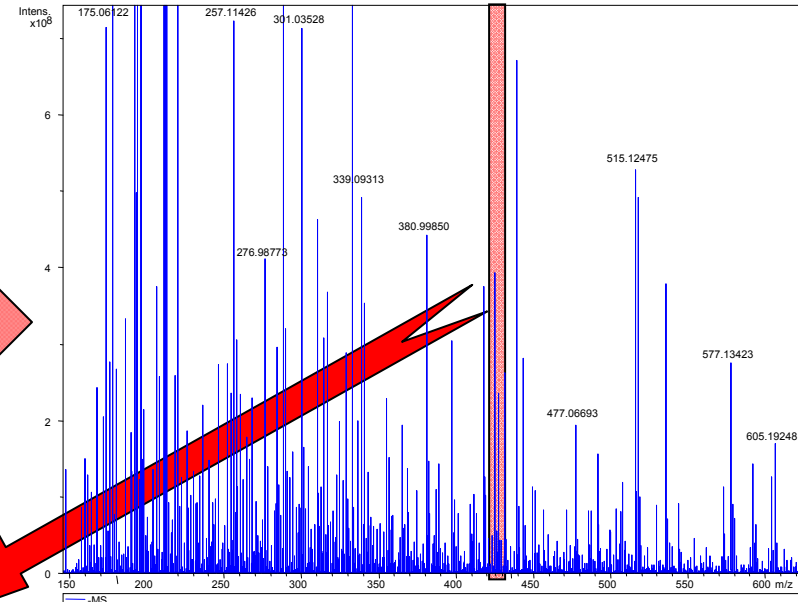


SIMILAR PEPTIDE PROFILE

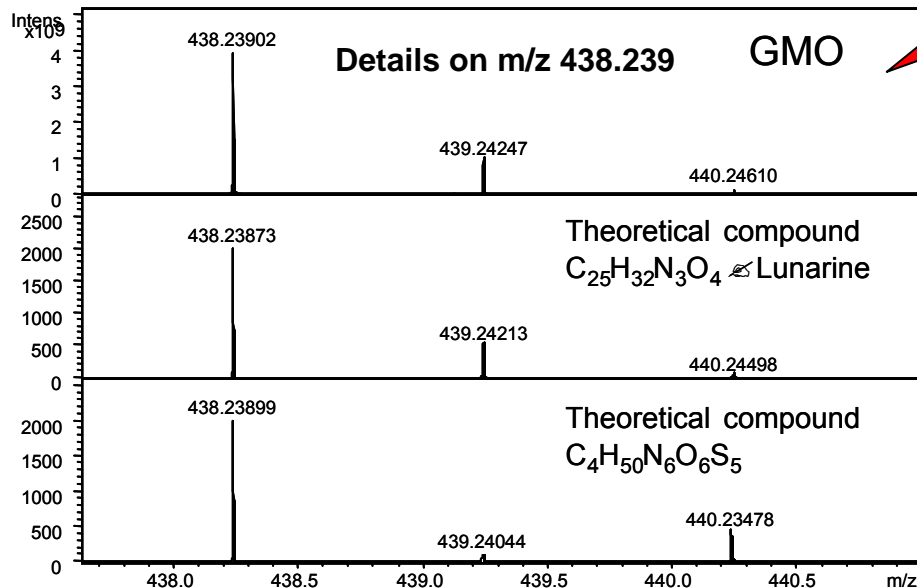


No differences were observed between the GM and wild soybean when a 15% abundance cutoff was used for the automatic deconvolution of the detected ions

METABOLOMICS by FT-ICR-MS, PLE and CE-TOF-MS: GM vs. wild corn

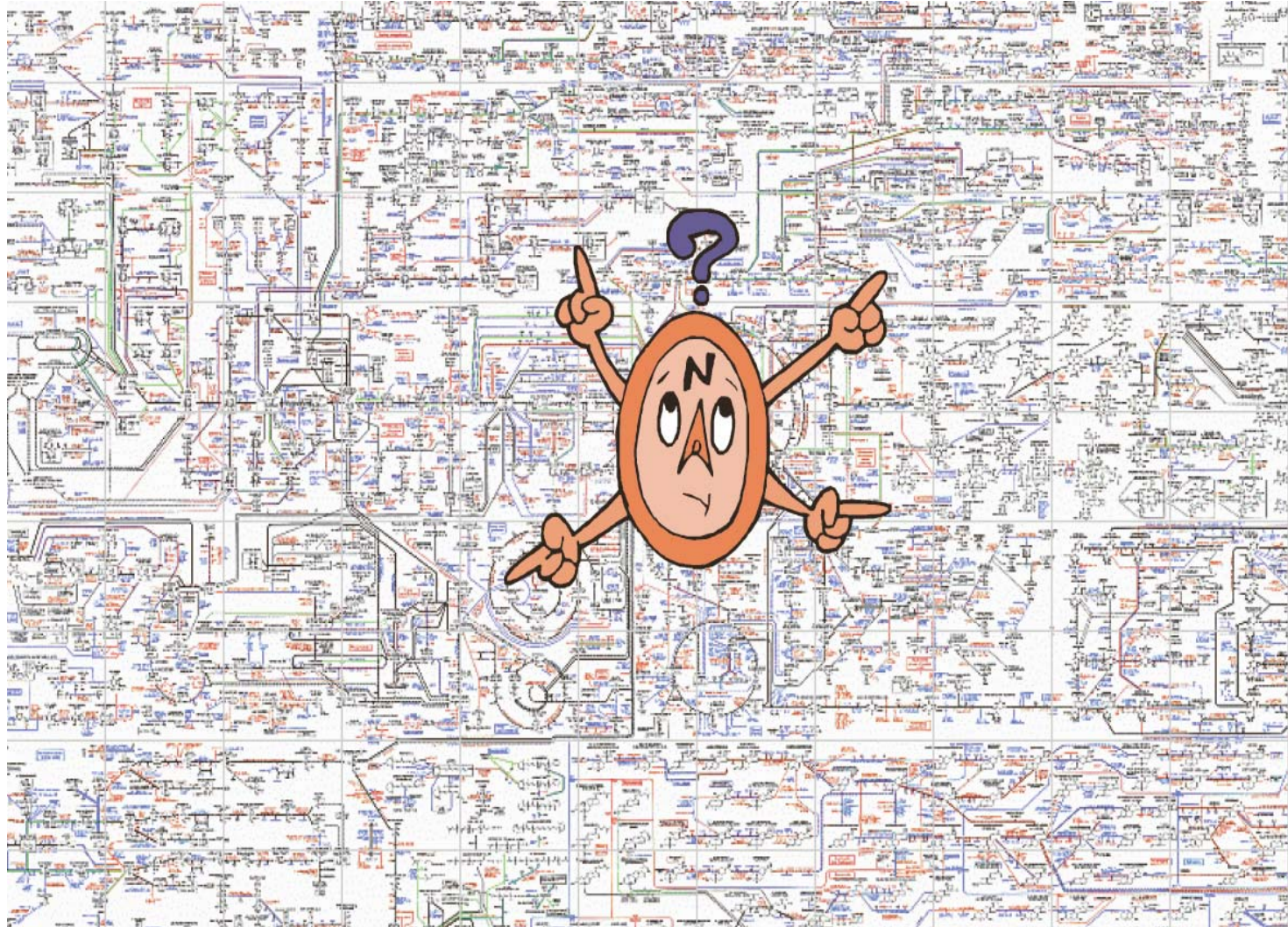


12 tesla FT-ICR-MS at GSF/Munich Germany
P. Schmitt Kopplin



Mass resolution: >600.000 in full scan
Mass accuracy: <0.1 ppm
>10.000 signals/mass spectra
>300 elementary composition assignments
(depending on the extraction conditions)

Although the high resolution and sensitivity provided by FT-MS allows the detection and identification of an impressive number of compounds, PLE and CE-TOF-MS can provide additional information useful to corroborate (or not) the metabolites identification.

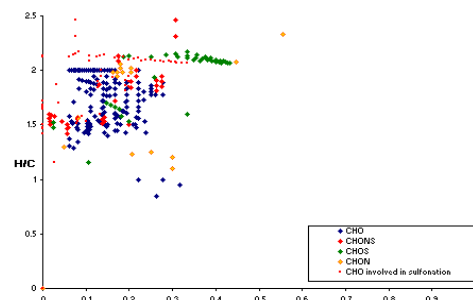
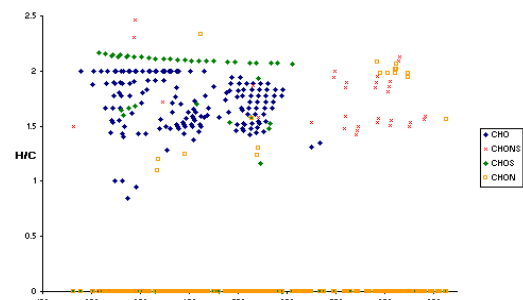


METABOLOMICS by FT-ICR-MS, PLE and CE-TOF-MS: GM vs. wild corn

FT-ICR-MS of wild maize

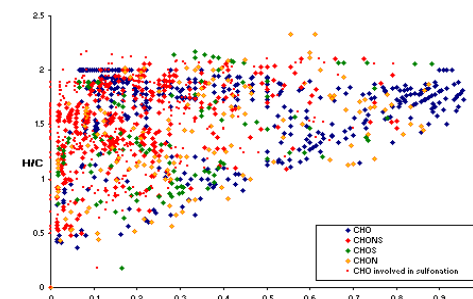
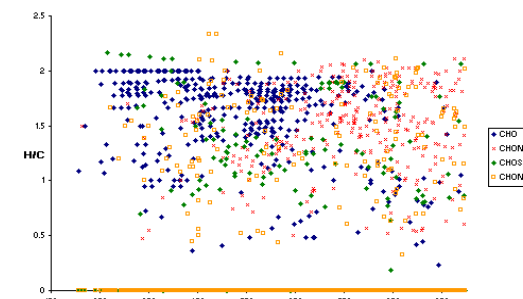
Mass resolution: >600.000 in full scan; Mass accuracy: <0.1 ppm; Signals/mass spectra: > 10.000
Elementary composition assignments: >300 (depending on the extraction conditions)

Extraction by PLE with:



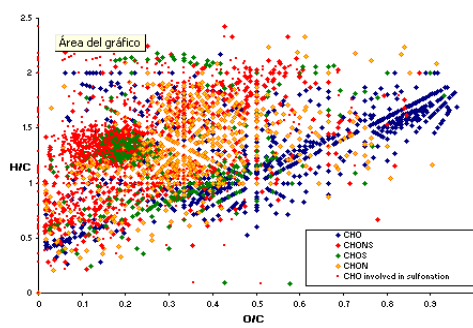
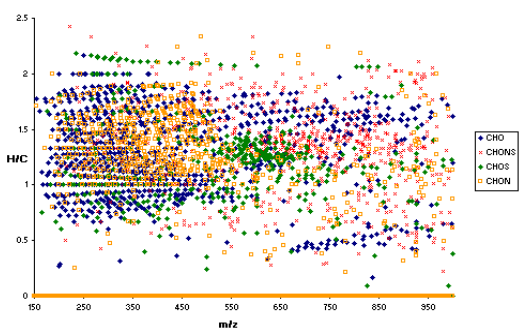
Tot	267
CHO	158
CHOS	60
CHON	17
CHONS	32

Hexane



Tot	1222
CHO	393
CHOS	385
CHON	145
CHONS	299

Methanol



Tot	3111
CHO	907
CHOS	972
CHON	612
CHONS	620

Water

PROCEDURE FOR THE TENTATIVE CHARACTERIZATION OF METABOLITES BASED ON FT-MS and CE-TOF-MS DATA

MOLECULAR ION DETERMINATION

ISOTOPIC PATTERN

MOLECULAR FORMULAE ASSIGNATION

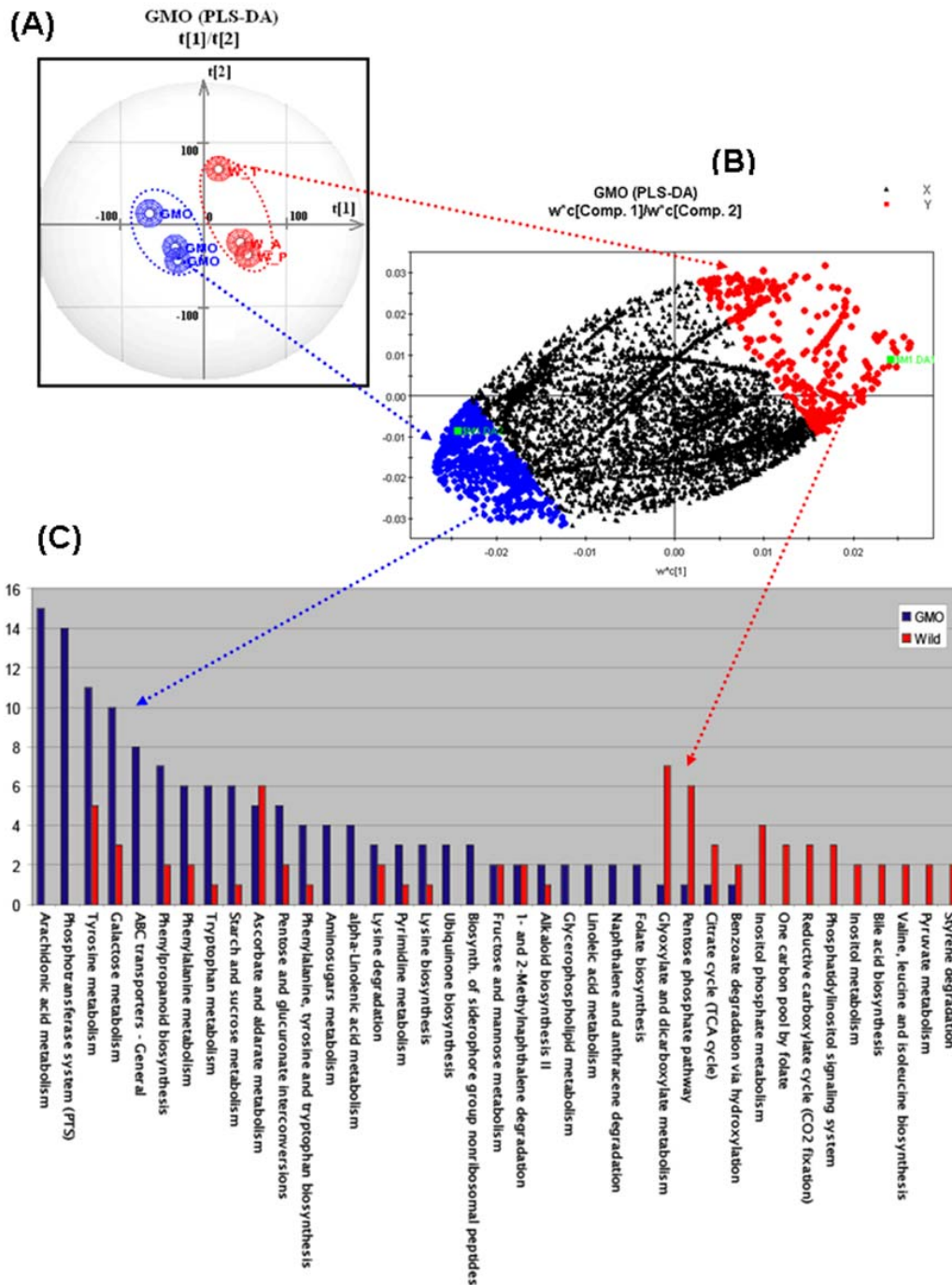
SEARCH IN DATABASES

EXPECTED ELECTROPHORETIC MOBILITY

DATA ANALYSIS

SAMPLES CLASSIFICATION/BIOMARKERS DETECTION





Partial least squares–discriminant analysis (PLS-DA)(Q2(cum)=0.52 and R2(Y)=0.99) with six different maize varieties analyzed by FT-MS.

Maize samples: A) PR33P66; B) PR33P66 Bt; C) Tietar; D) Tietar Bt; E) Aristis; and F) Aristis Bt.

The score scatter plot underlines a different pattern for the transgenic (they are represented in blue color) and wild lines (red color). The different properties of the discriminative masses (represented in blue and red in the loading plot) are investigated with MassTRIX.

The model was built up with the data measured in negative mode.

**Problem to be solved:
Number of available samples**

Publicaciones de nuestro grupo sobre GMOs

-C. Simó, R. González, C. Barbas, A. Cifuentes

Anal. Chem. 77 (2005) 7709-7716 ---**Proteomics**

-M. Herrero, E. Ibáñez, P.J. Martin-Alvarez, A. Cifuentes

Anal. Chem. 79 (2007) 5071-5077---**Metabolomics**

-T. Levandi, C. Leon, M. Kaljurand, V. Garcia-Cañas, A. Cifuentes

Anal. Chem. 80 (2008) 6329-6335 ---**Metabolomics**

- V. García-Cañas, M. Mondello, A. Cifuentes

Electrophoresis 31 (2010) 2249–2259 ---**Genomics**

-C. Leon, I. Rodriguez, M. Lucio, V. Garcia-Cañas, P. Schmitt-Kopplin, A. Cifuentes

J. Chromatogr. A 1216 (2009) 7314-7323---**Metabolomics**

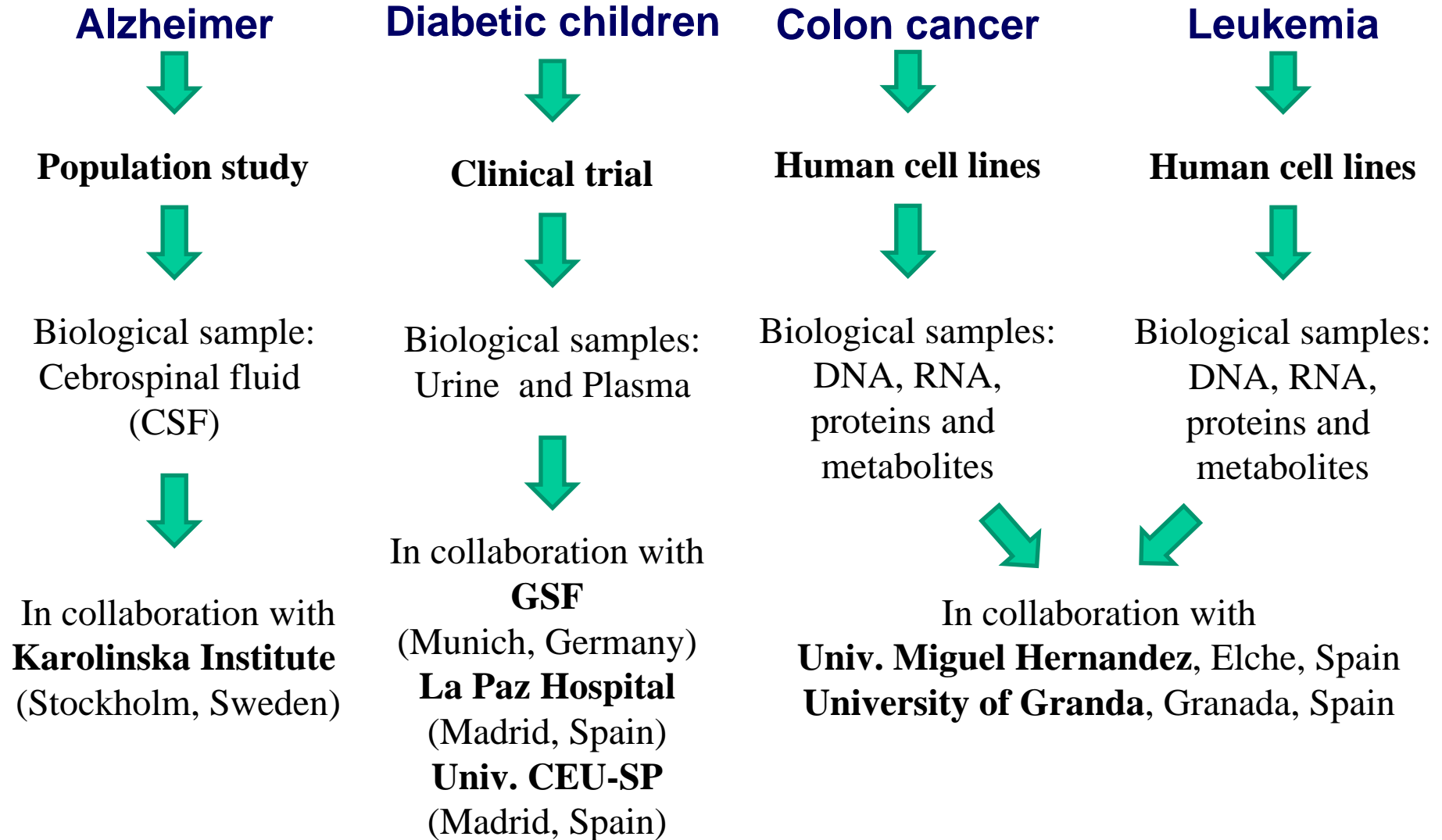
-C. Simó, E. Domínguez-Vega, M.L. Marina, M.C. García, G. Dinelli, A. Cifuentes

Electrophoresis 31 (2010) 1175–1183---**Proteomics**

-V. García-Cañas, C. Simó, C. León, E. Ibáñez, A. Cifuentes

Mass Spectrom. Rev. 30 (2011) 396– 416 –**Proteomics + Metabolomics**

Running Foodomics projects at our lab on bioactivity of new functional ingredients on:



GENERAL CONCLUSION

Foodomics is a suitable approach to solve new challenges in Food Science and Nutrition...

20th International Symposium on Electro- and Liquid-Phase Separation Techniques

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Thank you!

