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C-PASS
Conference on Photonics
for Advanced Spectroscopy and Sensing

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Challenges and Opportunities from **Food Volatilomics:** **Sensing the Quality**

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Challenges

Nature's complexity and food-omics: domains and investigations strategies

Opportunities

High resolution analysis of volatiles -> *volatilomics*

Artificial Intelligence algorithms and concepts to go beyond current Quality indexes



Delineating Quality traits of premium hazelnuts for confectionery by *omics*

- ✓ **Rancidity indexing:** by patterns of marker volatiles
- ✓ **Aroma blueprinting:** by AI *smelling*
- ✓ **Spoilage diagnosis:** by Augmented visualization and Computer Vision

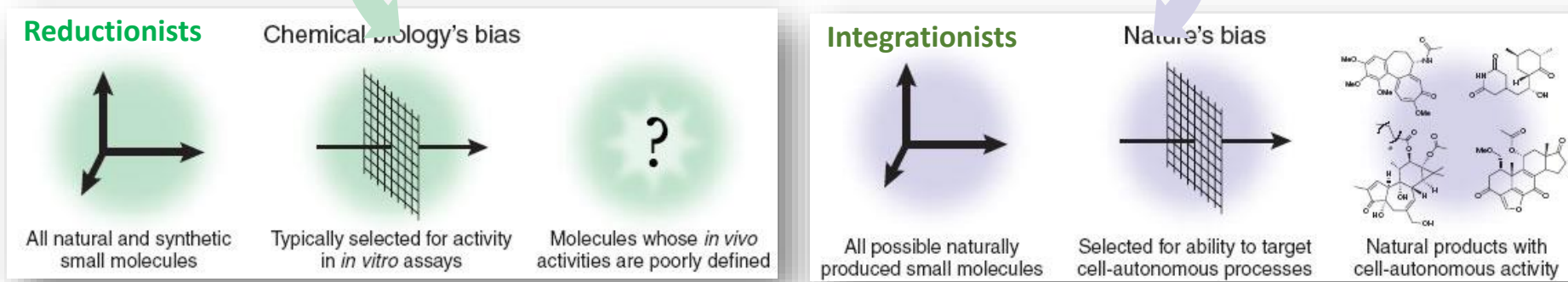
Combine challenges in a single step analytical process

Sensing Quality -> challenges and opportunities for Quality Control laboratories and at-line/on-line Quality monitoring

[1] Cuadros-Rodríguez, L.; Ruiz-Samblás, C.; Valverde-Som, L.; Pérez-Castaño, E.; González-Casado, A. Anal. Chim. Acta 2016, 909, 9–23.

[2] Dunkel, A.; Steinhaus, M.; Kotthoff, M.; Nowak, B.; Krautwurst, D.; Schieberle, P.; Hofmann, T. Angew. Chemie - Int. Ed. 53 (28) (2014) 7124–7143.

Decoding complex phenomena
Nature's complexity



Adapted from: Randall T. Peterson Commentary on Nature Chemical Biology 4, 635 (2008)

“...*Chemical biology and systems biology* have grown and evolved in parallel during the past decade, but the *mindsets of the two disciplines remain quite different*. As the inevitable intersections between the disciplines become more frequent, chemical biology has an opportunity to assimilate the most powerful ideas from systems biology.

Challenge

Can the *integrationist* mindset of systems biology liberate chemical biology from its *compulsion to reduce everything to individual small molecule-target interactions*?

Randall T. Peterson Commentary on Nature Chemical Biology 4, 635 (2008)

...the boundaries between chemistry and biology are vanishing...

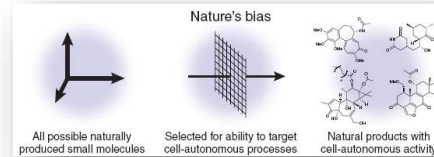
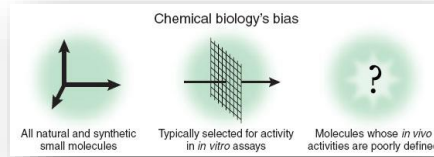
Prof. Thomas Hofmann

J. Agric. Food Chem. 2015, 63, 32, 7095–7096

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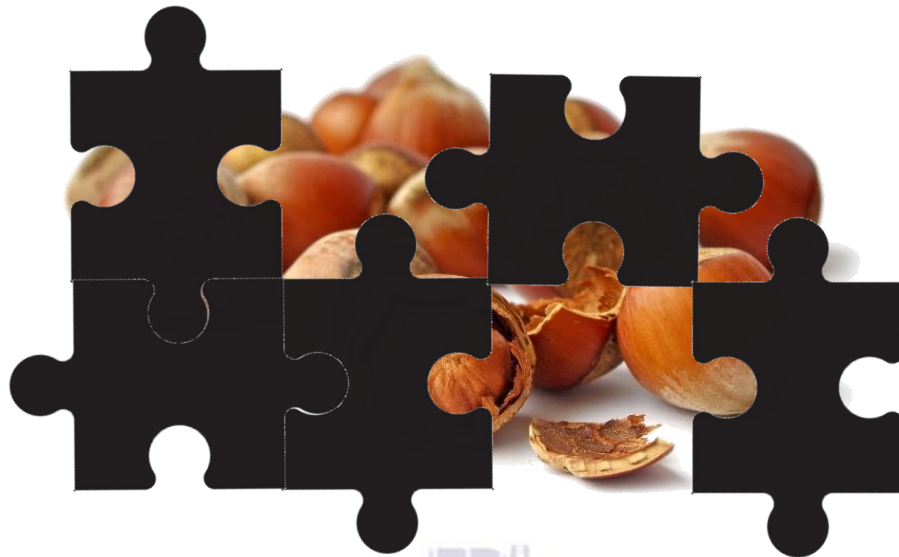
J. Agric. Food Chem. 2015, 63, 32, 7095–7096



Challenge

Reductionist approach
single target-molecule interaction

Integrationist approach
exploit the full information potential



Pre-targeted approaches
Investigation of known chemicals

Untargeted approaches
Investigation un-biased by knowledge

...the boundaries between chemistry
and biology are vanishing...

Prof. Thomas Hofmann

J. Agric. Food Chem. 2015, 63, 32, 7095–7096

Challenges & Opportunities

Food metabolomics

Chemical composition of food vs.

- ✓ crop botanical origin
- ✓ harvesting area
- ✓ climate impact
- ✓ post-harvest
- ✓ storage conditions



Nutrimetabolomics

Human metabolome by

- ✓ dietary patterns
- ✓ specific foods
- ✓ nutrients
- ✓ micro-organisms
- ✓ bioactives



Sensomics

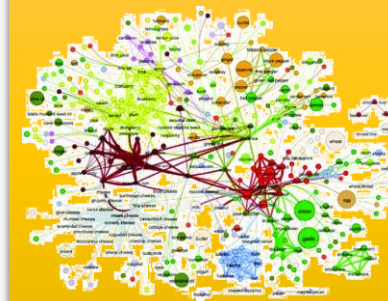
Food hedonic profile

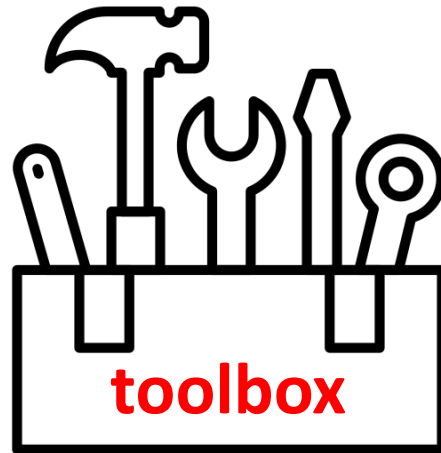
- ✓ potent odorants
- ✓ chemical odor code
- ✓ volatiles patterns
- ✓ odor activity value
- ✓ olfactometry



Food volatilomics

- ✓ spoilage
- ✓ sensory profile
- ✓ botanical tracers
- ✓ technological indicators
- ✓ authenticity





Food Volatilome -> encrypts information about Quality

The volatilome “contains all of the volatile metabolites and other volatile organic and inorganic compounds that originate from an organism” super-organism, or ecosystem¹. Volatiles are part of the sample’s metabolome

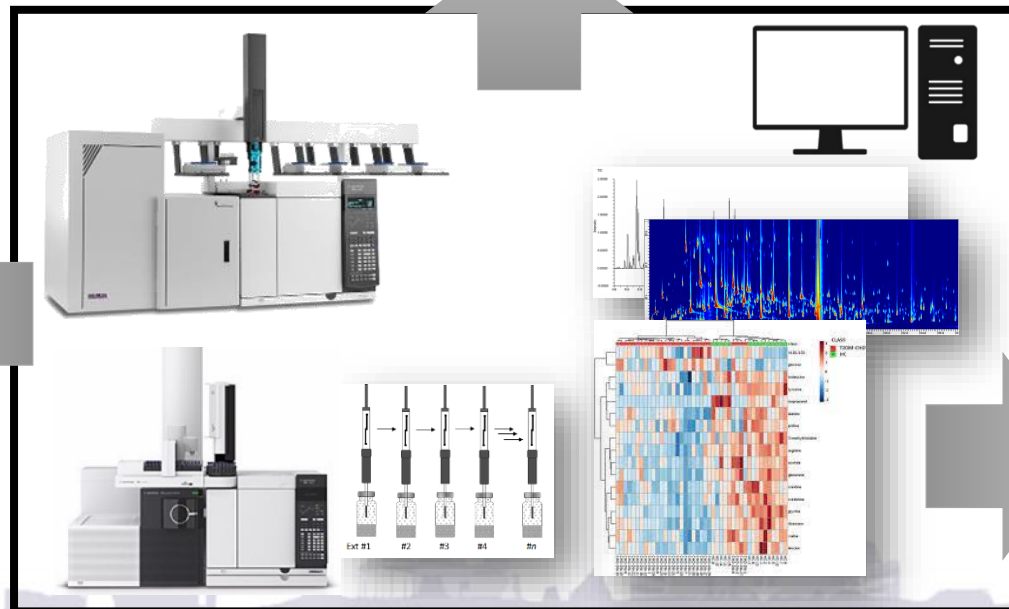
Hardware and configurations

- ✓ Analytes characteristics
- ✓ High resolution separation, identification, tracking and annotation
- ✓ Method sensitivity, quantitation accuracy, transferability
- ✓ *Ex-post* data interpretation

Sample preparation

- ✓ Targeted
- ✓ Untargeted
- ✓ Automation
- ✓ Green Analysis

Standard protocols



Data processing & AI

Comprehensive

Untargeted and targeted

Fingerprinting and profiling

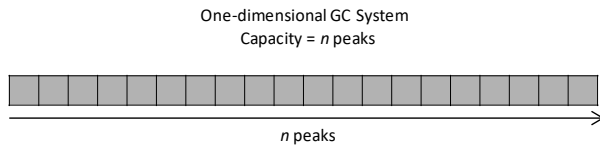
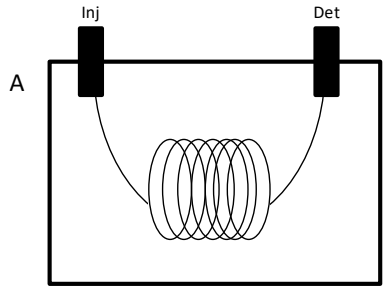
... **Step ahead**

AI smelling as decision makers

Computer Vision algorithms

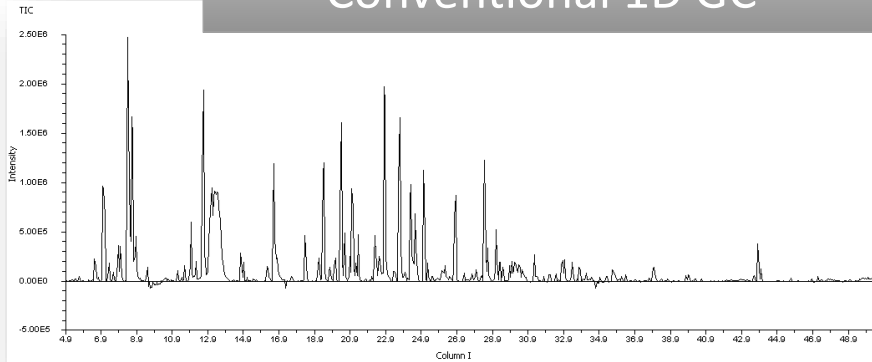


Comprehensive 2D GC

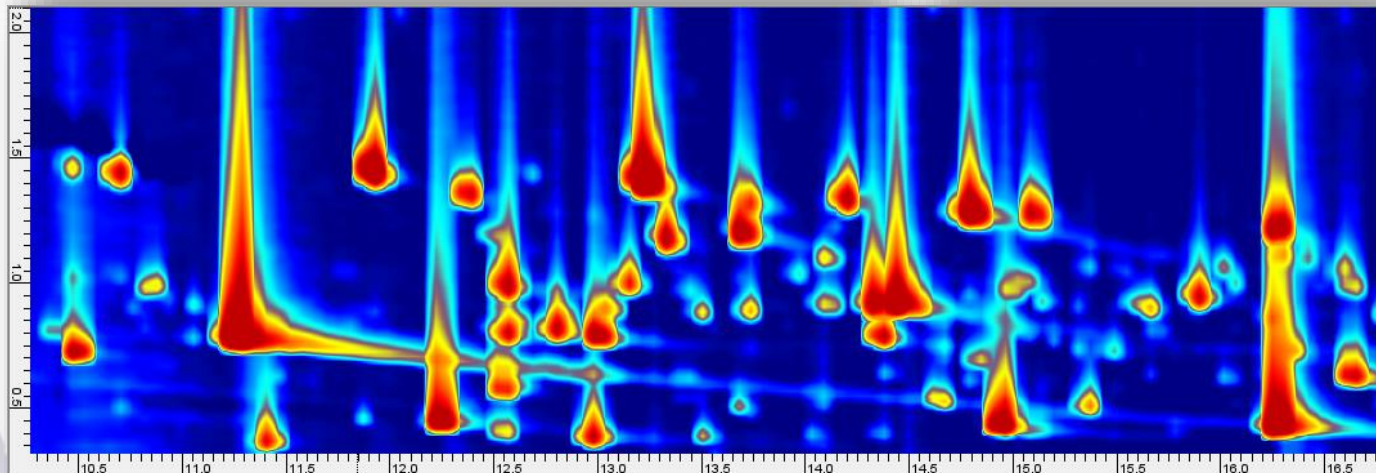
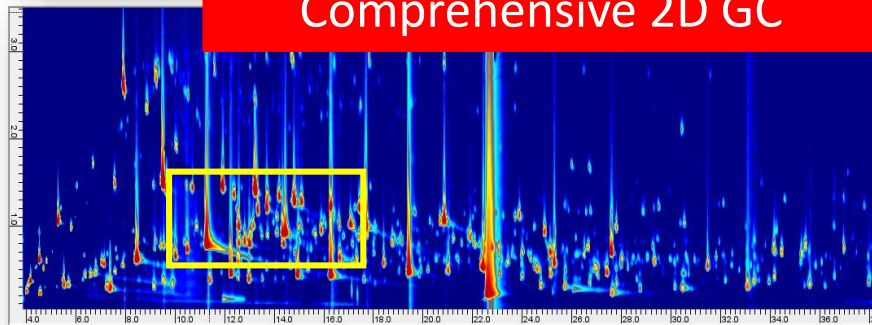


- ✓ **Separation power** and peak capacity are given by the product of the two chromatographic dimensions (GC×GC)¹
- ✓ **Selectivity** and **specificity** achieved by combining orthogonal discrimination principles in a single measure (physico-chemical discrimination)
- ✓ **Sensitivity** is maximized thanks to a band compression (in space - for thermal modulators) which produces signal-to-noise ratio enhancement
- ✓ **Quantification accuracy** is achieved in a large dynamic range of actual concentrations
- ✓ **Fingerprinting** is based on 3D/4D data arrays achieving higher accuracy and specificity

Conventional 1D GC



Comprehensive 2D GC



Opportunities

“High resolution” profiling
GC×GC separation power
accurate quantitative profiling

2D/3D Chromatographic fingerprinting¹
pattern recognition (forensics)
comprehensive sample comparison

Group-Type Analysis
Rational retention logic
Ordered elution patterns

Delimiting Quality traits of premium hazelnuts by *omics*

Challenges and opportunities to go beyond conventional Quality indexes

Raw ingredient for **confectionery** products
Turkey is the leading producer (about 75% of world production) **Italy follows** as second in the ranking

- ✓ **Industrial partner** world leader in the production of confectionery products based on hazelnuts
- ✓ Need for **objective evaluation** of **Quality**

Quality assessment at industrial level focuses on morphological aspects, presence of damaged kernels, perceivable sensory defects (mould, rancid, *cimiciato*, stale etc..)



Corylus avellana L.

Step-ahead in quality assessment
molecular resolution probes:

- ✓ identification¹ (origin, harvest area)
- ✓ qualification (oxidation status, shelf-life storage effectiveness, bacterial and mold grow)
- ✓ definition of aroma potential²

AI decision makers

- ✓ Fingerprinting
- ✓ *Computer Vision* in defected hazelnuts VOCs patterns
- ✓ *Smelling machine* - aroma blueprint

[1] Cuadros-Rodríguez, L.; Ruiz-Samblás, C.; Valverde-Som, L.; Pérez-Castaño, E.; González-Casado, A. *Anal. Chim. Acta* **2016**, *909*, 9–23.

[2] Cialliè Rosso, M.; Mazzucotelli, M.; Bicchi, C.; Charron, M.; Manini, F.; Menta, R.; Fontana, M.; Reichenbach, S. E.; Cordero, C. J. *Chromatogr. A* **2020**, *1614* (460739)

Delimiting Quality traits of premium hazelnuts by *omics*

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Corylus avellana L.

Since 2006
1,500 industrial samples

15,000 analyses

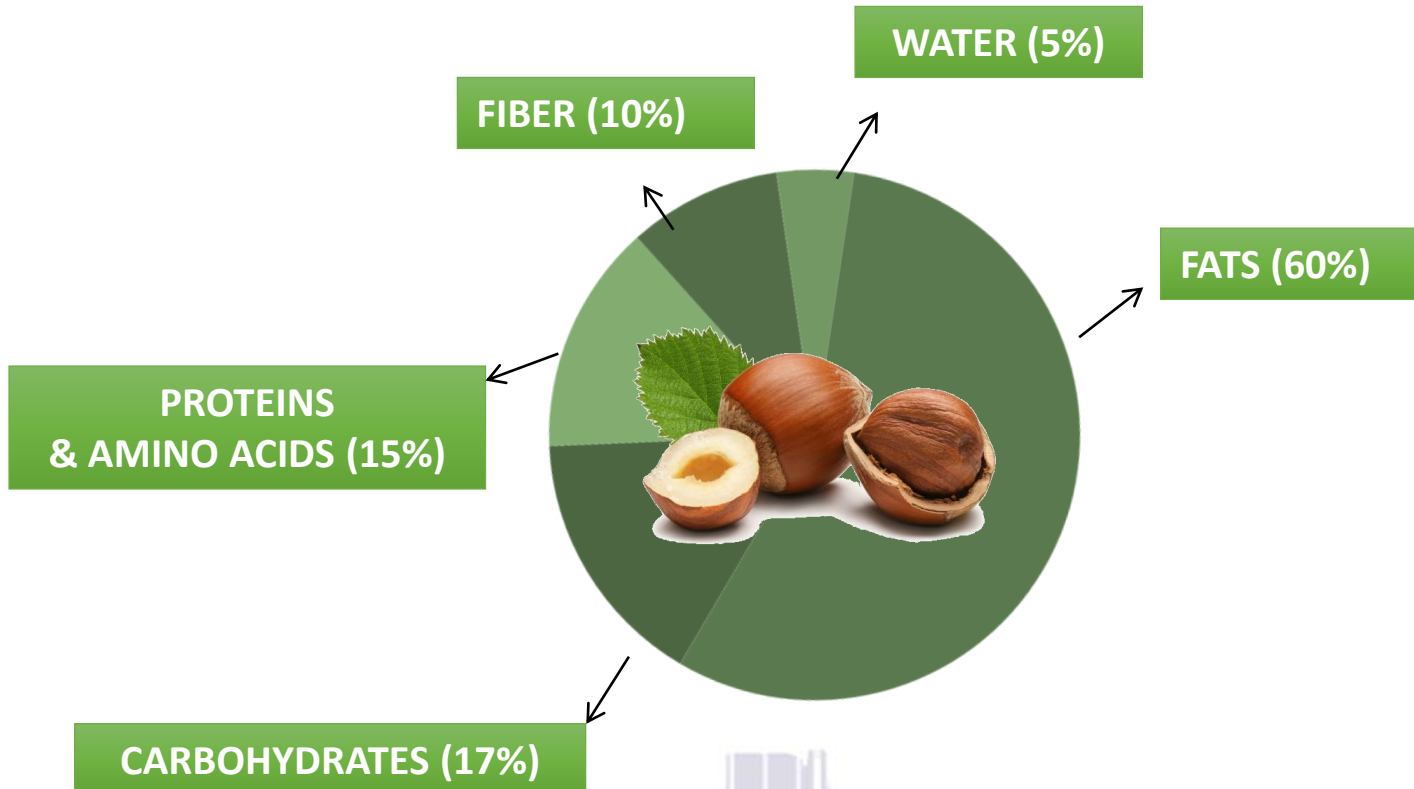
- ✓ 450 targeted analytes
- ✓ 70 robust markers
- ✓ 700 reliable chemical features
- ✓ **3,000 GB raw data**

botanical tracers
spoilage indicators
rancidity markers
aroma precursors
aroma compounds

antioxidants
primary metabolites



Challenges and opportunities to go beyond conventional Quality indexes



Hazelnuts volatilomics

Volatiles < 0.01%

- Hydrocarbons
- Terpenes
- Alcohols (linear and branched)
- Carbonyl derivatives
- Carboxylic acids
- Esters
- Lactones

Encrypts a lot of information

- geographical origin
- **phenotyping** and chemotyping
- multitrophic interactions (plants-insects)
- **presence of bacteria and moulds**
- **scent and odorous compounds**
- **distinctive aroma blueprint**

Challenges and opportunities to go beyond conventional Quality indexes

botanical tracers
spoilage indicators
rancidity markers
aroma precursors
aroma compounds

antioxidants
primary metabolites



Crop/Harvest post-harvest

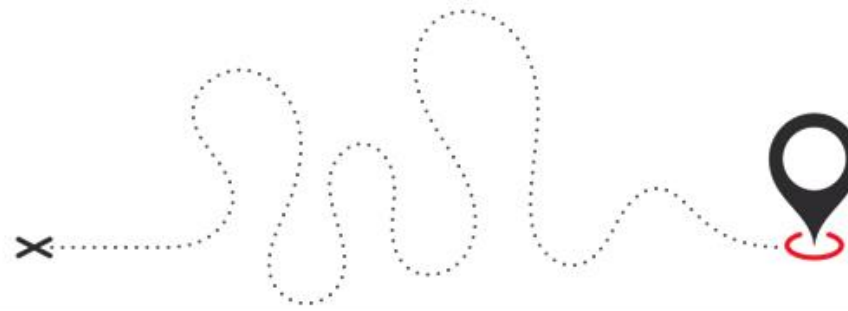


warehousing

logistics

controlled storage

processing



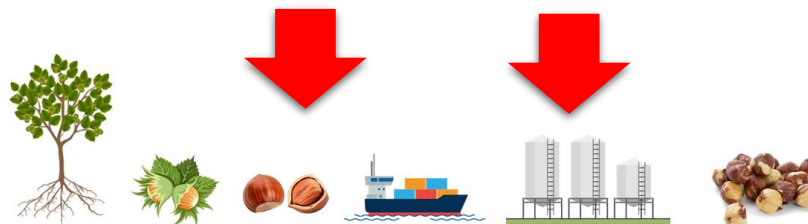
Rancidity Indexing



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Decision-maker
Raw hazelnuts quality
Rancidity level
Deployed to industry



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Journal of Food Composition and Analysis

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



Validation of a high-throughput method for the accurate quantification of secondary products of lipid oxidation in high-quality hazelnuts (*Corylus avellana* L.): A robust tool for quality assessment



AP

Secondary products
aldehydes

The Artificial Intelligence smelling machine



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Decision-maker

Raw/Roasted hazelnuts quality

Aroma quality and spoilage



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Journal of Chromatography A

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



Artificial Intelligence decision-making tools based on comprehensive two-dimensional gas chromatography data: the challenge of quantitative volatilomics in food quality assessment



Simone Squara^a, Andrea Caratti^a, Angelica Fina^a, Erica Liberto^a, Nicola Spigolon^b,
Giuseppe Genova^b, Giuseppe Castello^b, Irene Cincera^b, Carlo Bicchi^a, Chiara Cordero^{a,*}

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Spoilage diagnosis by Augmented visualization



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Decision-maker



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Journal of Chromatography A

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



Augmented visualization by computer vision and chromatographic fingerprinting on comprehensive two-dimensional gas chromatographic patterns: Unraveling diagnostic signatures in food volatilome



Andrea Caratti^{a,1}, Simone Squara^{a,1}, Carlo Bicchi^a, Qingping Tao^b, Daniel Geschwender^b, Stephen E. Reichenbach^{b,c}, Francesco Ferrero^d, Giorgio Borreani^d, Chiara Cordero^{a,*}

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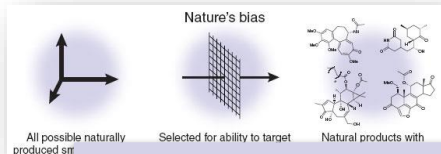
Challenges & Opportunities



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FOOD ANALYSIS LAB
QC/QA LABORATORY

Sensing Quality



Integrationist approach



Objective Quality traits
Robust marker patterns



Challenges

Real-time and **non invasive analysis** of food (at-line or on-line) should target **novel** yet **robust Quality markers** and marker **patterns**.

To align with the **industry needs** and the actual **confidence level** of **benchmark analytical tools**, **sensors** and **sensors arrays** should be:

- ✓ **sensitive** (ppt to % level in the matrix)
- ✓ **specific** and **selective** (molecular resolution and confirmatory)
- ✓ **reliable** (in quantification)
- ✓ **linear** within the dynamic range of concentrations (3 to 4 orders of magnitude)

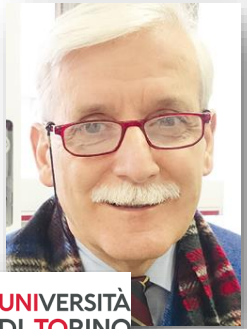
Contact Prof. Chiara Emilia Cordero

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Web: <http://www.dstfen.unito.it/do/home.pl>
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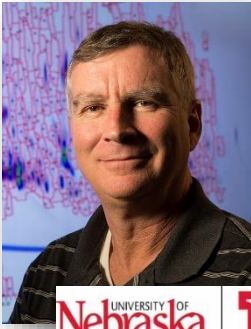
Thank you for your attention

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Dr. Simone Squara



Dr. Angelica Fina

