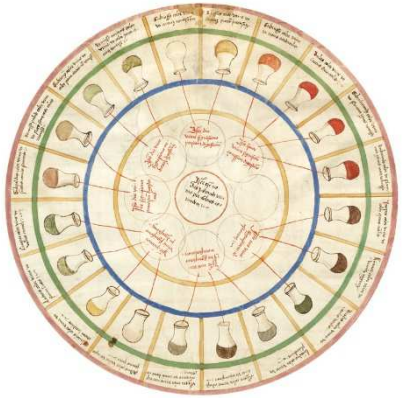
Analisi quantitativa universale di



matrici complesse

mediante risonanza magnetica

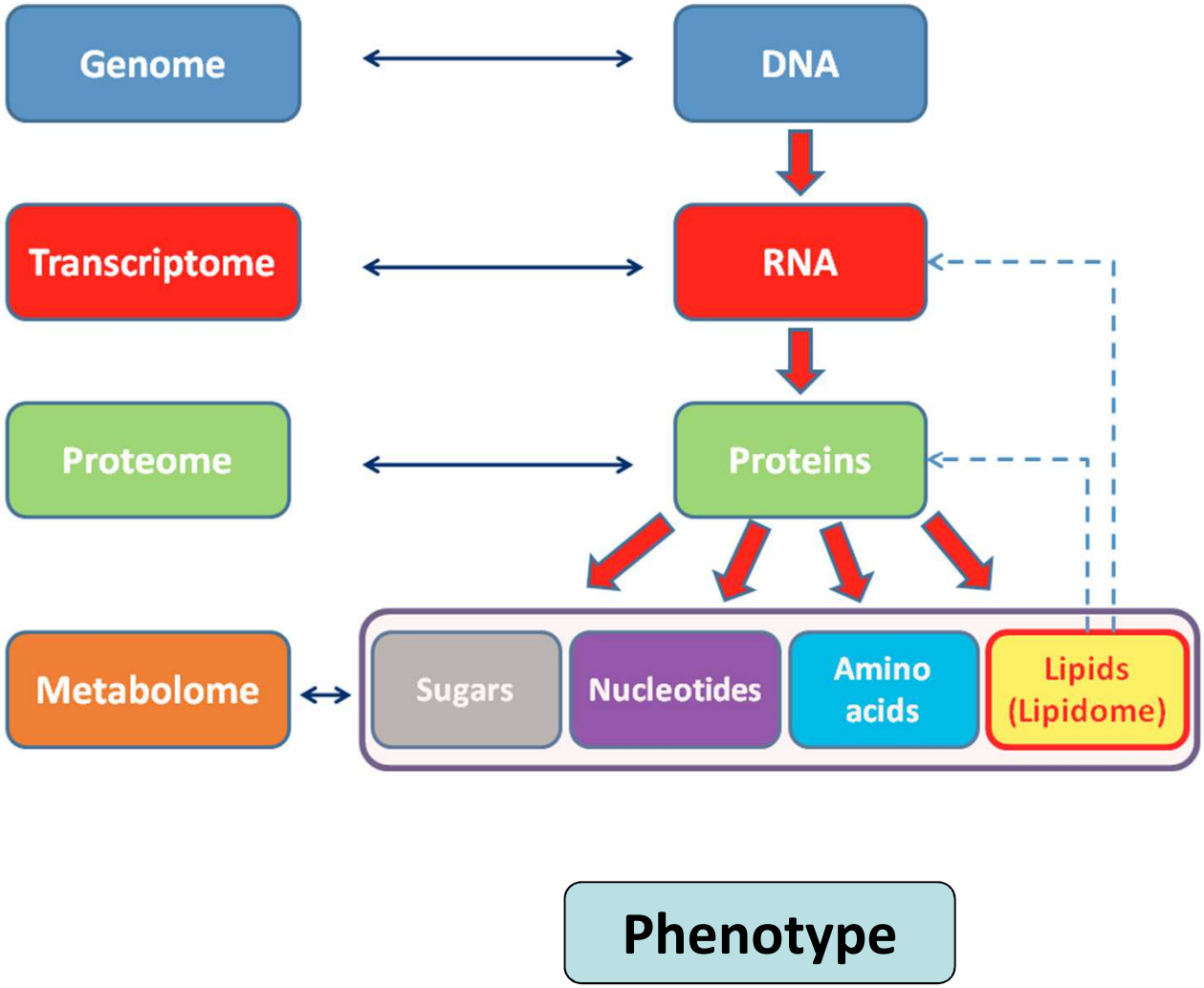
Metabolomics in terms of 'Systems Biology'

What can happen

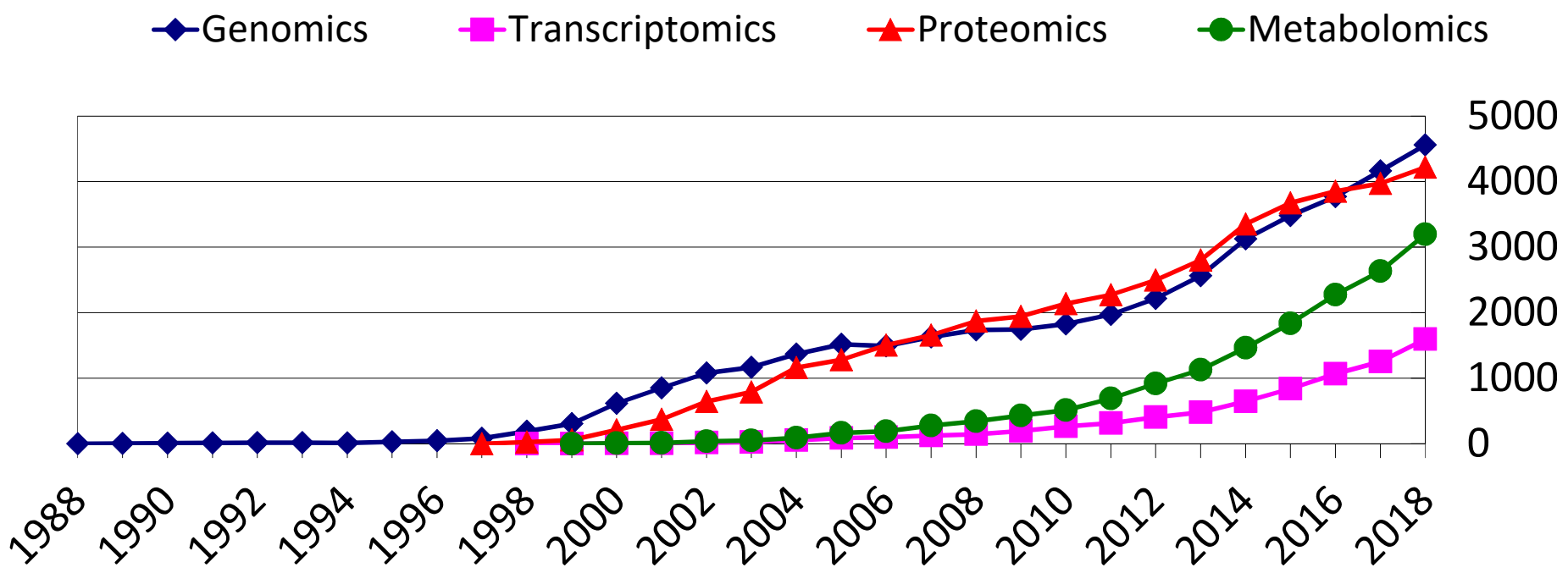
What appears to be happening

What makes it happen

What has happened and is happening

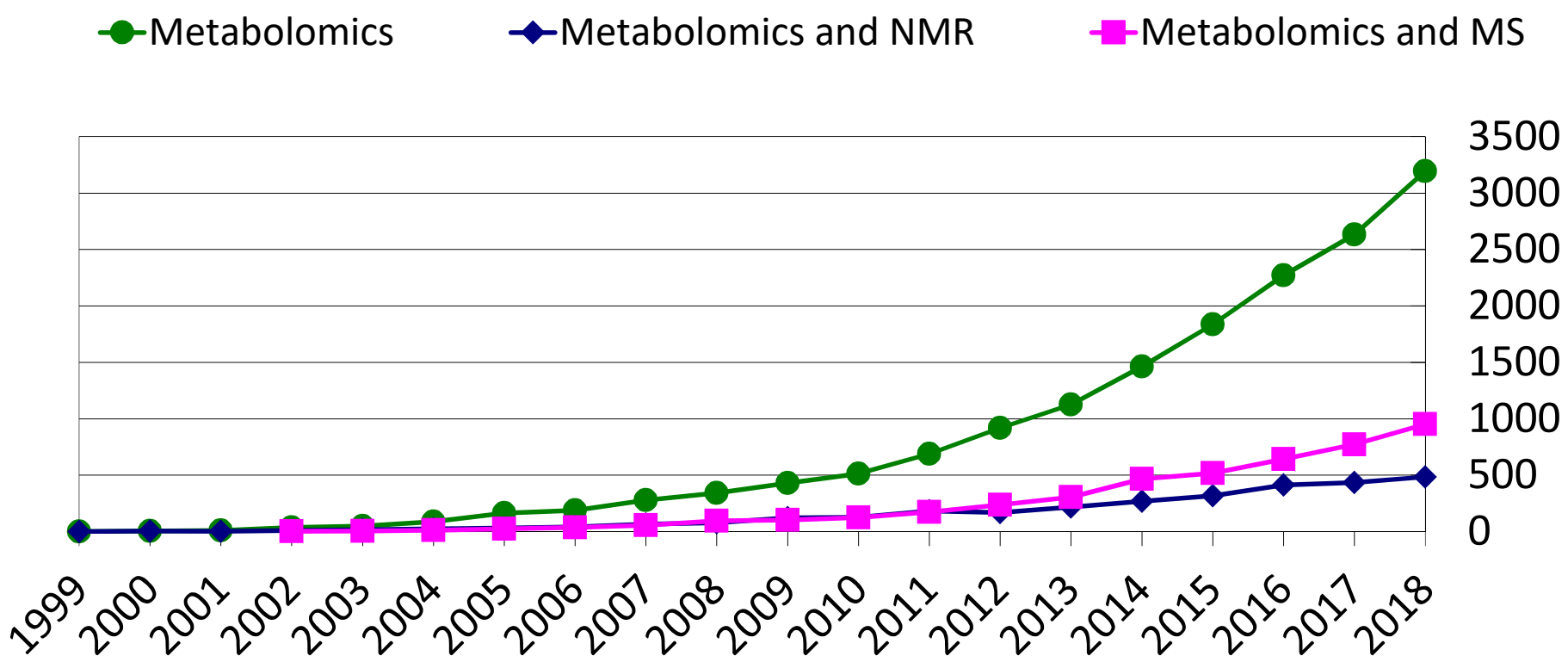


Metabolomics numbers since its inception



PubMed results for title/abstract searches

Metabolomics numbers since its inception

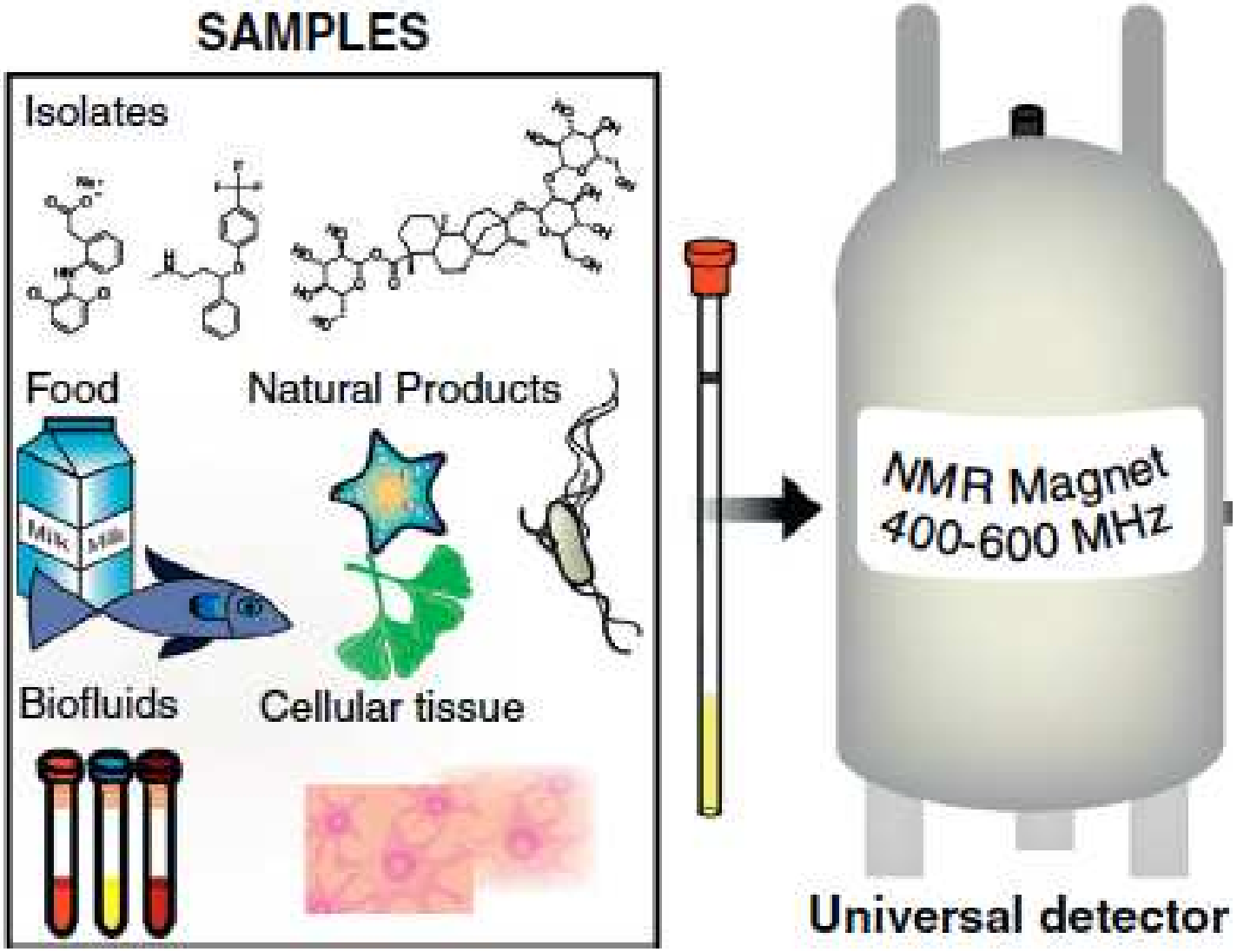


PubMed results for title/abstract searches

Universal quantitative NMR analysis of complex natural samples

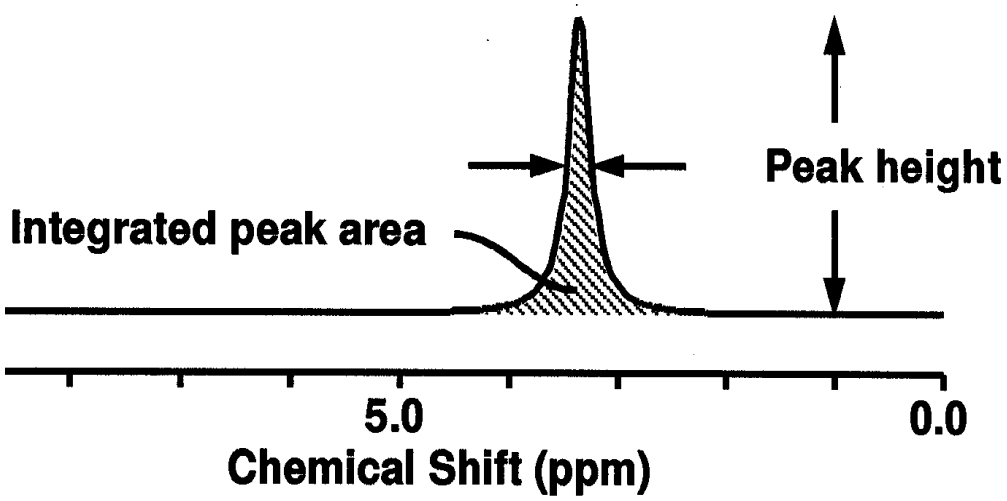
Drugs, NPS,
Oils, Fuels,
Explosives,
…

Plasma,
Urine,
Saliva,
CSF,
…



Current Opinion in Biotechnology 2014, **25**:51–59

L'NMR fornisce informazioni qualitative e quantitative



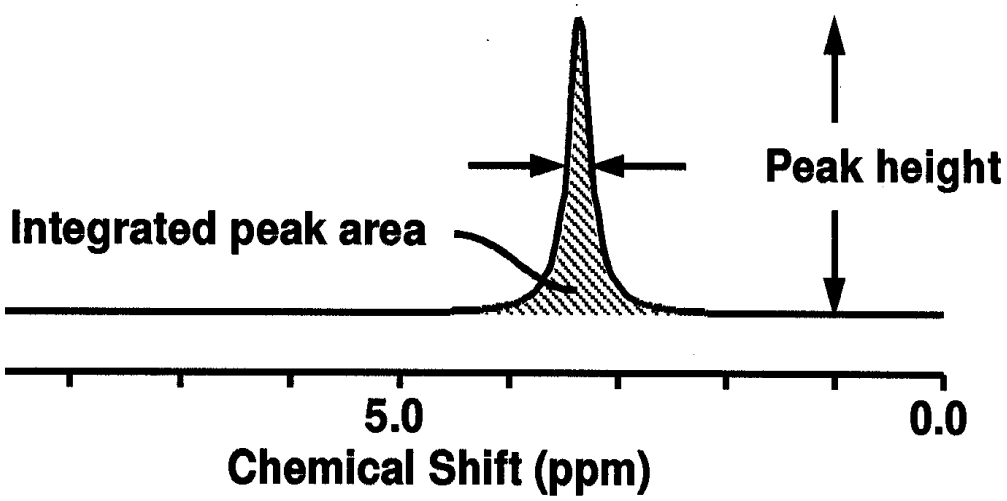
qNMR

L'intensità del segnale è direttamente proporzionale al numero dei nuclei che danno origine a quella specifica risonanza

Parametri di acquisizione da definire in qHNMR:

- Standard di riferimento (interno/esterno)
- Nucleo di osservazione (normalmente ^{1}H)
- Numero di scansioni (S/N > 250 per un'integrazione corretta)
- Tempo di acquisizione (3-5 volte T_2)
- Tempo di riciclo (5 volte T_1)
- Guadagno del ricevitore ottimale

L'NMR fornisce informazioni qualitative e quantitative



qNMR

L'intensità del segnale è direttamente proporzionale al numero dei nuclei che danno origine a quella specifica risonanza

Parametri di processamento da definire in qHNMR:

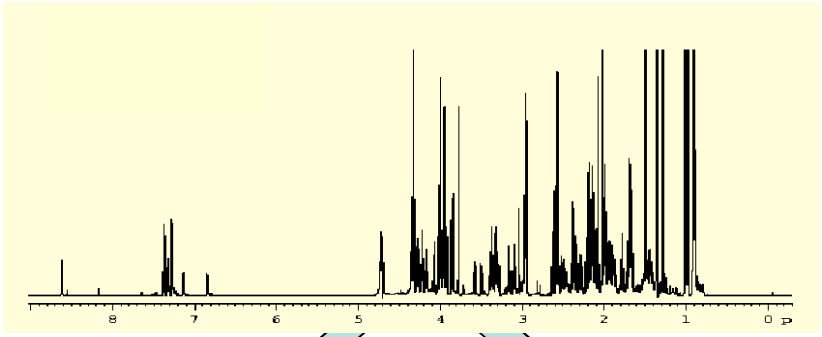
- Zero-filling
- Apodizzazione
- Correzione della fase
- Correzione della linea di base
- Definizione della regione di integrazione

Comparison of NMR vs MS for Metabolomics

Analytical Considerations	NMR	MS
Sensitivity		★★
Reproducibility – within lab	★	
Reproducibility – across labs	★★	
Quantitation	★★	
Sample Prep Requirements	★	
Sample Analysis Automation	★	
Versatility	★	

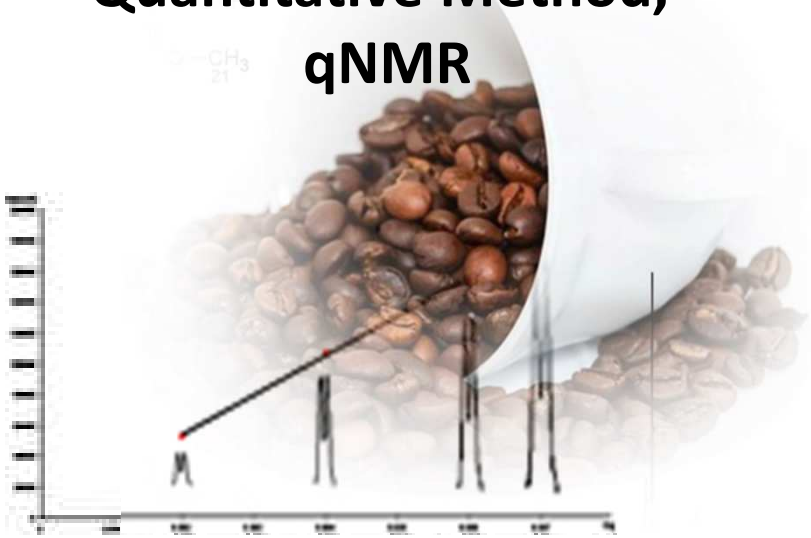
*Taken from D.G. Robertson, Toxicological Sciences, **85**, 809, 2005*

Two Routes to Metabolomics



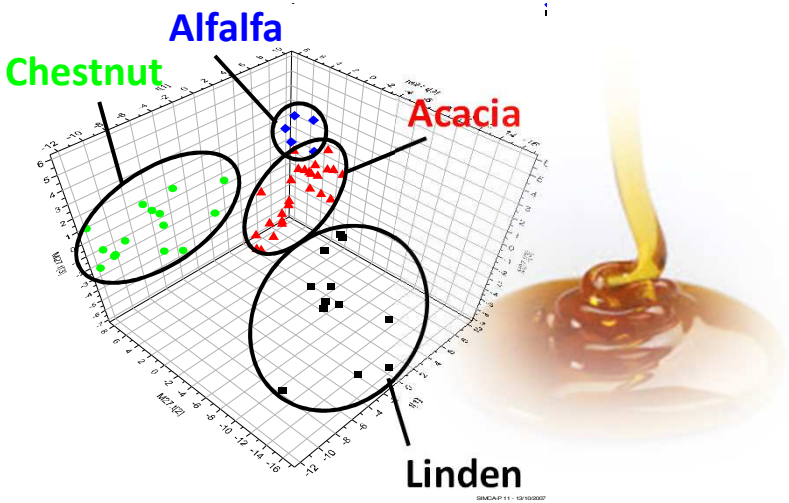
Targeted

Quantitative Method, qNMR

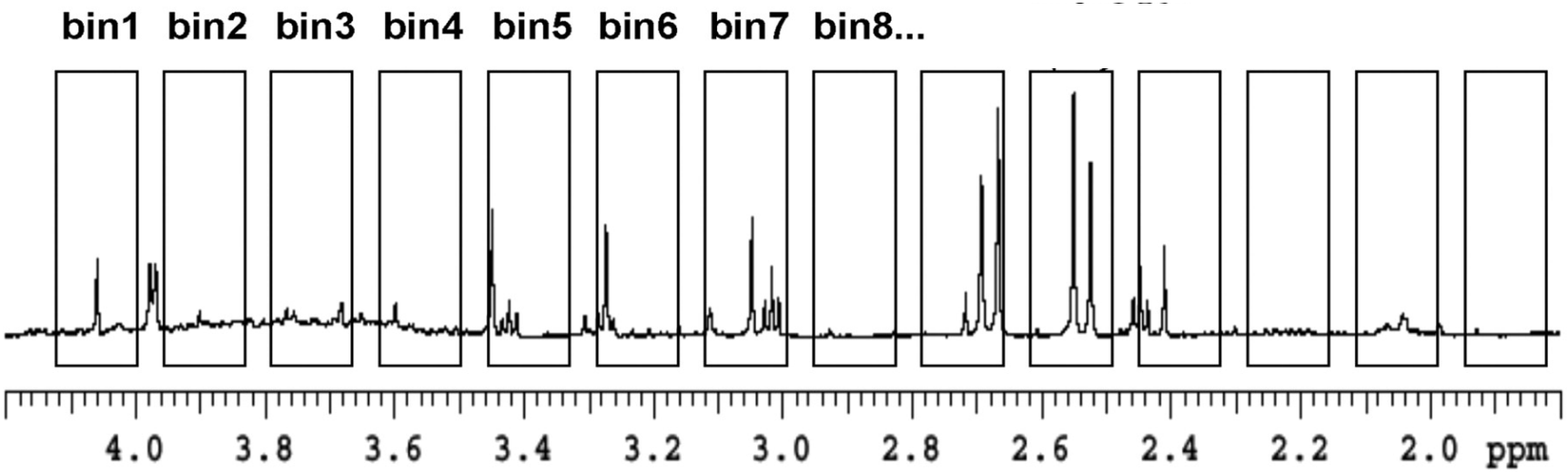


Untargeted

Chemometric Method



Spectral integration and construction of the data matrix



variables

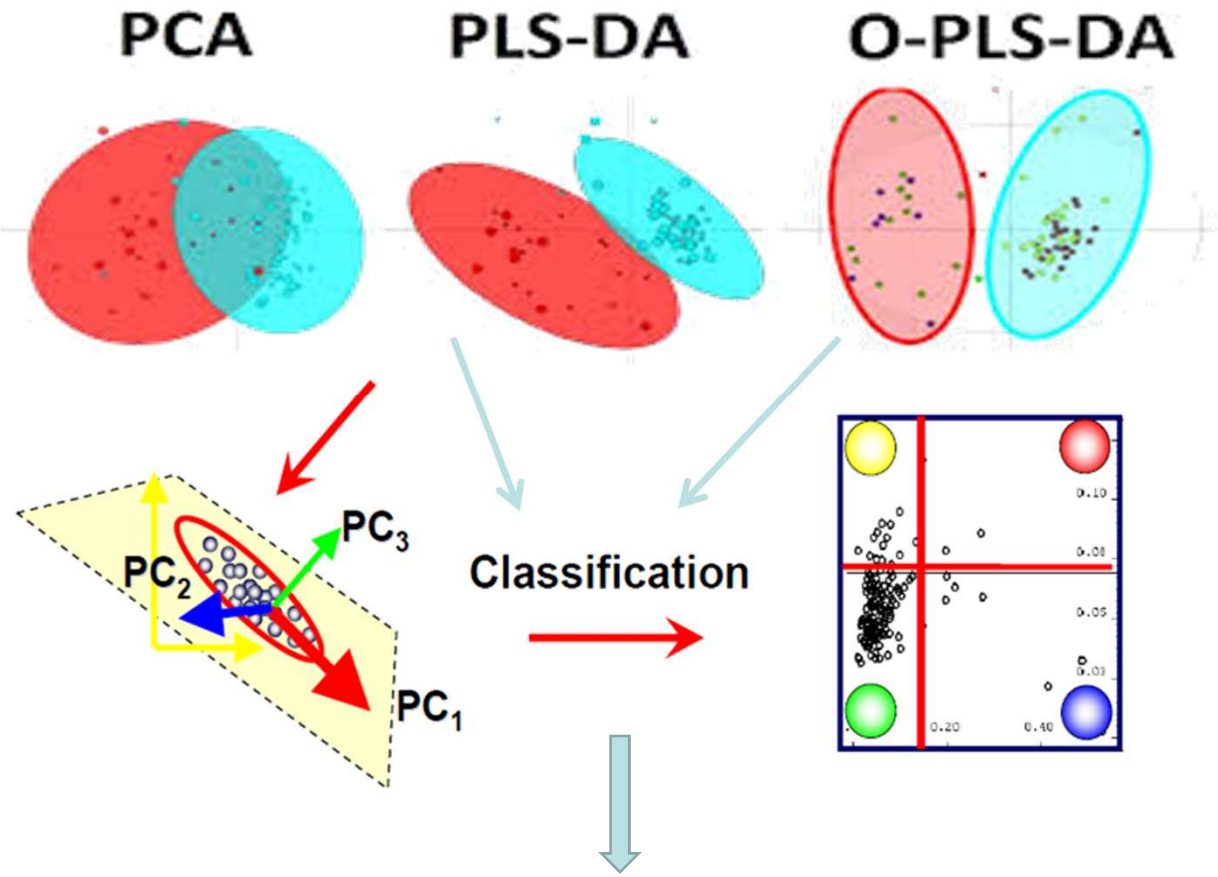
bin1 bin2 bin3 bin4 bin5 bin… bin250 bin…

samples

Sample 1
Sample 2
Sample 3
Sample 4
Sample 5
Sample ….
Sample 520
Sample …

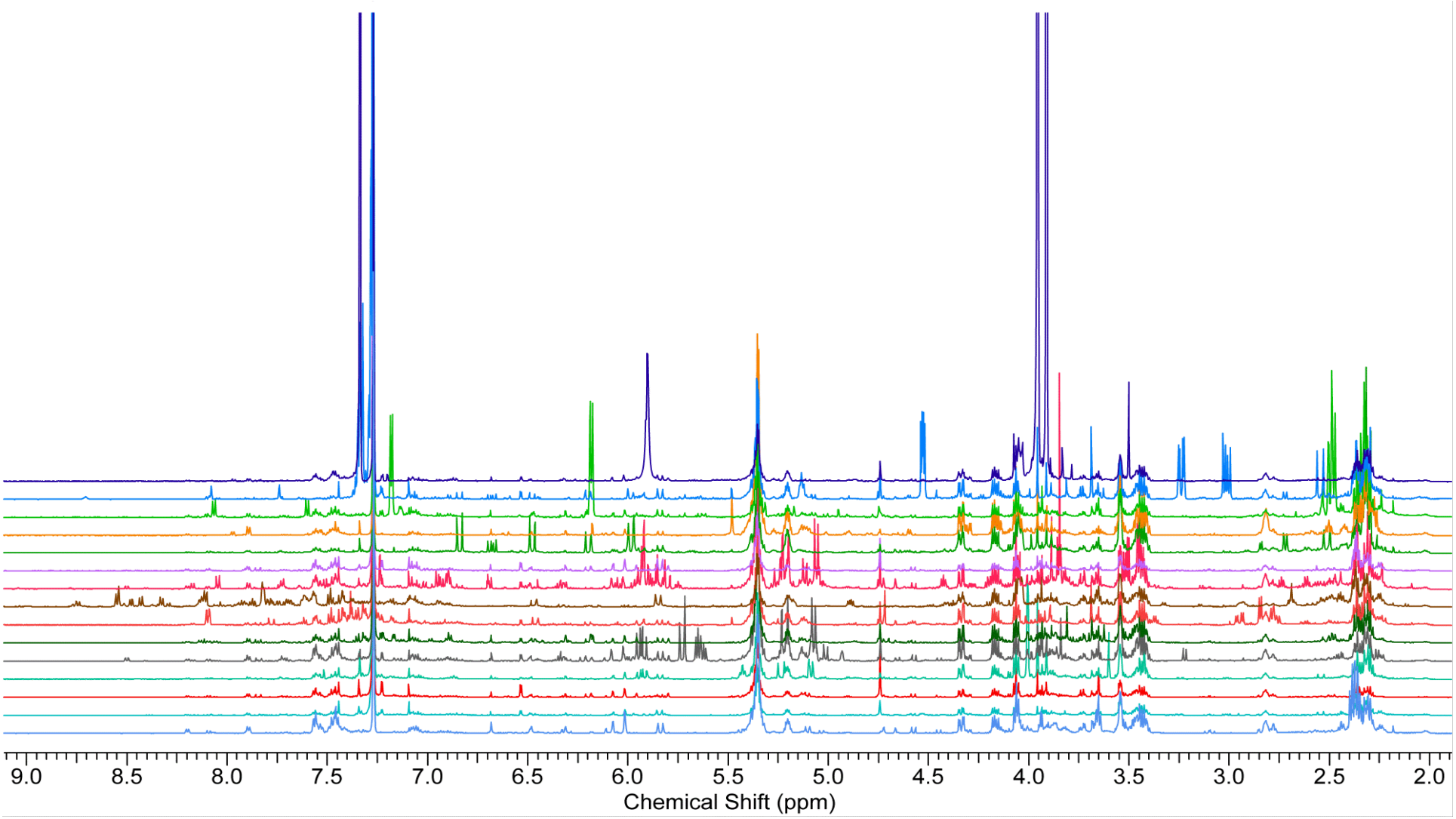
Discriminant Analysis (PLS-DA, O-PLS-DA)

”Supervised” Methods of Classification

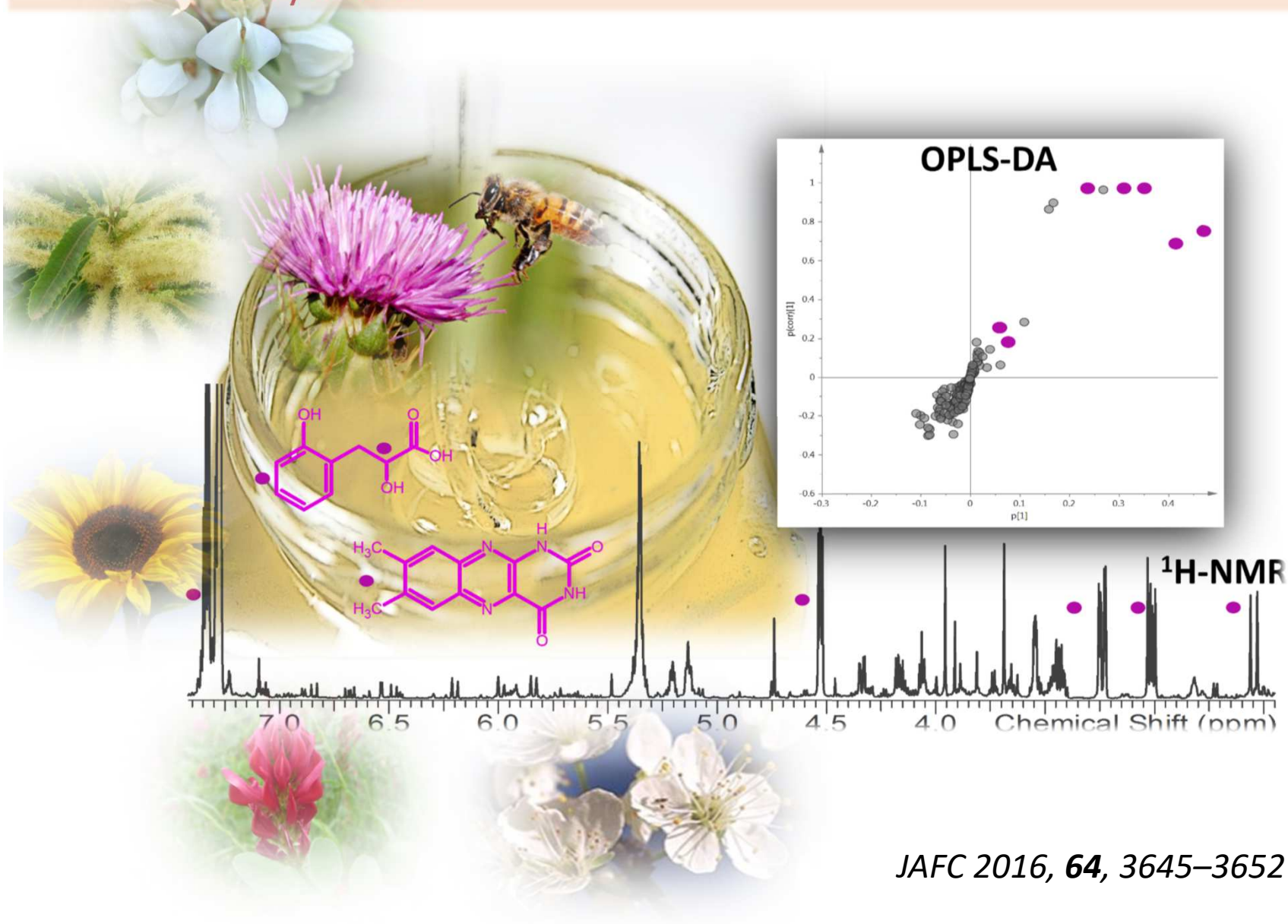


Models are generated that predict the class to which unknown samples belong

NMR Spectra of Monofloral Honeys



Objective Definition of Monofloral and Polyfloral Honeys Based on NMR Metabolomic Profiling

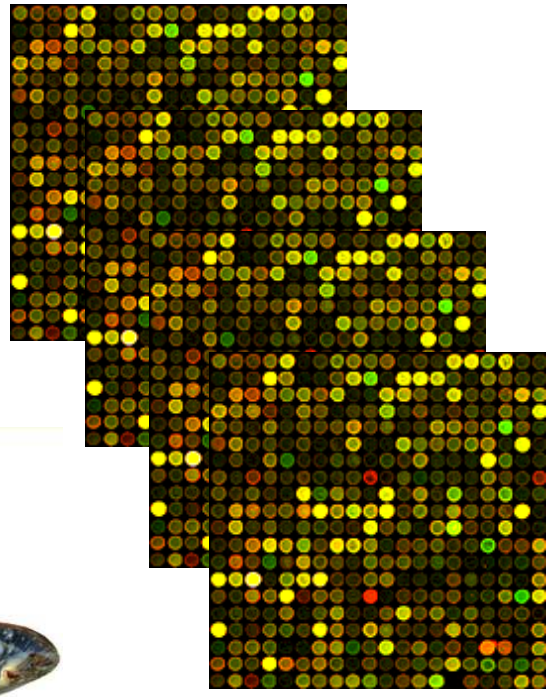


*JAFC 2016, **64**, 3645–3652 (2016)*

UNIVERSITÀ DEGLI STUDI DI PADOVA

LM in Biotecnologie Industriali
Percorso «ambientale»

MONITORAGGIO AMBIENTALE E ALIMENTARE

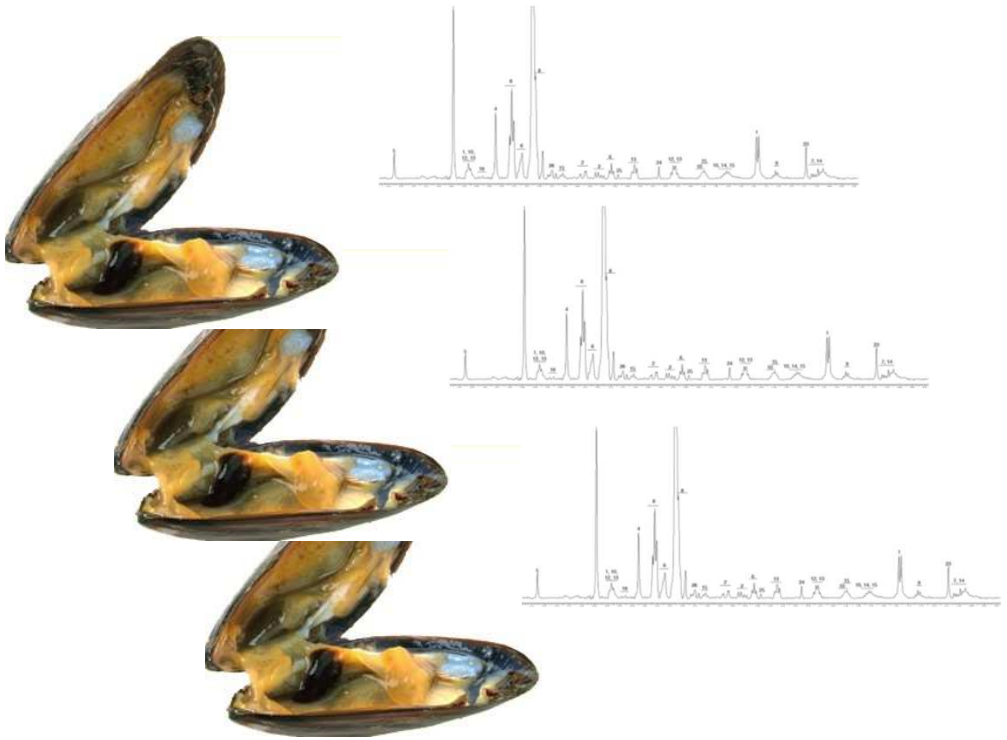


Valutazione dell'espressione genica per il controllo degli *stock* alimentari e dell'inquinamento delle acque.

MONITORAGGIO AMBIENTALE E ALIMENTARE

- Laguna di Venezia vs. Sacca di Scardovari
- Ghiaccio vs. acqua fredda salata

- Tessuto intero
- Branchie
- Ghiandola digestiva
- Plasma



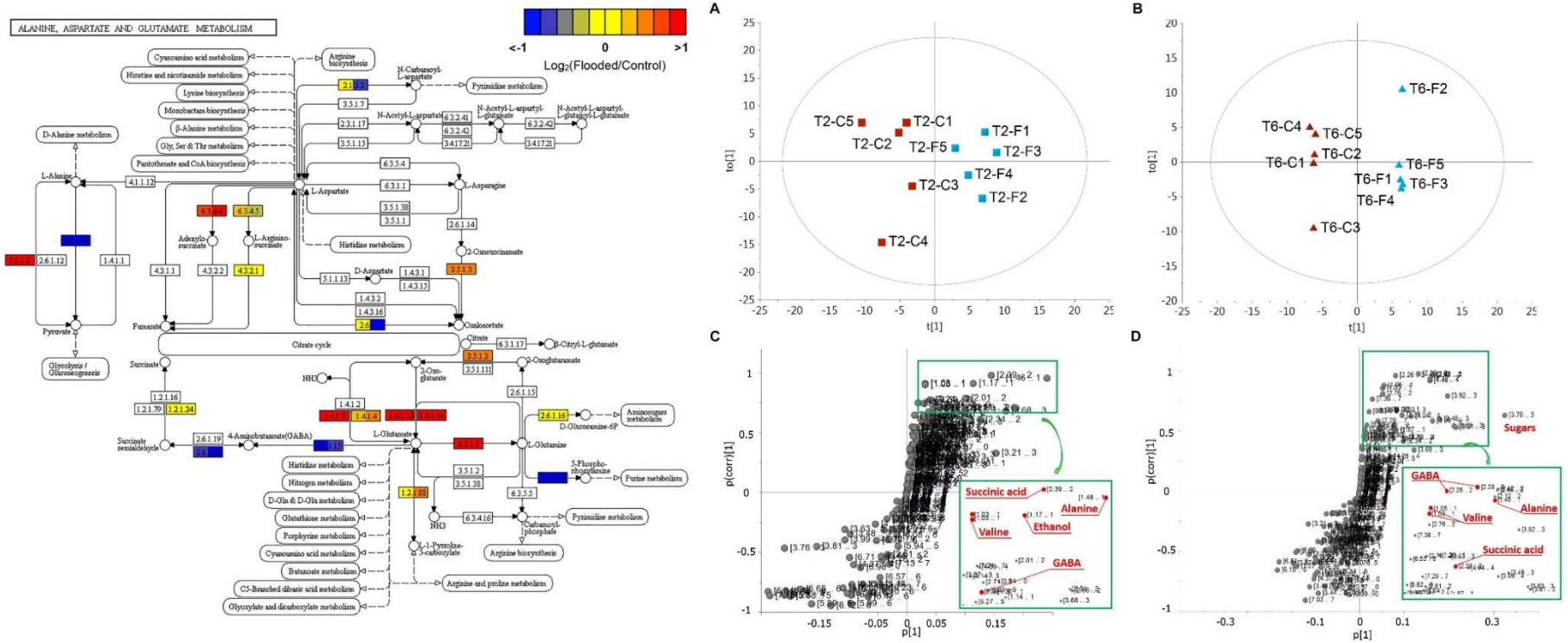
Valutazione del metaboloma e del lipidoma di diversi tessuti per il controllo della provenienza e della freschezza.

frontiers in Plant Science

Flooding Responses on Grapevine: A Physiological, Transcriptional, and Metabolic Perspective

ORIGINAL RESEARCH
published: 26 March 2019
doi: 10.3389/fpls.2019.00339

*Benedetto Ruperti[1,2,3], Alessandro Botton[1,2,3], Francesca Populin[1], Giulia Eccher[1], Matteo Brilli[4], Silvia Quaggiotti[1,3], Sara Trevisan[1], Nadia Cainelli[1], Paola Guarracino[5], Elisabetta Schievano[5] and Franco Meggio[1,2]**



NEONATAL SEPSIS

Early Human Development 90S1 (2014) S78–S83

Contents lists available at ScienceDirect

Early Human Development

journal homepage: www.elsevier.com/locate/earlhumdev

Urinary ^{1}H-NMR and GC-MS metabolomics predicts early and late onset neonatal sepsis

9 septic newborns (EOS + LOS)
vs 16 controls

urine at birth and at regular intervals

significant differences in metabolome of sepsis group and controls

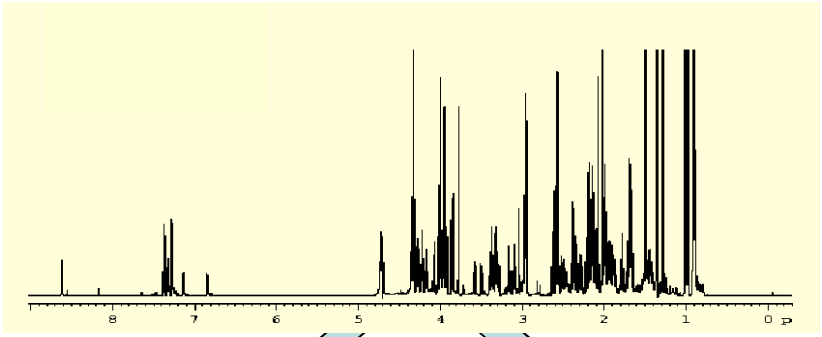
(urine collected at birth in EOS, within 72 h prior the onset of LOS)

Fanos, 2014

Neonatal sepsis – Future Directions

- Metabolomic targeted in MS/MS (plasma) and untarged NMR (urine) analysis in Early onset Sepsis
- If with NMR it is possible to predict EOS and which pathways are involved.
- To improve the prediction of EOS by Combining MS and NMR data.
- Integrate the NMR and MS data to evaluate the pathways that are involved.
- Early metabolomic marker of prognosis

Two Routes to Metabolomics



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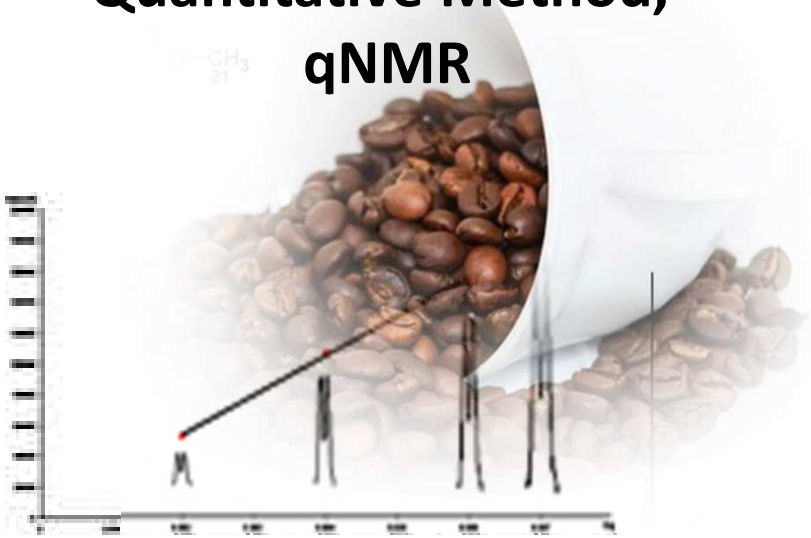
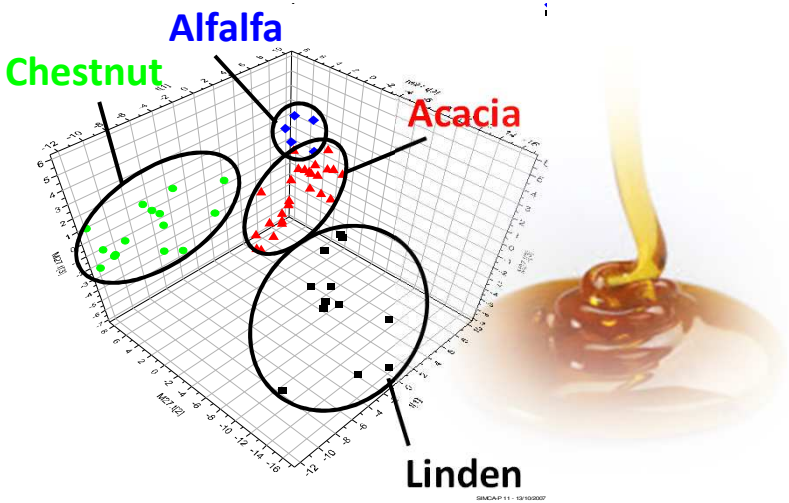
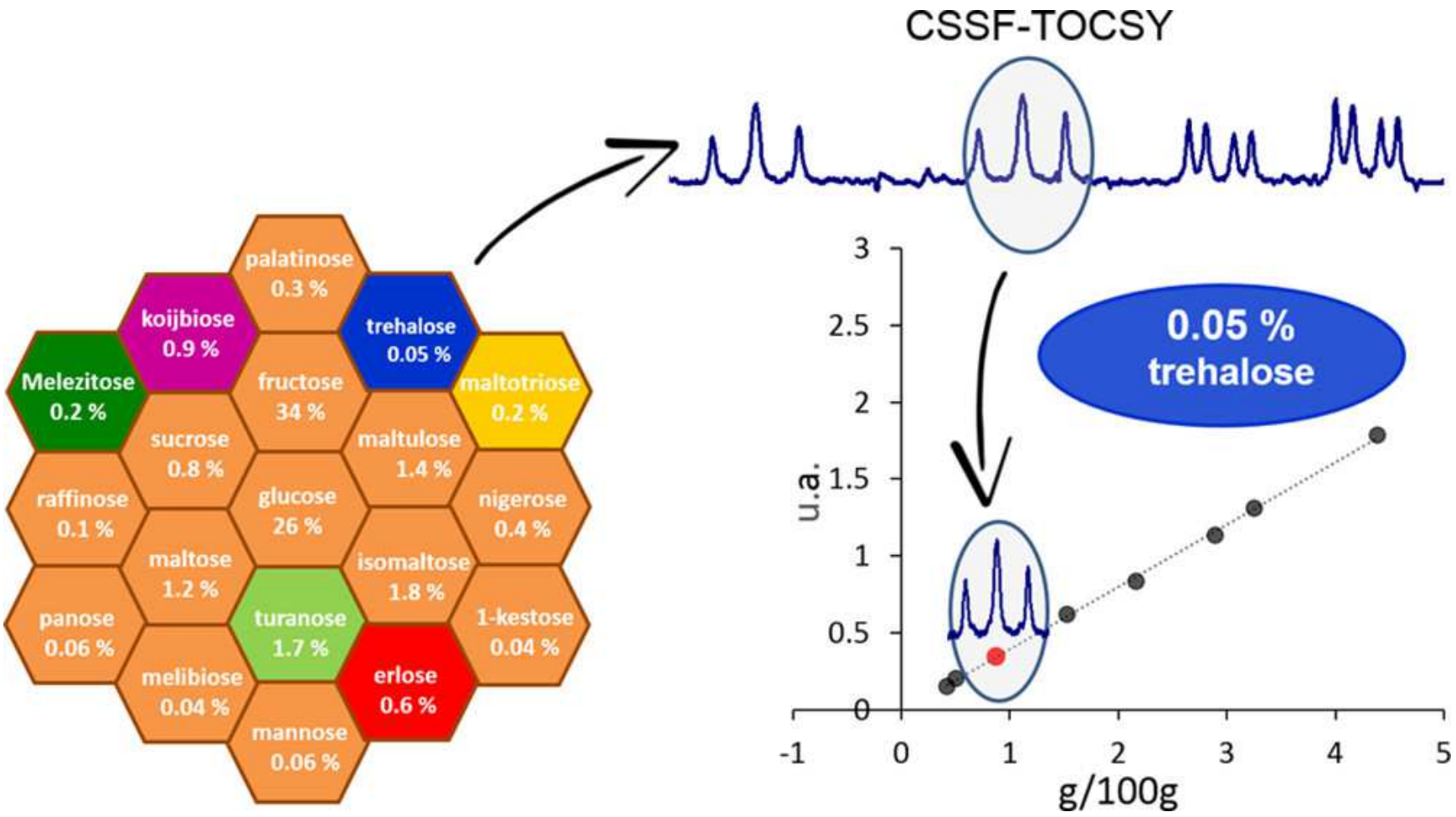


Untargeted

Chemometric Method



NMR Quantification of Carbohydrates in Complex Mixtures. A Challenge on Honey



Published in: Elisabetta Schievano; Marco Tonoli; Federico Rastrelli; *Anal. Chem.* **2017,** 89, 13405-13414.
DOI: 10.1021/acs.analchem.7b03656

NMR Quantification of Carbohydrates in Complex Mixtures. A Challenge on Honey

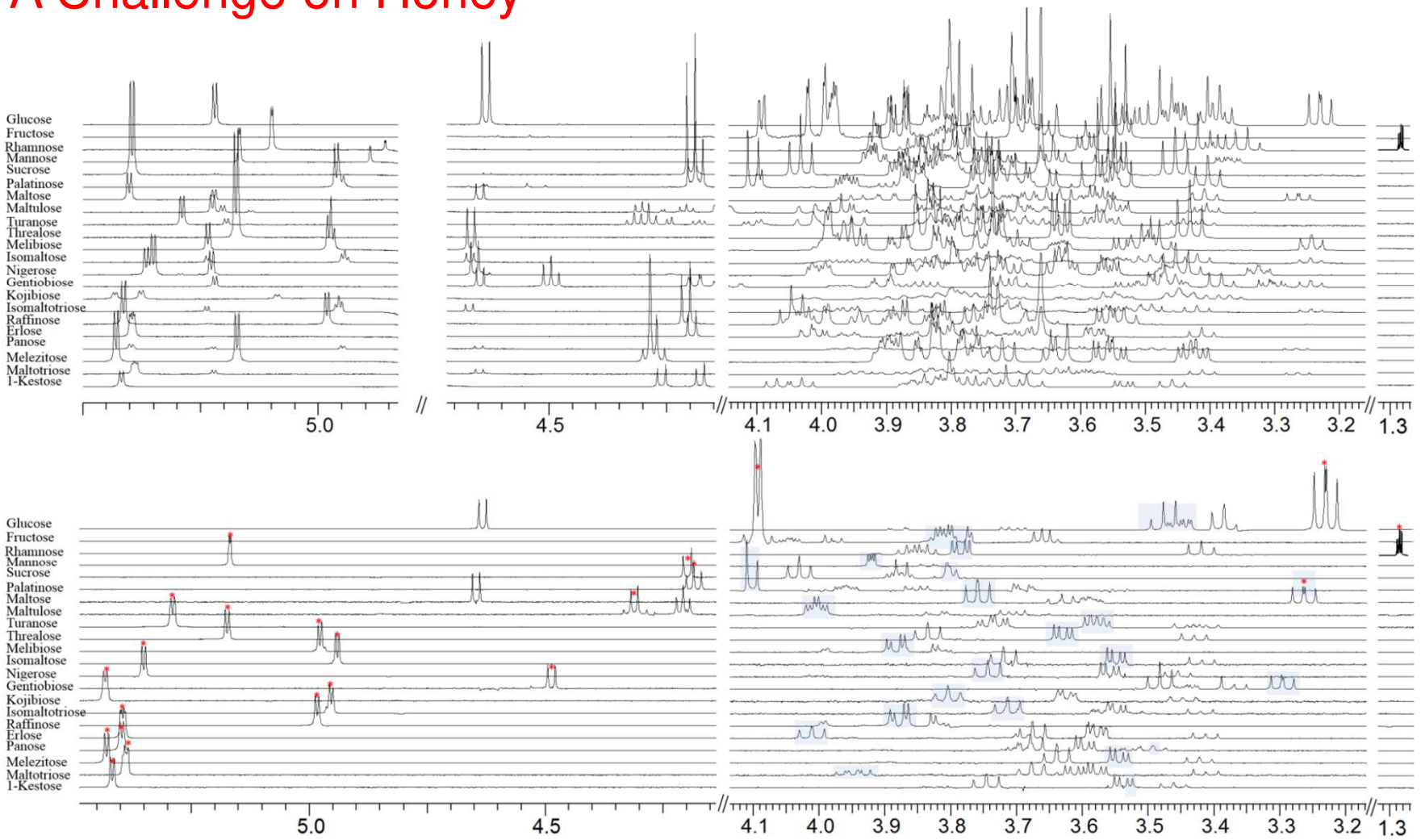
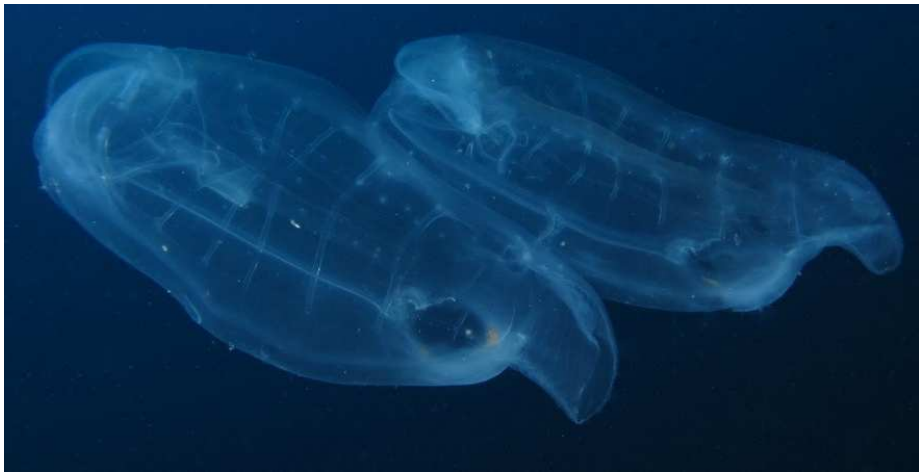


Figure S-4. Panel A: 1D conventional spectra of the 22 sugars under investigation. Panel B: CSSF-TOCSY of the 22 sugars. Red marks indicate the chosen excitation frequency of each sugar, while the rectangles indicate the integration regions.

Estrazione e valorizzazione della cellulosa da Tunicata

Prof. Lucia Manni
Prof. Elisabetta Schievano
Prof. Tommaso Carofiglio



Fondazione
ISTITUTO DI RICERCA
PEDIATRICA

European Research Council

Elisa Cimetta BIAMET - NBTECH laboratories

Master Thesis student position and PhD scholarship available

A Master thesis student position and PhD scholarship are available in the laboratory of Prof. Elisa Cimetta to define how hypoxia influences physicochemical properties of **exosomes** produced by paediatric cancer **Neuroblastoma** (NB).
The research is funded by a Starting Grant from the European Research Council (ERC StG 2017).

Current research in the lab is focused on the development of microfluidic platforms to test the effects of NB-derived exosomes on target cells cultures and to elucidate the molecular mechanisms/signaling through which the microenvironment shapes Neuroblastoma aggressiveness and progression.

The laboratories are located at the Department of Industrial Engineering (DII), University of Padua and at the Fondazione Istituto di Ricerca Pediatrica Citta' della Speranza (IRP). The proposed activities will be developed at the **IRP**.

Students will be trained in advanced molecular, biochemical and cell biology techniques, and will work in a diverse team with engineers, biologists and biotechnologists.

Informal enquiries to **elisa.cimetta@unipd.it**

Elisa Cimetta
Phone: 0498275817