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RDPA 2023

Recent Developments in Pharmaceutical Analysis

Comprehensive two-dimensional gas chromatography a *gestalt* technique in food metabolomics

<u>Chiara Cordero[1]</u>

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2: GC Image LLC (Lincoln NE, USA)
3: Dept. of Computer Science and Engineering, University of Nebraska, (Lincoln NE, USA)

Foreword

Do we need more powerful approaches to 1D-GC separations in food investigations? Does comprehensive multidimensional chromatography open new opportunities to food metabolomics?

Gestalt: *something that is made of many parts and yet is somehow more than or different from the combination of its parts*

Key-concepts

- ✓ Analytical dimensions of a GC×GC platform
- ✓ Investigation strategies: a change of perspective from 1D -> 2D
  - *Pattern recognition* -> chromatographic fingerprinting
  - *Computer vision*
  - *Artificial Intelligence smelling* based on sensomics

Shelling nuts: an *omics* approach to unravel hazelnut quality and flavor by advanced chromatographic fingerprinting

Conclusive remarks

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

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

REVIEW ARTICLE
JOURNAL OF SEPARATION SCIENCE

Comprehensive two-dimensional gas chromatography as a boosting technology in food-omic investigations

Federico Stilo[1] | Carlo Bicchi[1] | Stephen E. Reichenbach[2,3] | Chiara Cordero[1]

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Data mining
machine learning
unsupervised/supervised

Data processing
targeted/untargeted
profiling/fingerprinting

Analytical platform

Columns combination
Modulation technology
Detection:
- (HR)-Mass Spectrometry
- Olfactometry
- Parallel detection

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

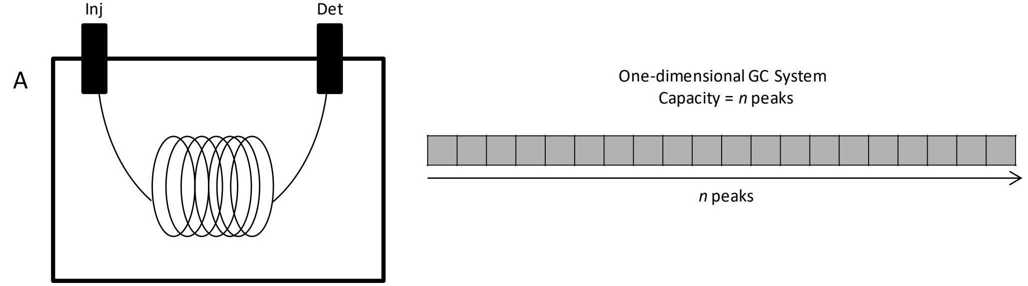
Is …*something that is made of many parts and yet is somehow more than or different from the combination of its parts*[1]… useful

Does comprehensive multidimensional chromatography offer new opportunities in food components profiling and fingerprinting?

Does it facilitate the access to higher level information?

[1] Merriam-Webster.com Dictionary, Merriam-Webster, https://www.merriam-webster.com/dictionary/gestalt. Accessed 5 Apr. 2022

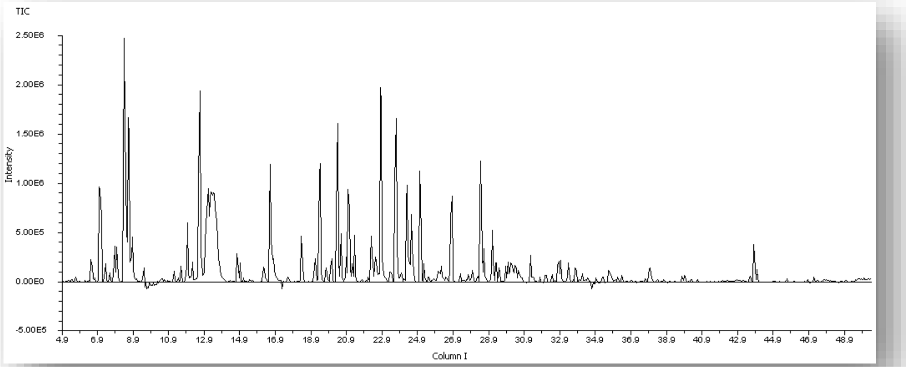
Comprehensive 2D GC



- ✓ Separation power (peak capacity) is given by the product of the two chromatographic dimensions (GC×GC)[1]
- ✓ Independent (almost) displacement in both dimensions produces rational retention patterns for homologue series[1]
- ✓ Band compression (in space - for thermal modulators) produces signal-to-noise ratio enhancement - sensitivity
- ✓ Bi-dimensional peak patterns exploits a 3D space where fingerprinting could be more accurate that in a 2D space (as for 1D-GC profiles)

[1] Giddings, J.C. (1987), Concepts and comparisons in multidimensional separation. J. High Resol. Chromatogr., 10: 319-323.

Conventional 1D GC



Profiling[1]
detailed analysis of the chemical pattern

Target(ed) analysis[2]
GC-MS metadata (retention and spectra)
analytes <u>identity</u> and <u>amount</u>

Chromatographic fingerprinting[1,3]
general and rapid high-throughput screening -> discriminate/classify samples

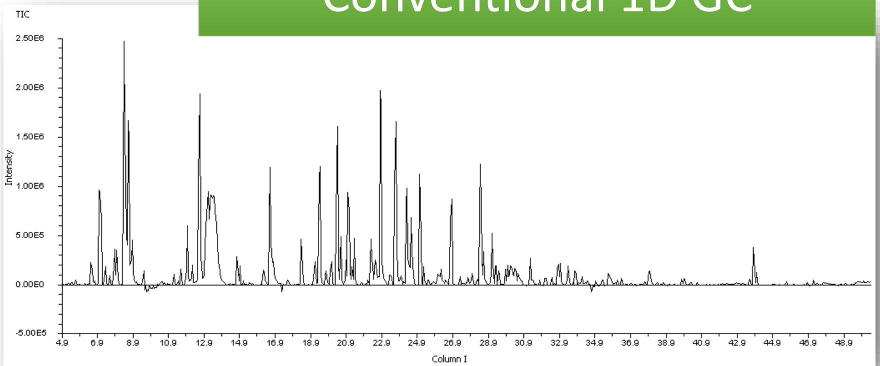
Limits
high chemical dimensionality[4]
complexity of food samples

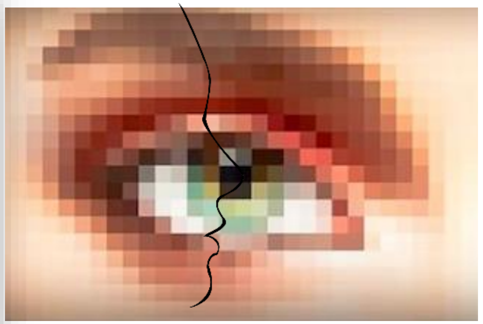
isomers/isobars might co-elute and analytes discrimination becomes challenging

Need of multiple dimensions (separation / detection) to explore compositional complexity[4]

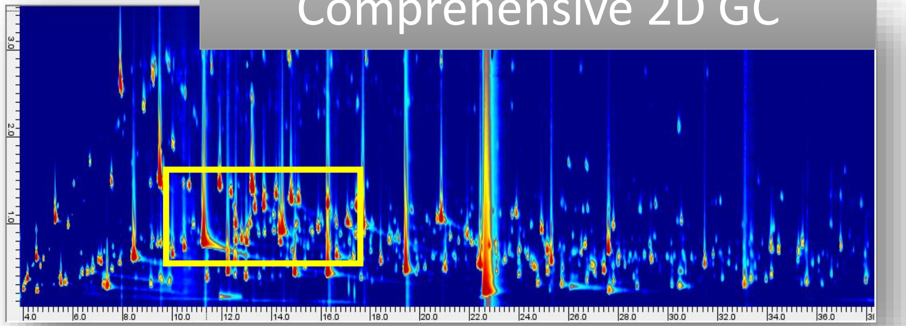
[1] Harrigan G., Goodacre R. (2003) Metabolic profiling: its role in biomarker discovery and gene function analysis. Kluwer Academic Publishers: Boston
[2] S.E. Reichenbach et al. J. Chromatogr. A 1226 (2012) 140– 148
[3] Stilo, F., Bicchi, C., Jimenez-Carvelo, A.M., Cuadros-Rodriguez, L., Reichenbach, S.E., Cordero, C. TrAC Trends Anal. Chem. 134 (2021) 116133
[4] Giddings, J. C. (1995) J. Chromatogr. A. 703, 3–15.

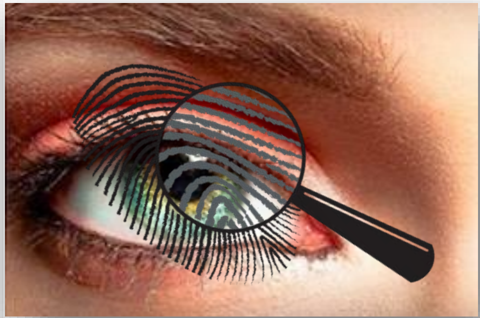
Conventional 1D GC

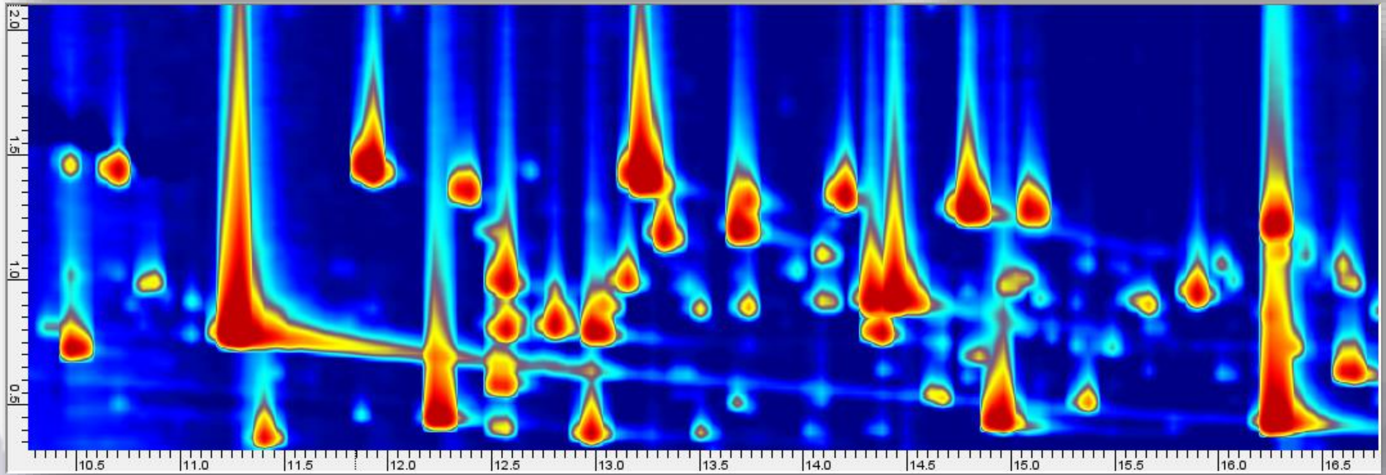




Comprehensive 2D GC





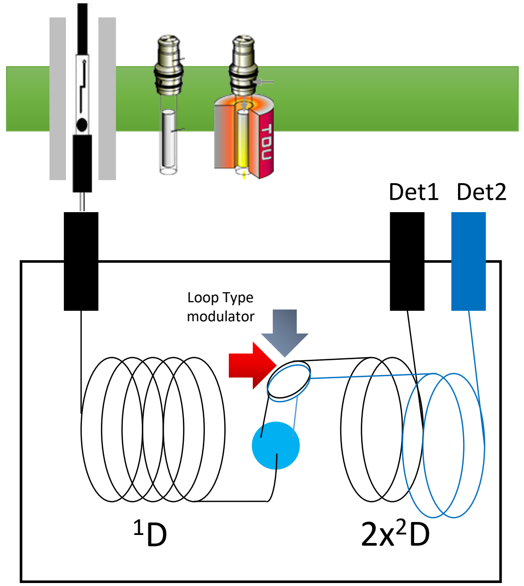


"High resolution" profiling
GC×GC <u>separation power</u>
accurate quantitative profiling

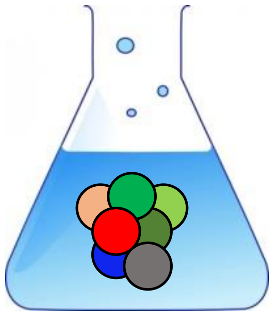
2D/3D Chromatographic fingerprinting[1]
<u>pattern recognition (forensics)</u>
comprehensive sample comparison

Group-Type Analysis
Rational retention logic
Ordered elution patterns

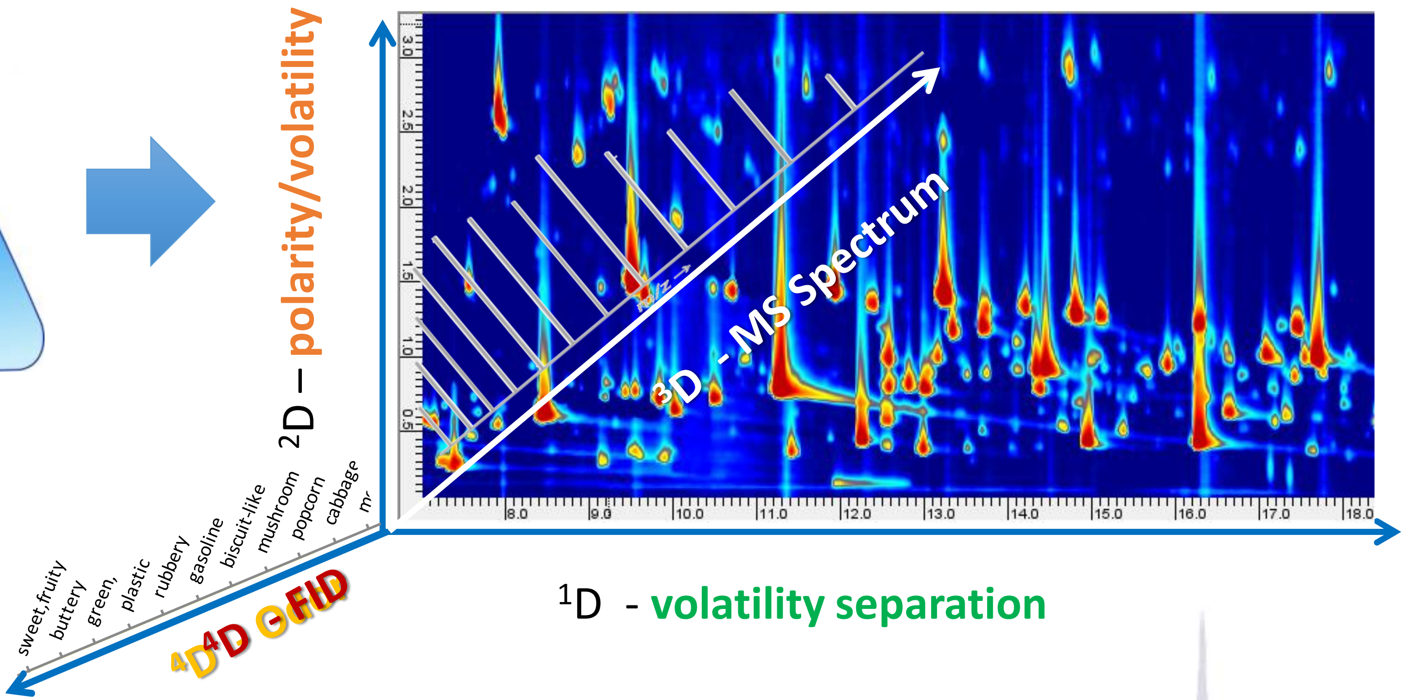
[1] Stilo, F., Bicchi, C., Jimenez-Carvelo, A. M., Cuadros-Rodriguez, L., Reichenbach, S. E., & Cordero, C. (2021). TrAC Trends in Analytical Chemistry, 134, 116133.



Sample prep - GC×2GC-MS/FID
Sample prep - GC(O)×GC-MS



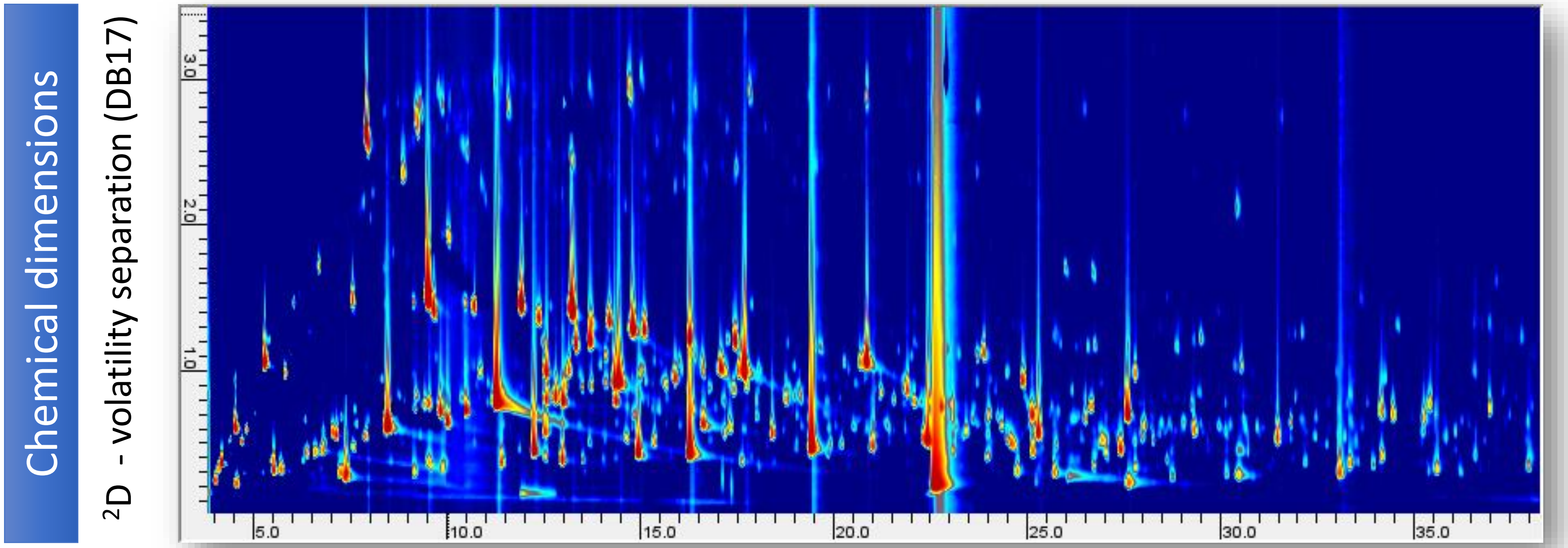
Information dimensions
spectral signature (identity)
volatility/polarity
sensory descriptor (bio-assay)



[1] J.C. Giddings J. Chromatogr. A 703(1995) 3–15.

Rational information space

Raw hazelnut volatiles - Rancid sample Origin Turkey
HS-SPME (CAR/PDMS/DVB) - 125 mg - 50°C/50 min

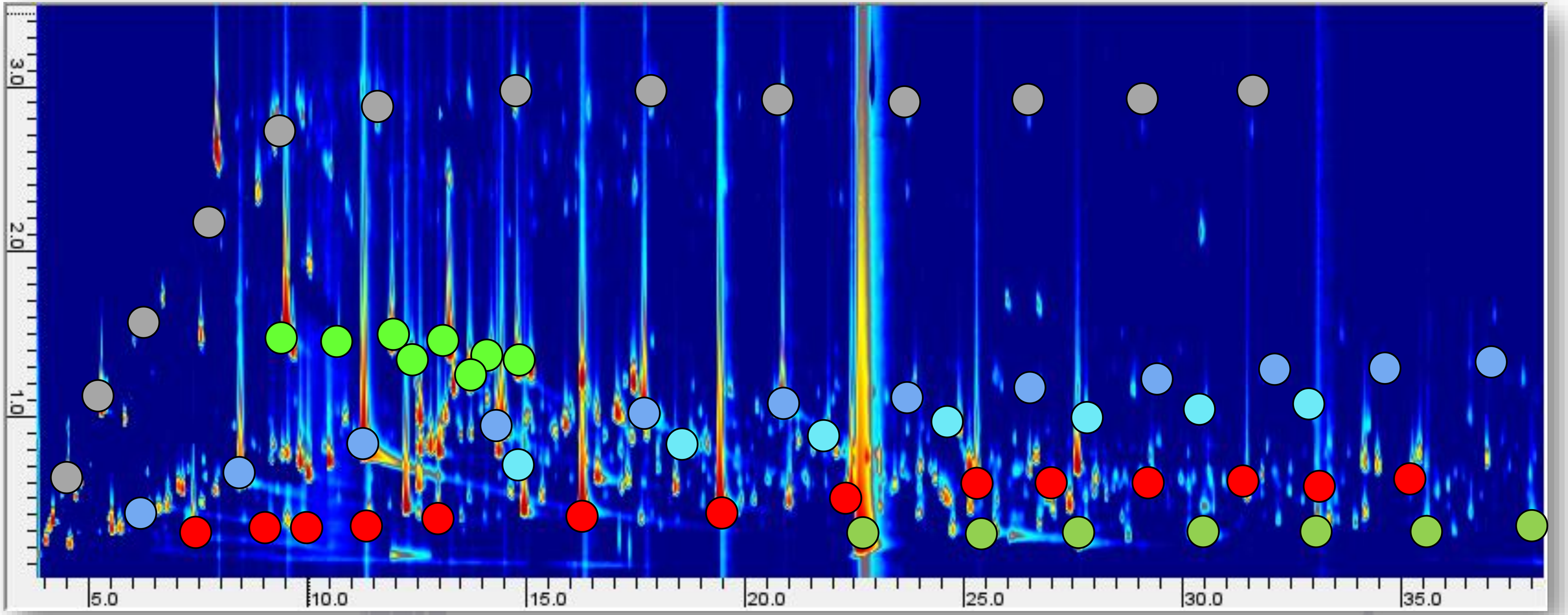


About 700 detectable features (2D peaks) over 20 S/N
Of them 250 reliably identified by 70 eV spectrum and I^T coherence
Various chemical classes highly correlated with **autoxidation** processes , enzymatic **peroxidation**, **aroma compounds** and **potent odorants**

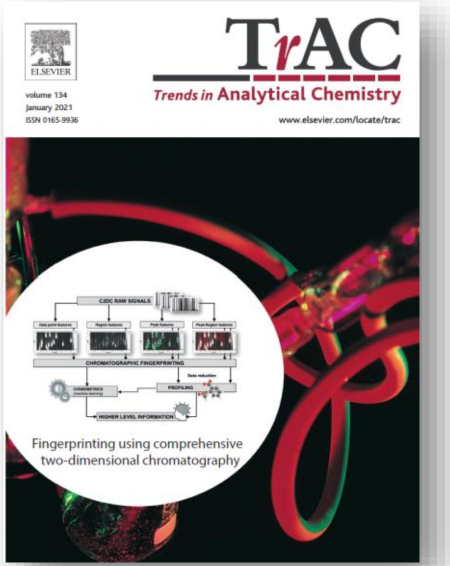
Rational information space

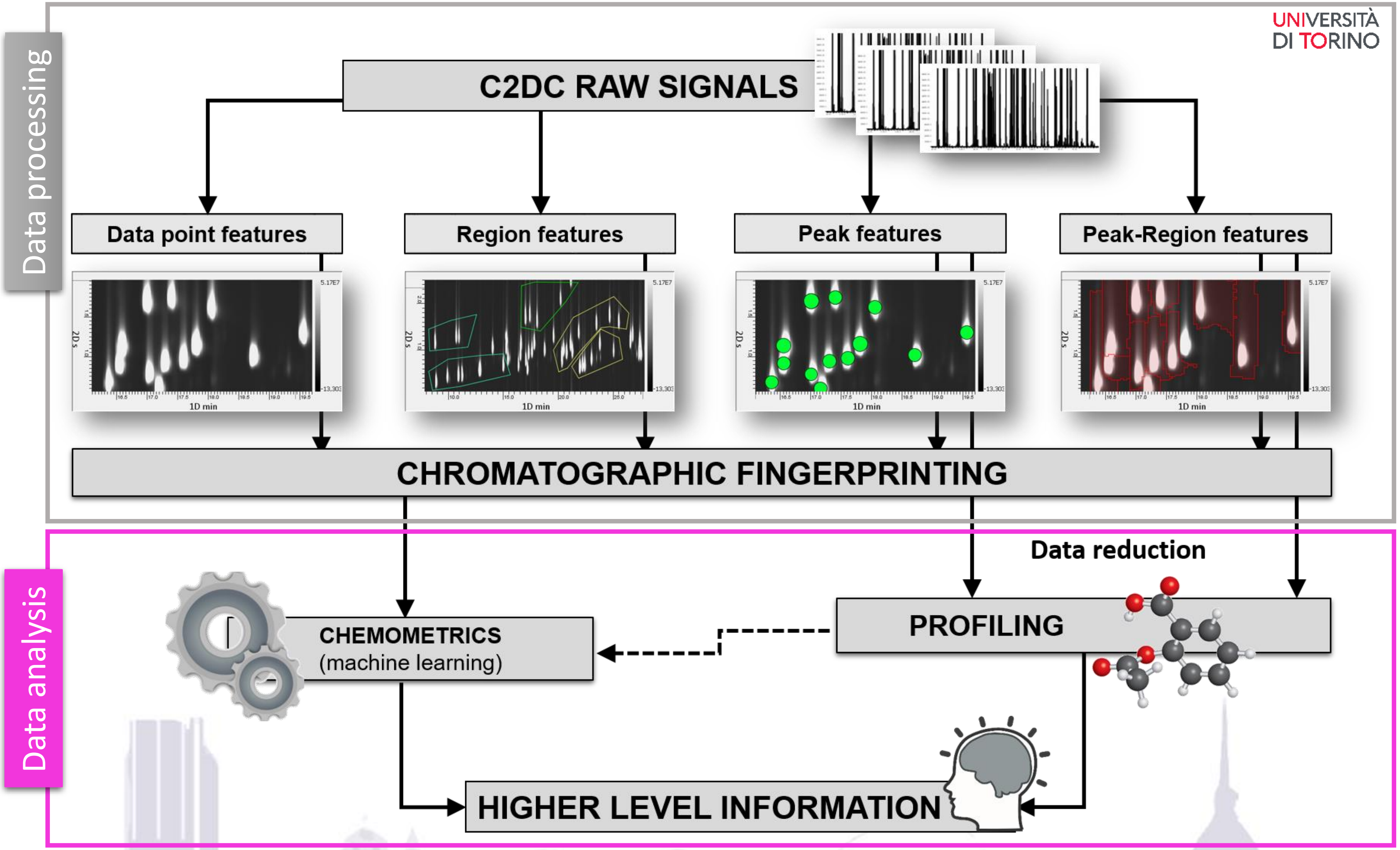
Raw hazelnut volatiles - Rancid sample Origin Turkey HS-SPME (CAR/PDMS/DVB) - 125 mg - 50°C/50 min

Information dimensions



Pattern recognition





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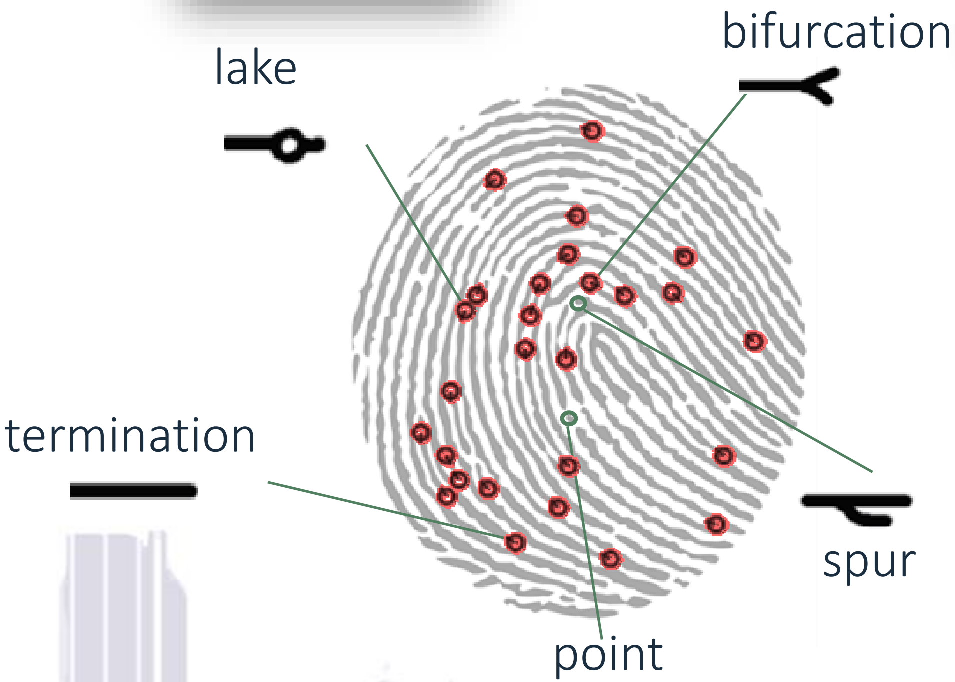
Pattern recognition

A **fingerprint** is the pattern of ridges and valleys on the surface of a fingertip
-> Everyone has unique fingerprints

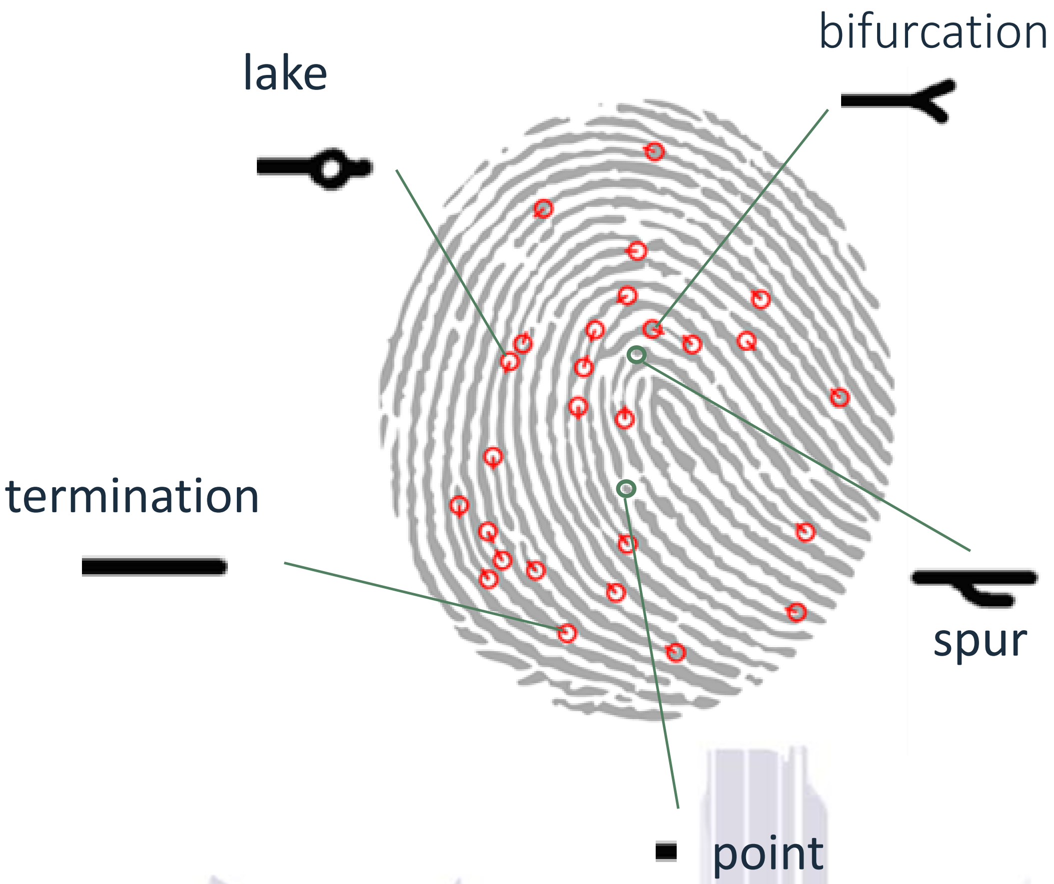
Crime scene fingerprint



Database fingerprints

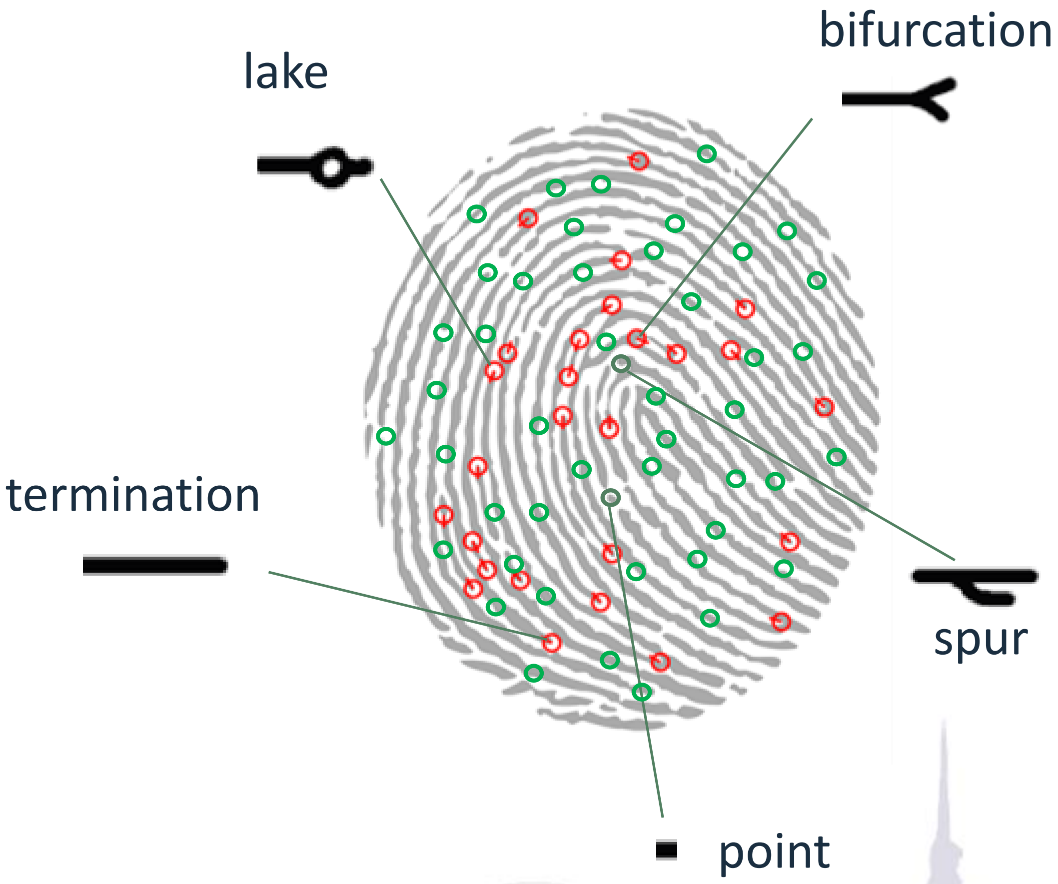
Pattern recognition

Targeted - minutiae



Untargeted - Targeted

UT - extended investigation



Pattern recognition

Untargeted/*Targeted* Fingerprinting[1-4] - comprehensive mapping

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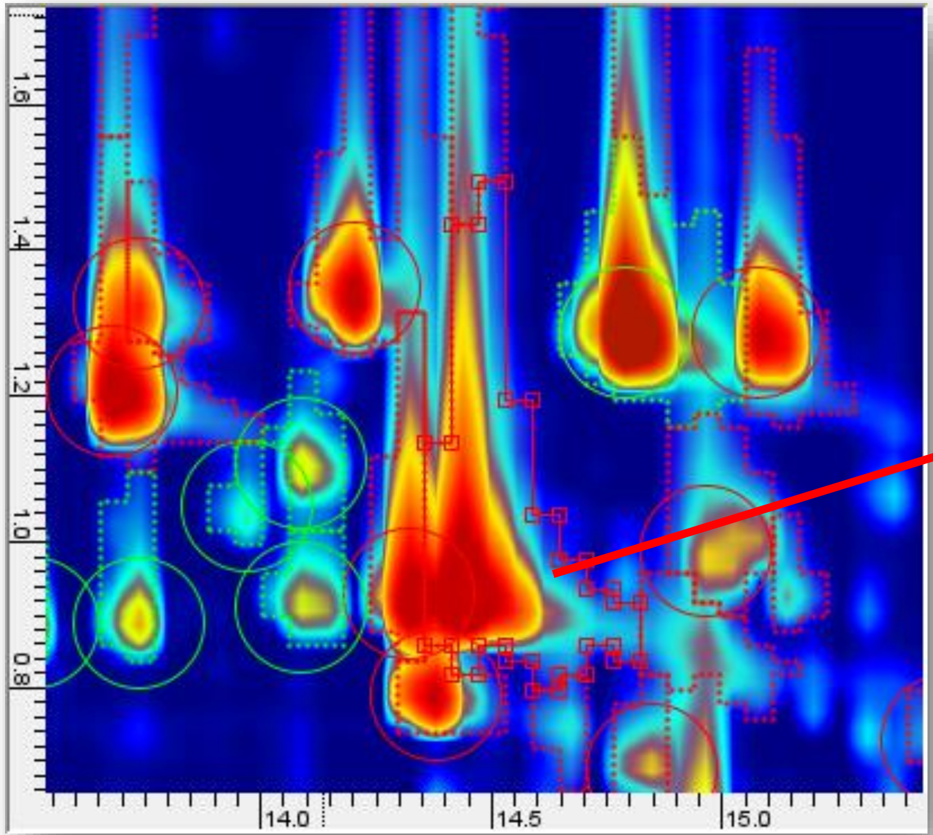

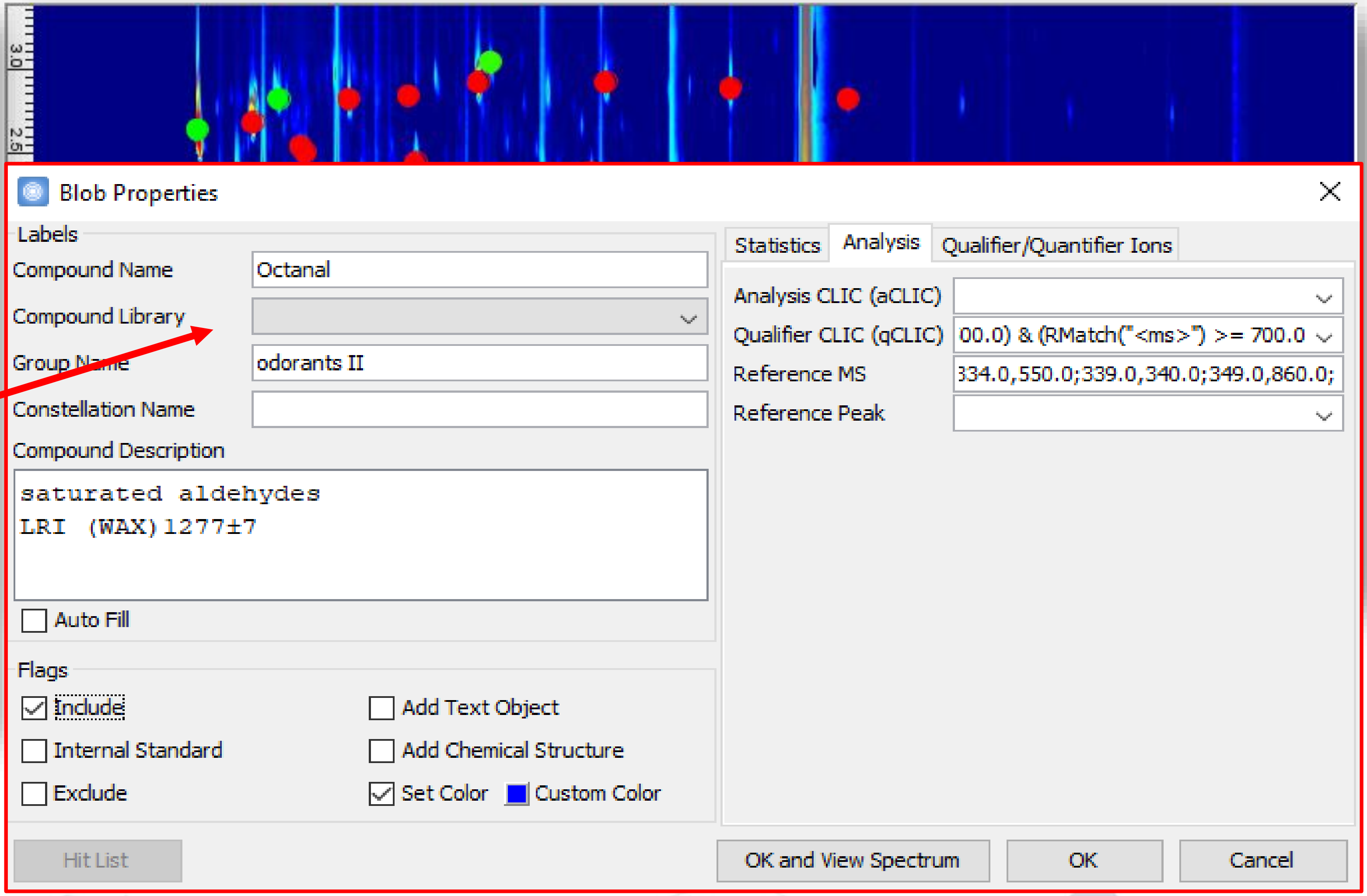

[1] Magagna, F., Valverde-Som, L., Ruíz-Samblás, C., Cuadros-Rodríguez, L., Reichenbach, S. E., Bicchi, C., & Cordero, C. (2016). Analytica Chimica Acta, 936, 245–258.
[2] Reichenbach, S. E., Tian, X., Tao, Q., Ledford, E. B., Wu, Z., & Fiehn, O. (2011). Talanta, 83(4), 1279–1288
[3] Reichenbach, S. E., Zini, C. A., Nicolli, K. P., Welke, J. E., Cordero, C., & Tao, Q. (2019). Journal of Chromatography A, 1595, 158–167
[4] Cordero, C., Guglielmetti, A., Bicchi, C., Liberto, E., Baroux, L., Merle, P., … Reichenbach, S. E. (2019). Journal of Chromatography A, 1597, 132–141

Pattern recognition

Untargeted/Targeted Fingerprinting - comprehensive mapping

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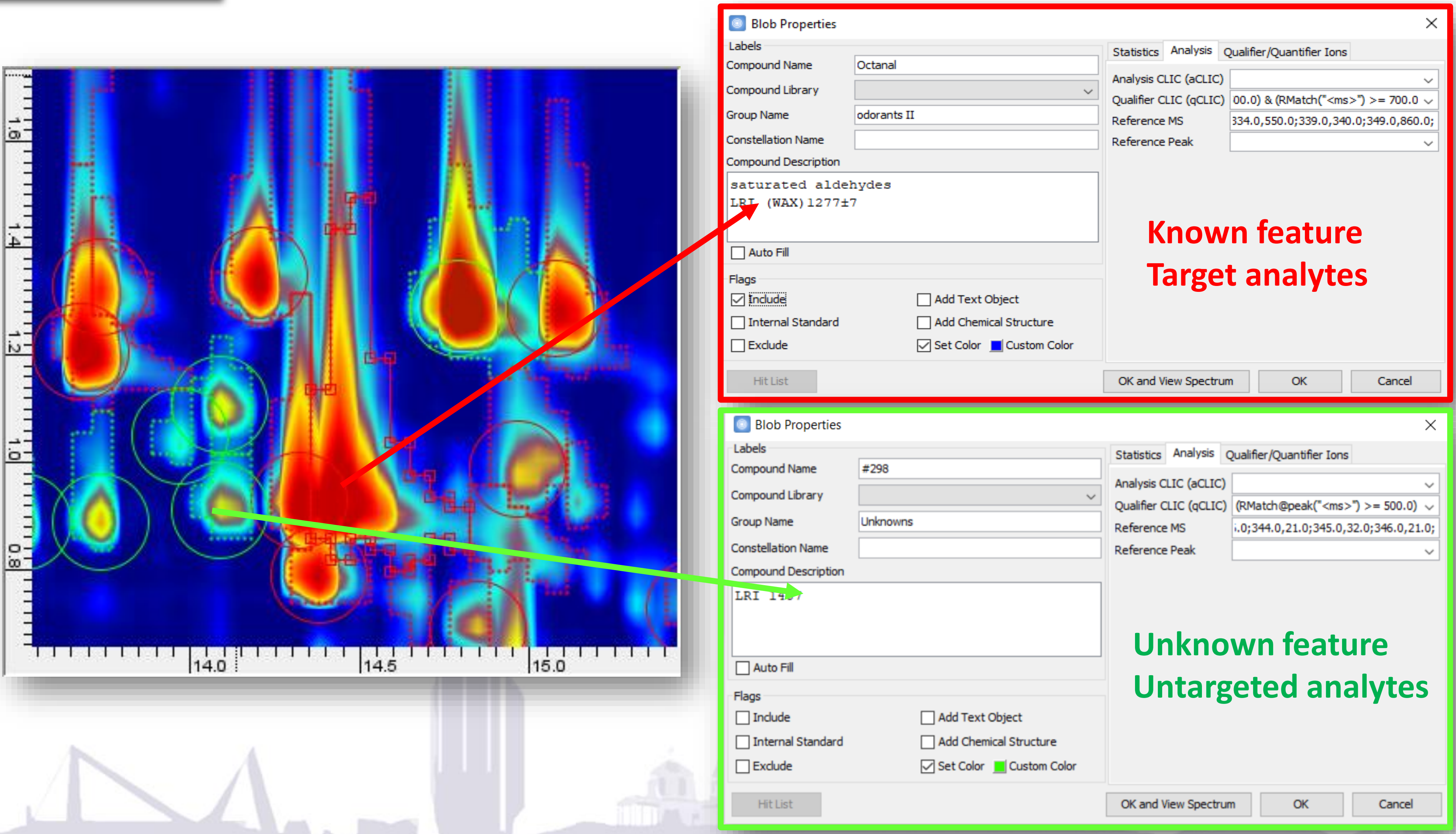
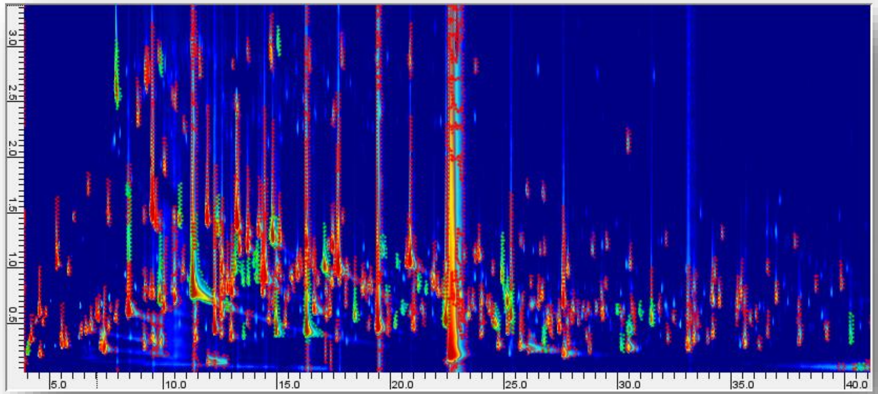
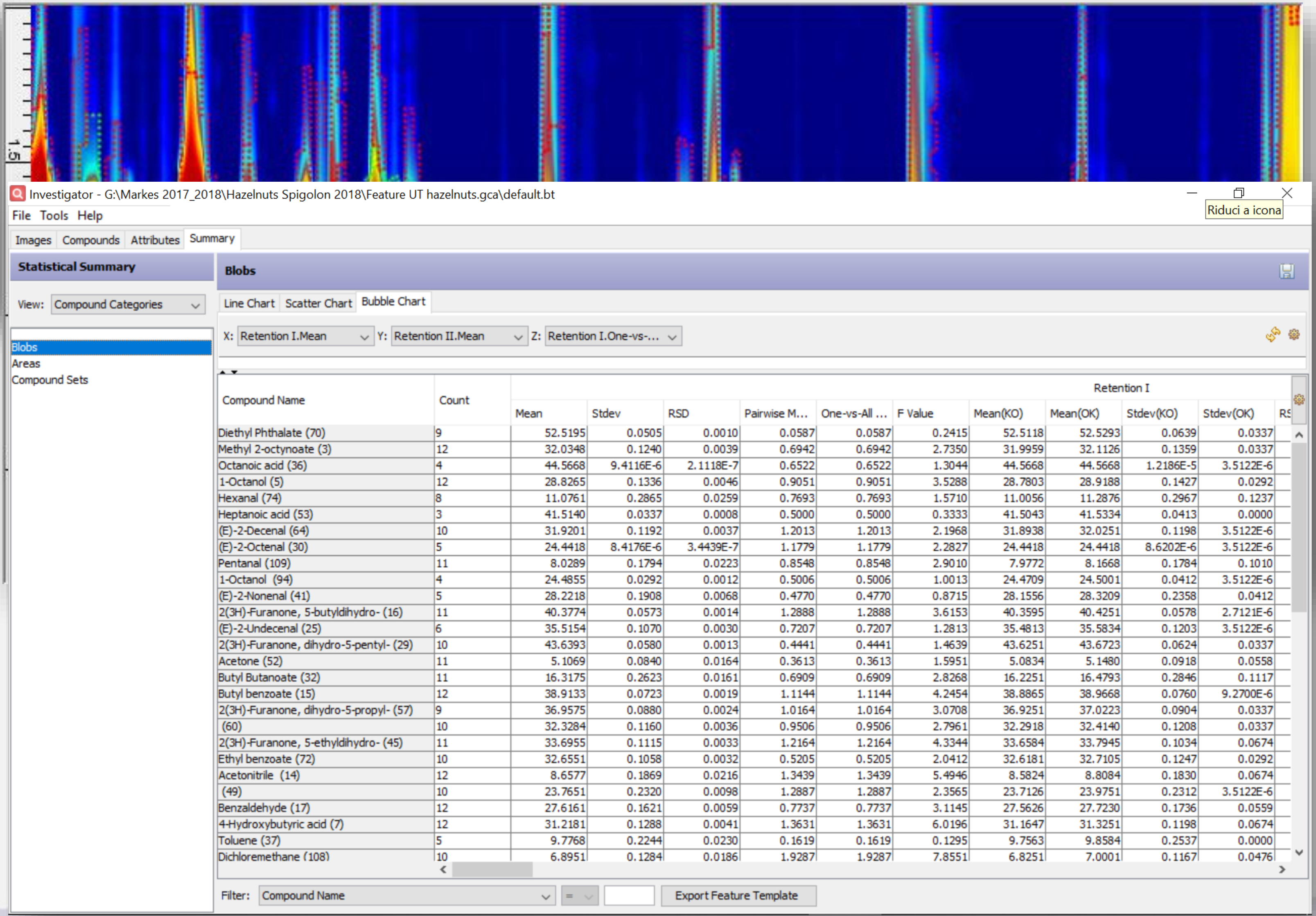


Pattern recognition





Compound Name	Count	Retention I Mean	Stdev	RSD	Pairwise M...	One-vs-All ...	F Value	Mean(KO)	Mean(OK)	Stdev(KO)	Stdev(OK)
Diethyl Phthalate (70)	9	52.5195	0.0505	0.0010	0.0587	0.0587	0.2415	52.5118	52.5293	0.0639	0.0337
Methyl 2-octynoate (3)	12	32.0348	0.1240	0.0039	0.6942	0.6942	2.7350	31.9959	32.1126	0.1359	0.0337
Octanoic acid (36)	4	44.5668	9.4116E-6	2.1118E-7	0.6522	0.6522	1.3044	44.5668	44.5668	1.2186E-5	3.5122E-6
1-Octanol (5)	12	28.8265	0.1336	0.0046	0.9051	0.9051	3.5288	28.7803	28.9188	0.1427	0.0292
Hexanal (74)	8	11.0761	0.2865	0.0259	0.7693	0.7693	1.5710	11.0056	11.2876	0.2967	0.1237
Heptanoic acid (53)	3	41.5140	0.0337	0.0008	0.5000	0.5000	0.3333	41.5043	41.5334	0.0413	0.0000
(E)-2-Decenal (64)	10	31.9201	0.1192	0.0037	1.2013	1.2013	2.1968	31.8938	32.0251	0.1198	3.5122E-6
(E)-2-Octenal (30)	5	24.4418	8.4176E-6	3.4439E-7	1.1779	1.1779	2.2827	24.4418	24.4418	8.6202E-6	3.5122E-6
Pentanal (109)	11	8.0289	0.1794	0.0223	0.8548	0.8548	2.9010	7.9772	8.1668	0.1784	0.1010
1-Octanol (94)	4	24.4855	0.0292	0.0012	0.5006	0.5006	1.0013	24.4709	24.5001	0.0412	3.5122E-6
(E)-2-Nonenal (41)	5	28.2218	0.1908	0.0068	0.4770	0.4770	0.8715	28.1556	28.3209	0.2358	0.0412
2(3H)-Furanone, 5-butyldihydro- (16)	11	40.3774	0.0573	0.0014	1.2888	1.2888	3.6153	40.3595	40.4251	0.0578	2.7121E-6
(E)-2-Undecenal (25)	6	35.5154	0.1070	0.0030	0.7207	0.7207	1.2813	35.4813	35.5834	0.1203	3.5122E-6
2(3H)-Furanone, dihydro-5-pentyl- (29)	10	43.6393	0.0580	0.0013	0.4441	0.4441	1.4639	43.6251	43.6723	0.0624	0.0337
Acetone (52)	11	5.1069	0.0840	0.0164	0.3613	0.3613	1.5951	5.0834	5.1480	0.0918	0.0558
Butyl Butanoate (32)	11	16.3175	0.2623	0.0161	0.6909	0.6909	2.8268	16.2251	16.4793	0.2846	0.1117
Butyl benzoate (15)	12	38.9133	0.0723	0.0019	1.1144	1.1144	4.2454	38.8865	38.9668	0.0760	9.2700E-6
2(3H)-Furanone, dihydro-5-propyl- (57)	9	36.9575	0.0880	0.0024	1.0164	1.0164	3.0708	36.9251	37.0223	0.0904	0.0337
(60)	10	32.3284	0.1160	0.0036	0.9506	0.9506	2.7961	32.2918	32.4140	0.1208	0.0337
2(3H)-Furanone, 5-ethyldihydro- (45)	11	33.6955	0.1115	0.0033	1.2164	1.2164	4.3344	33.6584	33.7945	0.1034	0.0674
Ethyl benzoate (72)	10	32.6551	0.1058	0.0032	0.5205	0.5205	2.0412	32.6181	32.7105	0.1247	0.0292
Acetonitrile (14)	12	8.6577	0.1869	0.0216	1.3439	1.3439	5.4946	8.5824	8.8084	0.1830	0.0674
(49)	10	23.7651	0.2320	0.0098	1.2887	1.2887	2.3565	23.7126	23.9751	0.2312	3.5122E-6
Benzaldehyde (17)	12	27.6161	0.1621	0.0059	0.7737	0.7737	3.1145	27.5626	27.7230	0.1736	0.0559
4-Hydroxybutyric acid (7)	12	31.2181	0.1288	0.0041	1.3631	1.3631	6.0196	31.1647	31.3251	0.1198	0.0674
Toluene (37)	5	9.7768	0.2244	0.0230	0.1619	0.1619	0.1295	9.7563	9.8584	0.2537	0.0000
Dichloremethane (108)	10	6.8951	0.1284	0.0186	1.9287	1.9287	7.8551	6.8251	7.0001	0.1167	0.0476

Targeted and **untargeted** peak(-region) features are cross-aligned between all samples and metadata collected for further processing.

Contents lists available at ScienceDirect

Analytica Chimica Acta

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

ELSEVIER

Combined untargeted and targeted fingerprinting with comprehensive two-dimensional chromatography for volatiles and ripening indicators in olive oil

Federico Magagna [a, 1], Lucia Valverde-Som [b, 1], Cristina Ruíz-Samblás [b], Luis Cuadros-Rodríguez [b], Stephen E. Reichenbach [c], Carlo Bicchi [a], Chiara Cordero [a, *]

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Shelling nuts

Artificial Intelligence decision-making tools:
Can multidimensional chromatography play a (key) role?

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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:

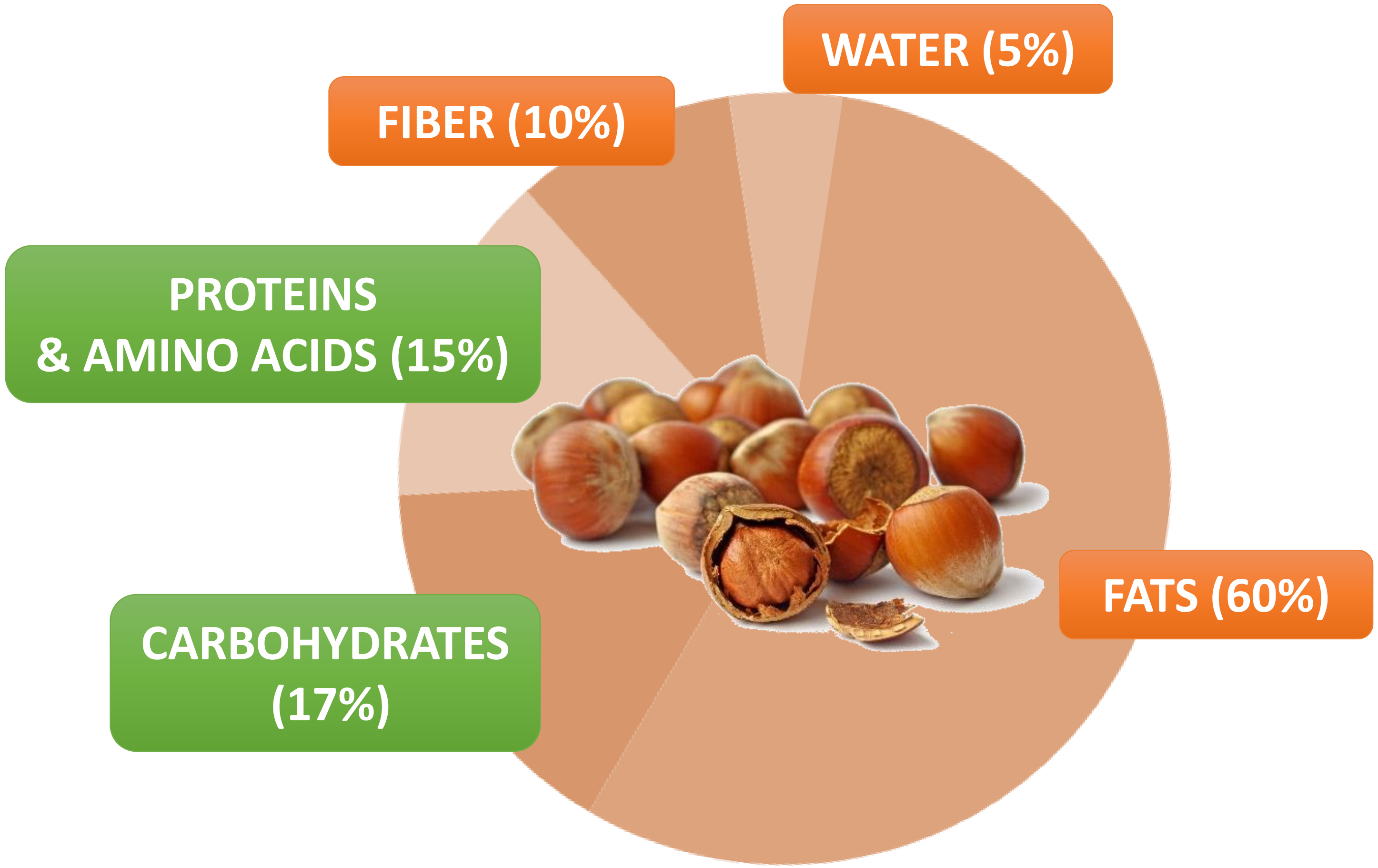
- ✓ qualification (oxidation status, shelf-life storage effectiveness, bacterial and mold grow)
- ✓ *identitation*[1] (cultivar, origin, harvest area)
- ✓ definition of *aroma potential*[2]

***AI* decision makers**

1. *Computer Vision* in defected hazelnuts VOCs patterns
2. *Smelling machine* - aroma blueprint
3. Aroma precursors pattern

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

Shelling nuts



Volatiles < 0.001%

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

Encrypts a lot of information

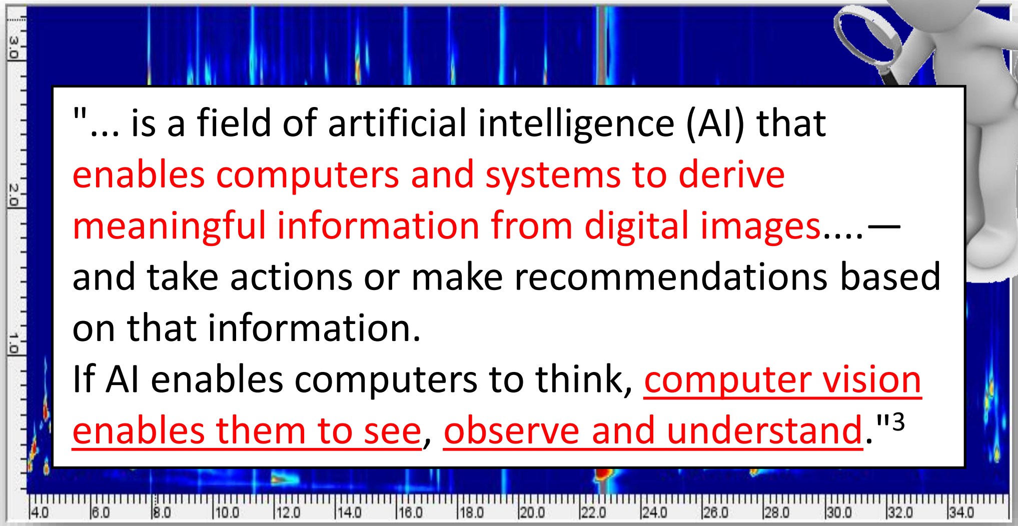
- geographical origin
- **phenotyping** and chemotyping
- multitrophic interactions (plants-insects)
- **presence of bacteria and moulds**
- **scent and odorous compounds**

- **distinctive aroma blueprint**

Shelling nuts

Computer Vision

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



"... is a field of artificial intelligence (AI) that enables computers and systems to derive meaningful information from digital images....— and take actions or make recommendations based on that information.
If AI enables computers to think, computer vision enables them to see, observe and understand."[3]

_AI_ decision-makers
Computer Vision in defected hazelnuts volatilome patterns

1. Dunkel, A.; Steinhaus, M.; Kotthoff, M.; Nowak, B.; Krautwurst, D.; Schieberle, P.; Hofmann, T. Angew. Chemie - Int. Ed. 53 (28) (2014) 7124–7143.
2. Nicolotti, L.; Mall, V.; Schieberle, P. J. Agric. Food Chem., 67 (2019) 4011–4022
3. https://www.ibm.com/topics/computer-vision

Shelling nuts

Volatiles patterns diagnostic of spoilage

Computer Vision tools
Prompt identification of non-conform samples and confident rejection

Computer Vision strategy
Classification trees

Good (OK) Rancid (KO) Spoiled (KO)

Collection of defected hazelnuts

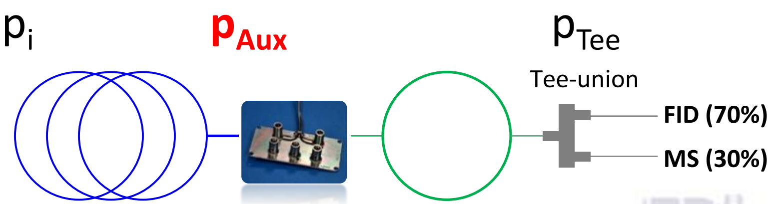
- ✓ harvest years
- ✓ origin
- ✓ shelf-life stage

Flash profiling

Mould
Mould-rancid-solvent
Rancid
Rancid-stale
Solvent
Uncoded KO

Shelling nuts

Platform

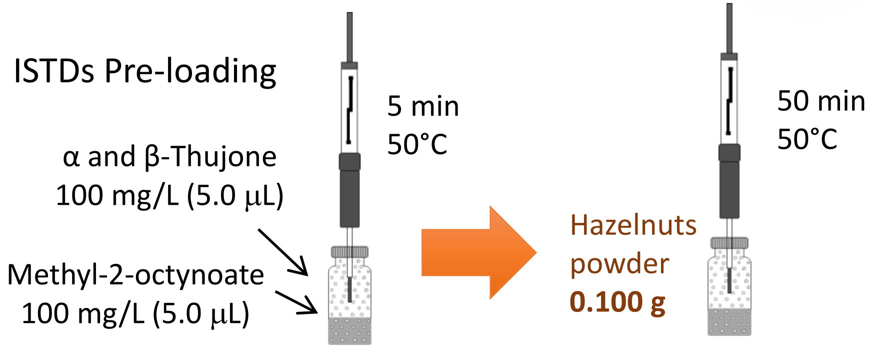


[1]D - Polar Heavy Wax (J&W)
20 m × 0.18 mm × 0.18 µm
He carrier @ **0.4 mL/min**

[2]D - Medium polarity OV17
1.8 m × 0.18 mm × 0.18 µm
He carrier @ **8 mL/min**

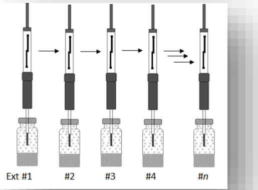
Tools

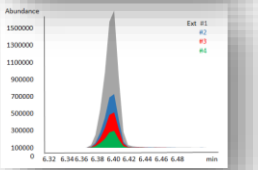
Headspace SPME



Multiple Headspace SPME - quantitation

MHS-SPME enables **accurate quantitation** of **several markers (ESTD and response factors)**





secondary products of lipid oxidation (hexanal, heptanal, octanal, nonanal, (E)-2-octenal, (E)-2-nonenal);

key-aroma compunds (3-methylbutanal, ethyl 2-methylbutanoate, (E)-β-damascenone, 2-nonanone, heptanoic acid etc);

markers of defected hz (nonanoic acid, butyric acid, 4-heptanol, 1-pentanol, propanoic acid, 2-heptanol, pentanoic acid etc)

Shelling nuts


Contents lists available at ScienceDirect
Food Chemistry
journal homepage: www.elsevier.com/locate/foodchem

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Journal of Chromatography A
journal homepage: www.elsevier.com/locate/chroma

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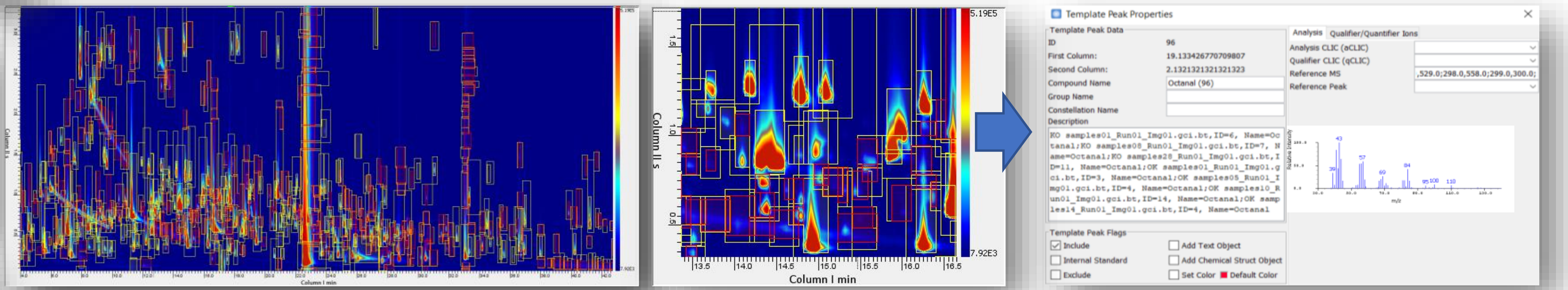
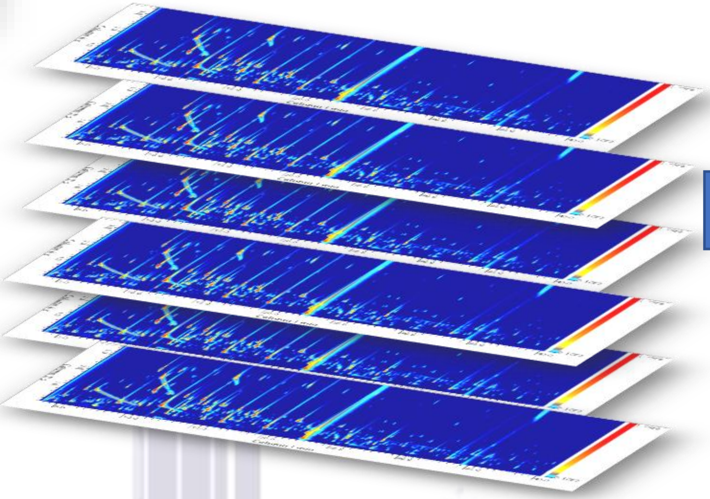
Untargeted/Targeted (UT) fingerprinting on single chromatograms

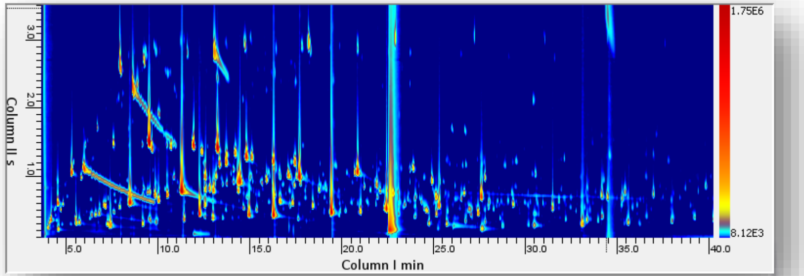


Generation of composite class-images from samples groups - one for each sensory defect

- ✓ patterns re-alignment by reliable 2D peaks and raw data summation (composite image)



Cumulative class-image "Mould"



The effect of dominant variables (origin, harvest year, cultivar, shelf-life etc..) is minimized while the "signature" of *mold* sensory defect emphasized - easier detection

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Composite class-images from samples groups - one for each sensory defect


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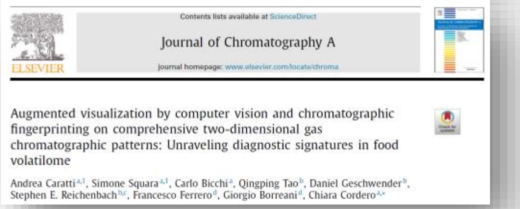
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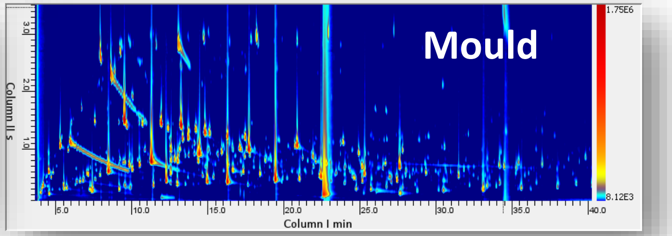

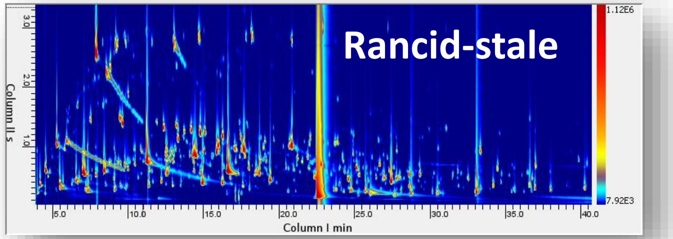

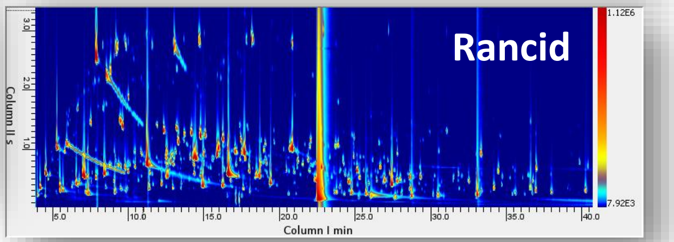

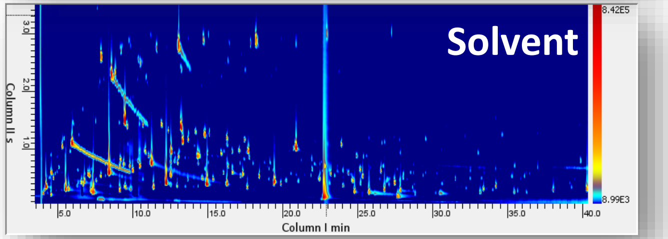

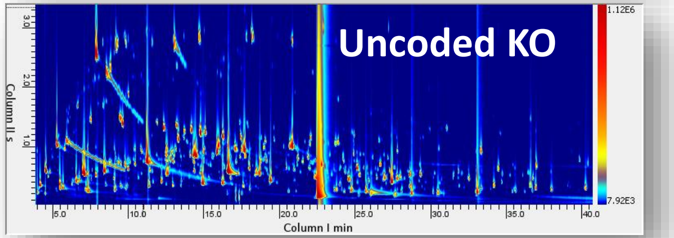

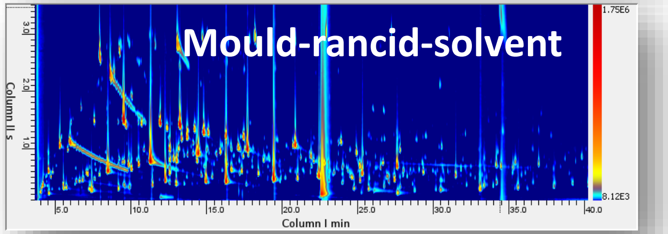

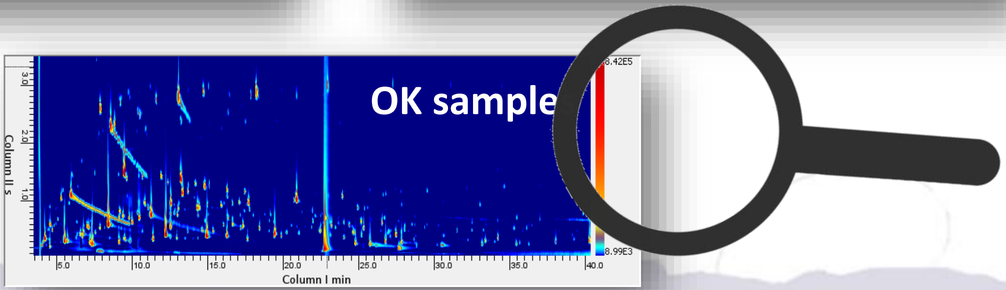

Mould
Mould-rancid-solvent
Rancid
Rancid-stale
Solvent
Uncoded KO

Reference OK samples

Shelling nuts


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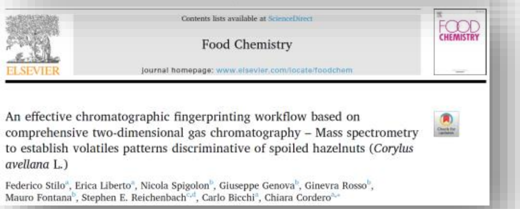
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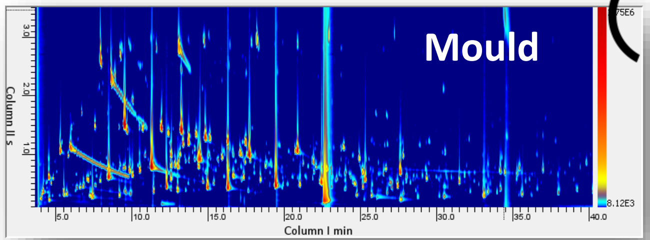
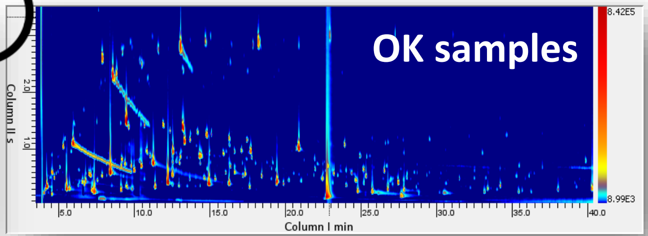
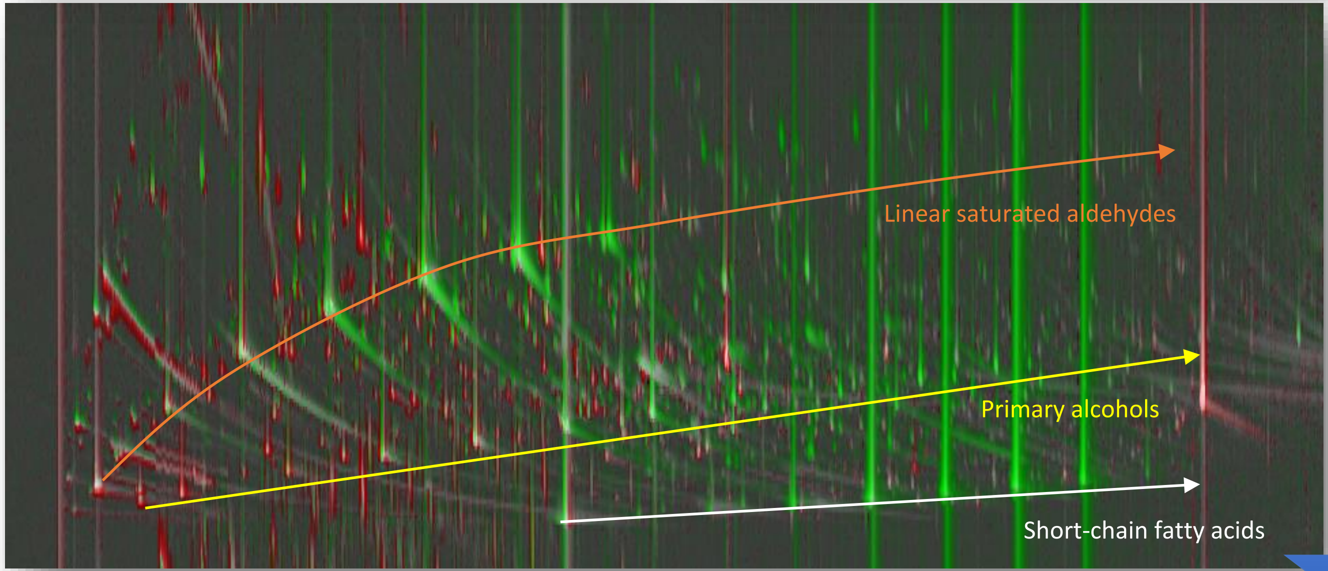
Datapoint features fingerprinting combined to peak-regions UT fingerprinting

Computer vision and chemical patterns

Computer Vision







First Image

BlobID	Compound ...	Retention I	Retention II	Peak Value
9	Heptanoic acid	41.417	0.661	1027913.00
10		10.908	1.351	2002502.00
11		14.642	1.562	1919573.00
12	Nonanoic acid	47.367	0.721	1150889.00
13		21.000	0.931	1722252.00

Second Image

BlobID	Compound ...	Retention I	Retention II	Peak Value
97	Heptanoic acid	41.533	0.631	165949.000
98	1-Decene	10.208	2.883	165851.000
99	3-Penten-2-...	12.658	1.021	163385.000
100	Oxirane, pe...	13.592	1.682	162084.000
101	1-Nonene	7.467	2.132	161864.000

Augmented visualization

Shelling nuts

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

Artificial Intelligence smelling

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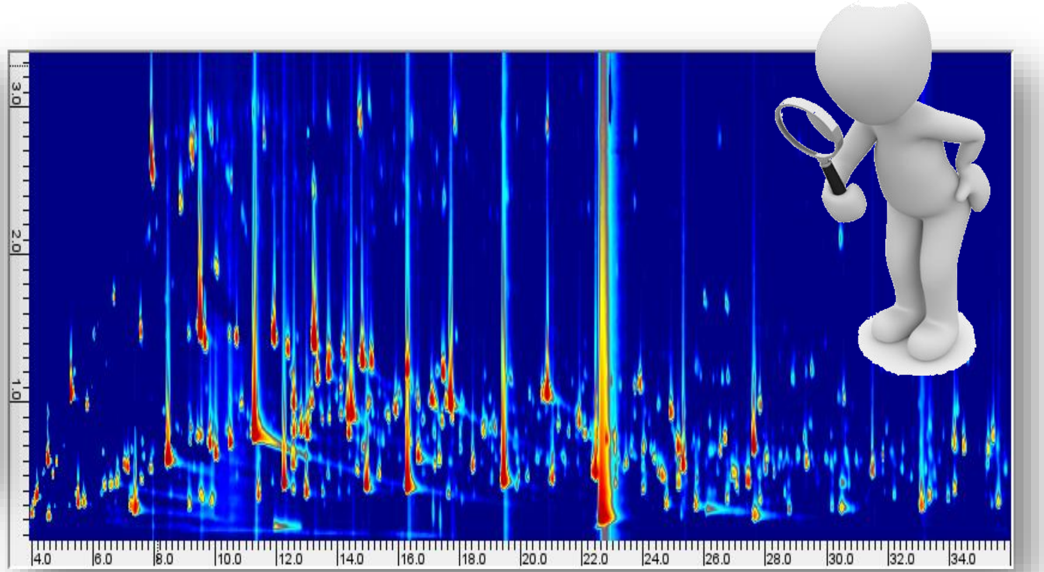

AI decision makers
AI Smelling machine - aroma blueprint

Contents lists available at ScienceDirect

Journal of Chromatography A

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

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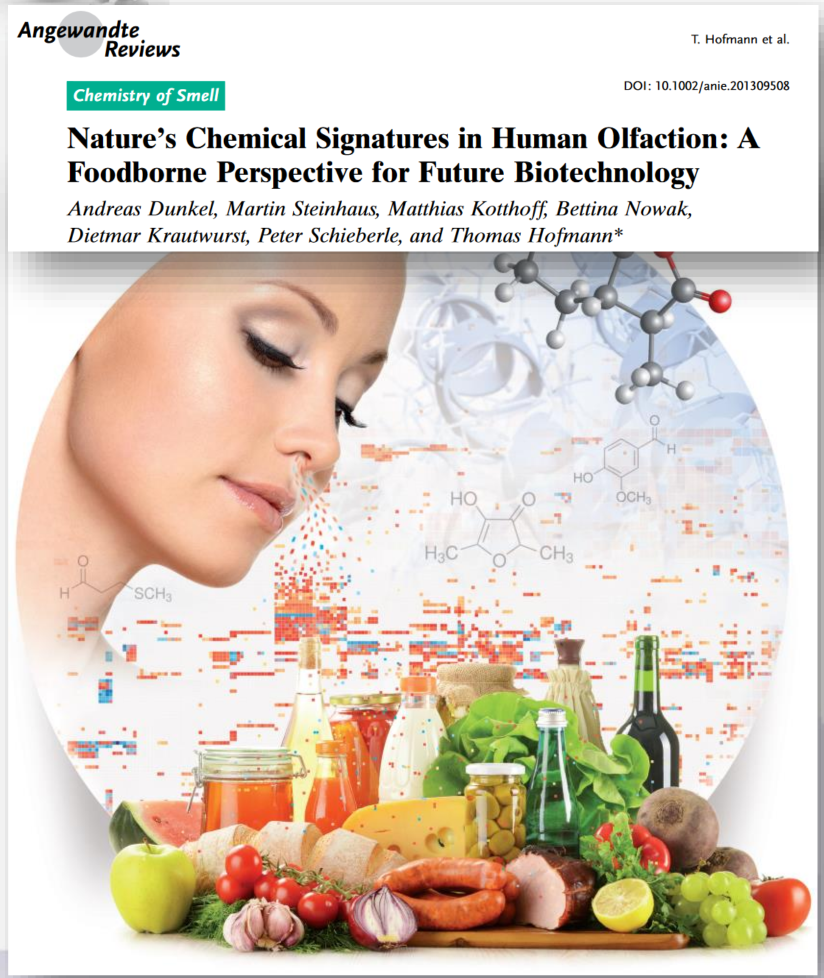
Artificial Intelligence decision-making tools based on comprehensive two-dimensional gas chromatography data: the challenge of quantitative volatilomics in food quality assessment

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,*]

Shelling nuts

Sensomics[1]

AI Smelling



Angewandte Reviews

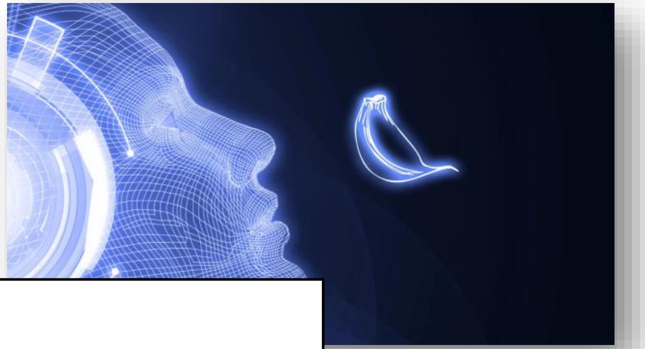
T. Hofmann et al.

DOI: 10.1002/anie.201309508

Chemistry of Smell

Nature's Chemical Signatures in Human Olfaction: A Foodborne Perspective for Future Biotechnology

*Andreas Dunkel, Martin Steinhaus, Matthias Kotthoff, Bettina Nowak, Dietmar Krautwurst, Peter Schieberle, and Thomas Hofmann**



Artificial Intelligence smelling machine

Context: *Sensomics*[1]

Principle: key-odorants and odorants patterns evoke specific smells/aroma qualities while contributing to define the overall flavor perception of a food - identity

Methods: extract, isolate, quantify potent odorants by reliable and robust methodologies

Outcome: **Sensomics-Based Expert System[2] (SEBES)** that predicts key-aroma signatures of food without using human olfaction.

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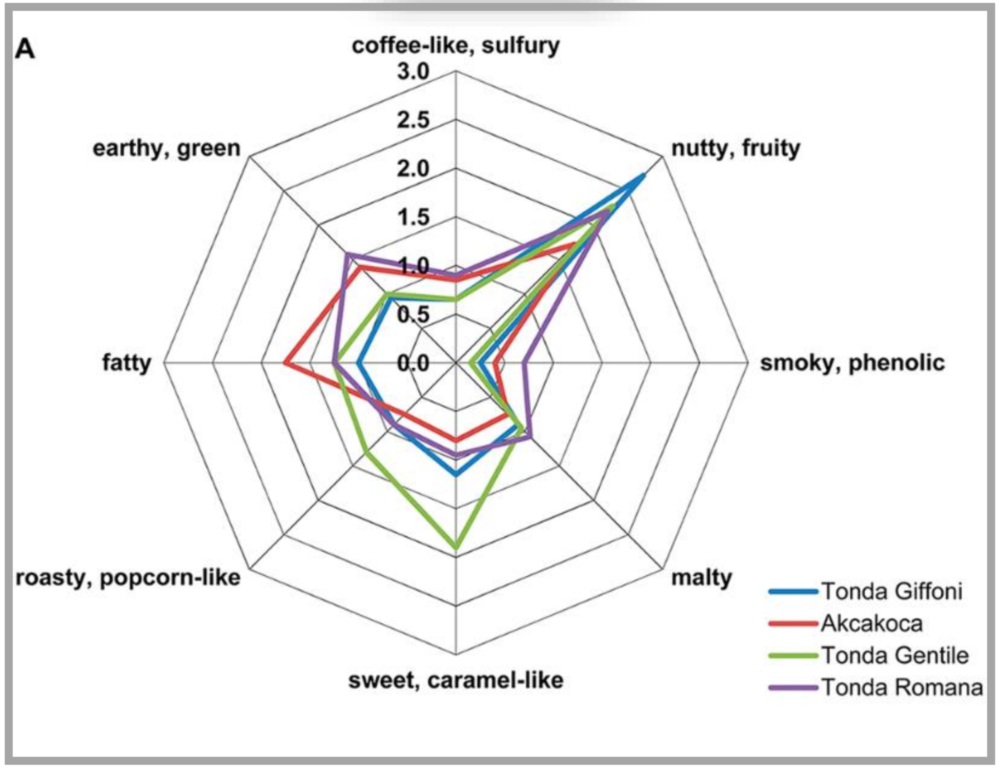
[1] Dunkel, A.; Steinhaus, M.; Kotthoff, M.; Nowak, B.; Krautwurst, D.; Schieberle, P.; Hofmann, T. Angew. Chemie - Int. Ed. 53 (28) (2014) 7124–7143.
[2] Nicolotti, L.; Mall, V.; Schieberle, P. J. Agric. Food Chem., 67 (2019) 4011–4022

Shelling nuts

Develop a sensomics-based expert system acting as AI *smelling machine*



Aroma profile of raw hazelnuts from different cultivar/origin[1]

Key-aroma compounds - raw hazelnuts odorants occurring in amounts that exceed the OT (Odor Activity Value > 1).
Their omission in aroma recombinates does not reproduce the flavour blueperint of the original product.

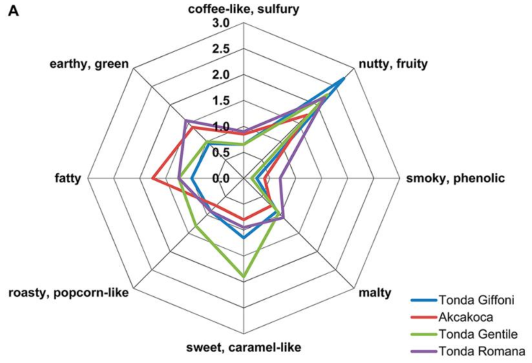
	'Tonda Romana'	'Tonda Gentile'	Akçakoca
hexanal	3	<1	8
3-methyl-4-heptanone	141	126	93
5-methyl-(E)-2-hepten-4-one	2	2	2
2-acetyl-1-pyrroline	24	24	24
dimethyl trisulfide	1	1	1
2-propionyl-1-pyrroline	22	22	22
2-furfuryl mercaptan	8	8	8
3-(methylthio)propionaldehyde	15	15	15
3,5-dimethyl-2-ethylpyrazine	1	1	1
2,3-diethyl-5-methylpyrazine	9	9	9
3,7-dimethylocta-1,6-dien-3-ol	12	12	12
2-acetyl-1,4,5,6-tetrahydropyridine	46	46	46
2-acetyl-3,4,5,6-tetrahydropridine	36	36	36
3-methylbutanoic acid	2	1	1
(E,E)-2,4-nonadienal	6	3	29

1. Kiefl, J.; Schieberle, P. J. Agric. Food Chem. 2013, 61 (22), 5236–5244.

Shelling nuts

Storage quality markers
1-heptanol (*green*, *chemical*), 2-octanol (*metal*, *burnt*), 1-octen-3-ol (*mushroom*), (E)-2-heptenal (*fatty*, *almond*), hexanal (*leaf-like, green*), heptanal (*fatty*), octanal (*fatty*) and nonanal (*tallowy*, *fruity*).

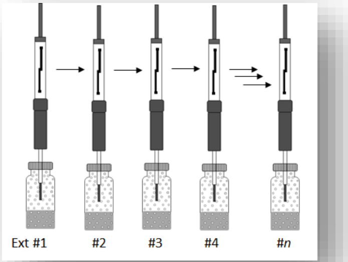
Key-aroma compounds



Spoiled hazelnuts markers
octanoic acid positively correlated to **mould**; γ-nonalactone, γ-hexalactone, acetone, and 1-nonanol are decisive to classify **OK** and **rancid** samples; heptanoic and hexanoic acids and γ-octalactone are present in high abundance **rancid-solvent** and **rancid-stale** samples.

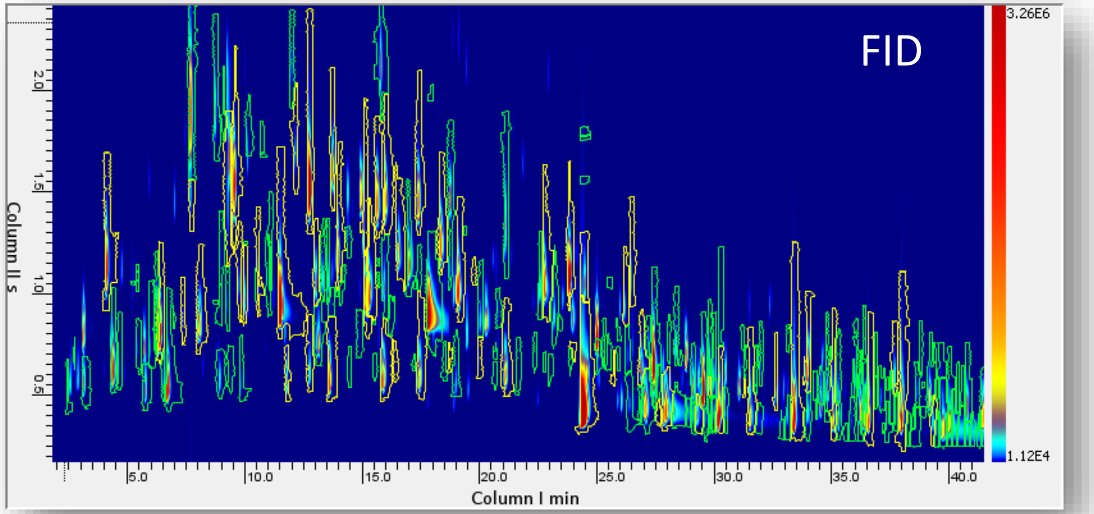
Strategy

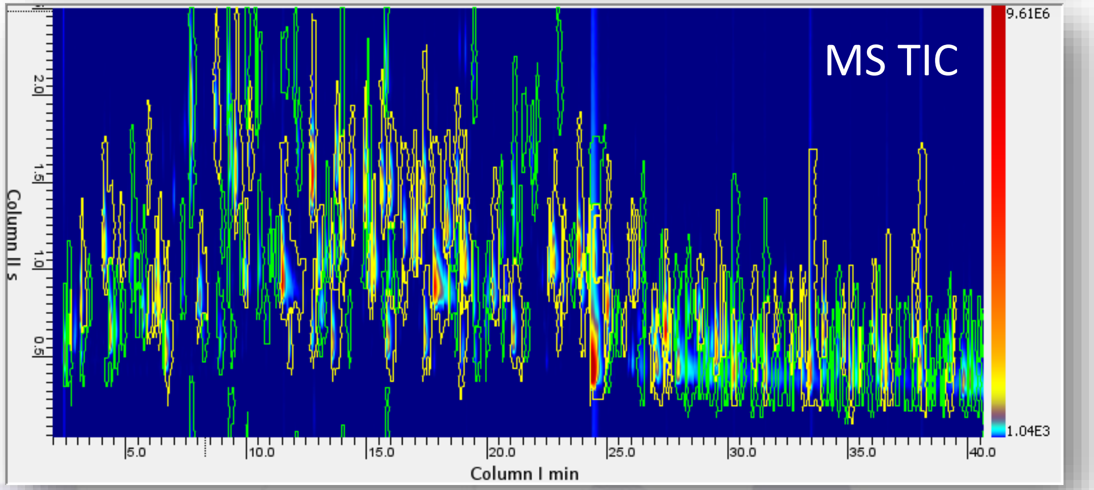
Multiple Headspace SPME
Accurate quantification / ESTD and RF



46 analytes key-aromas markers

Differential-flow modulator parallel detection qMS/FID





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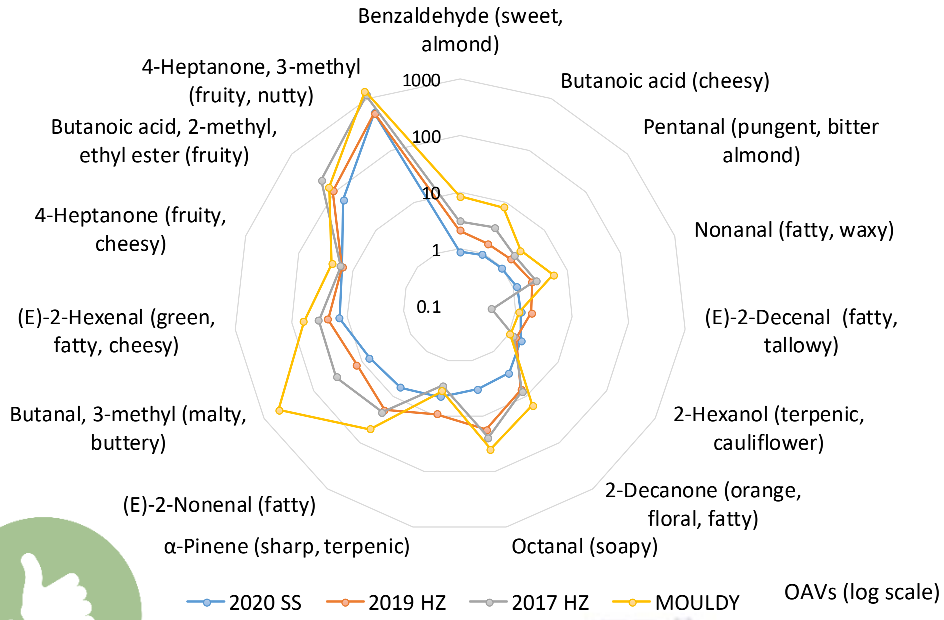
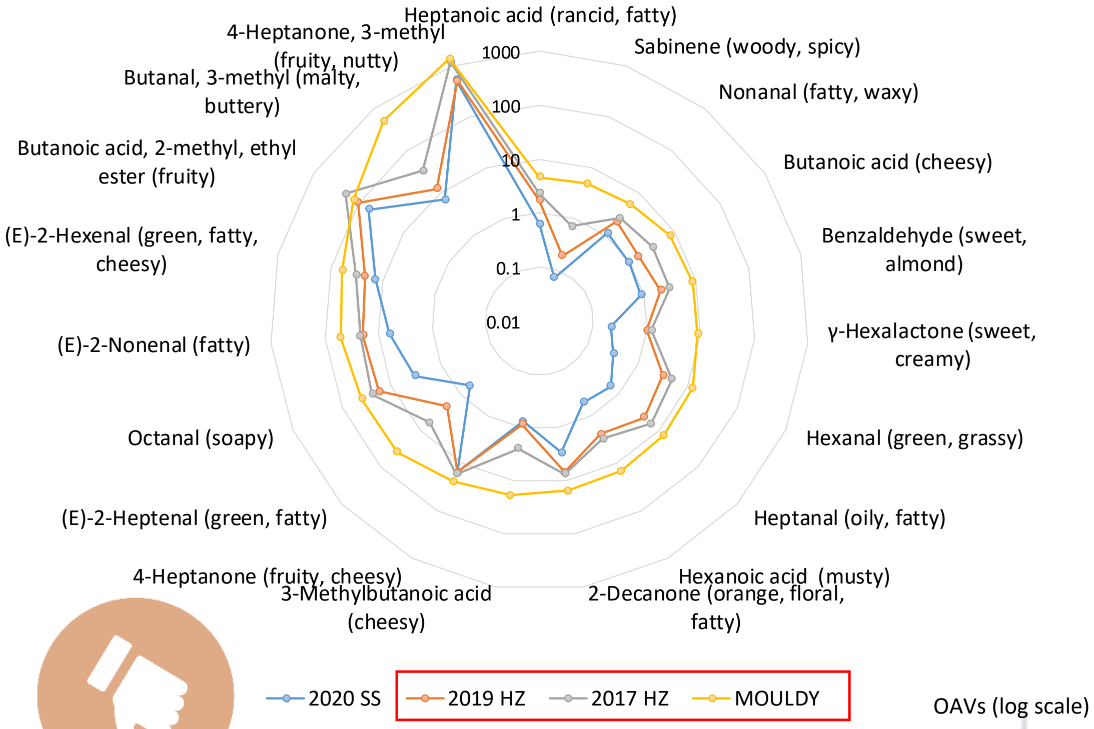
Shelling nuts

Artificial Intelligence smelling
Aroma blueprint - OAVs >1

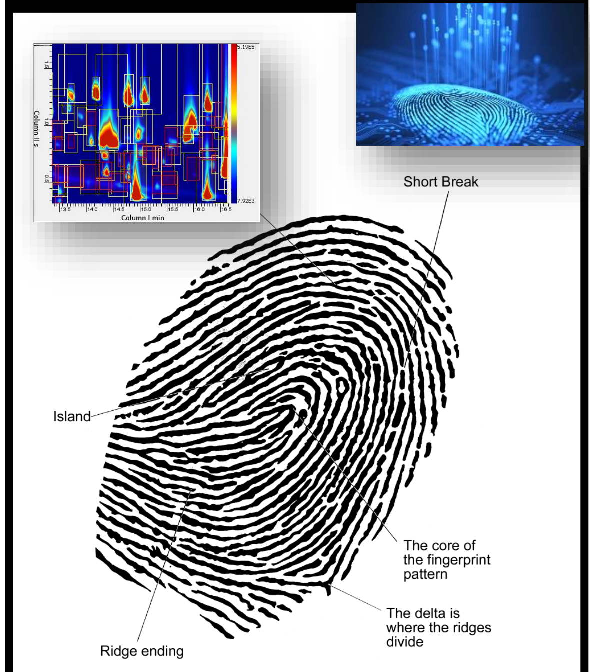




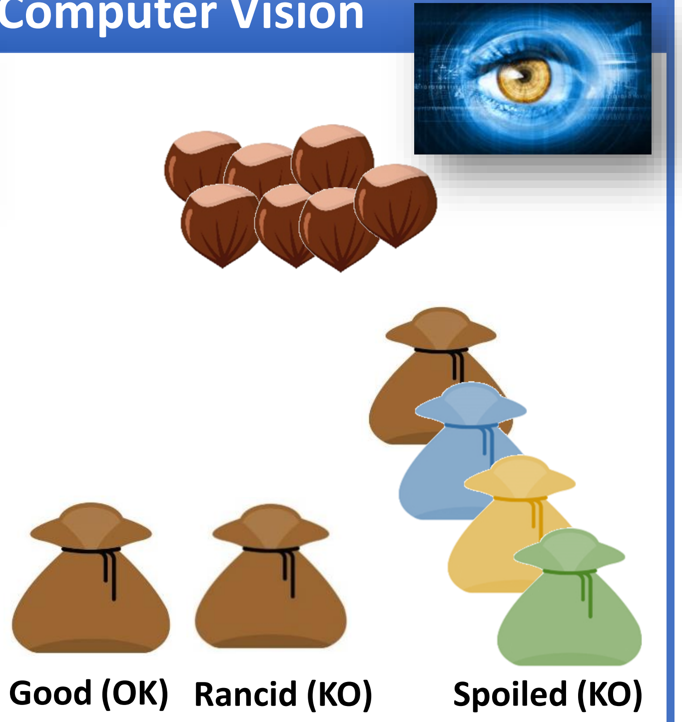
Artificial Intelligence smelling
Aroma blueprint of spoiled hazelnuts OAVs >1

Shelling nuts

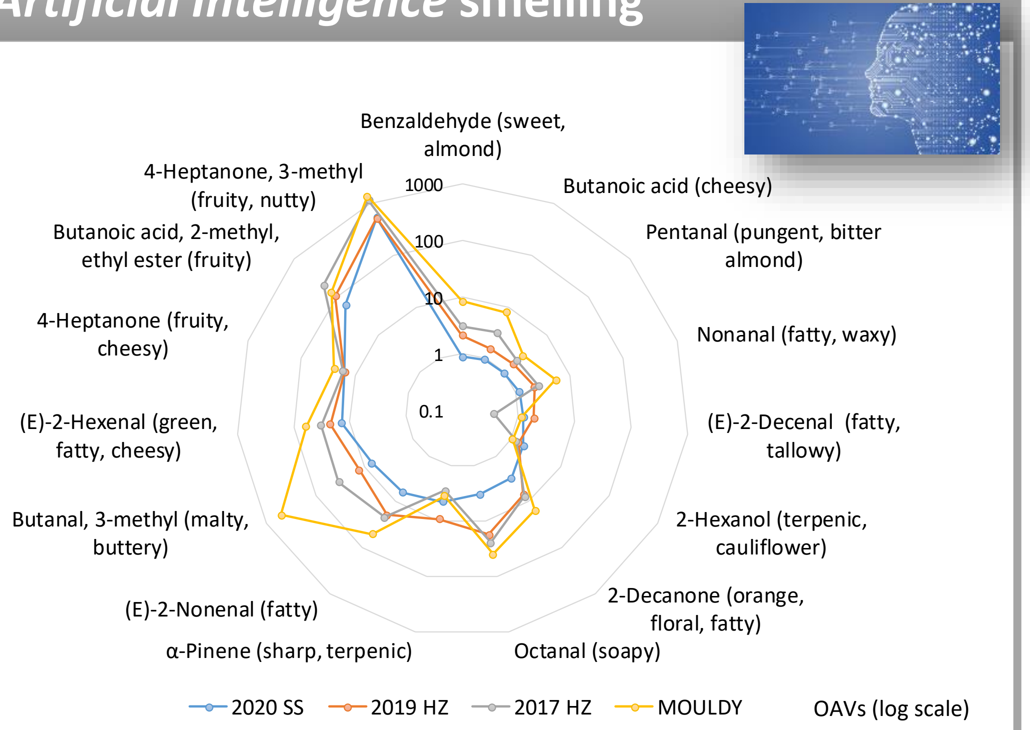
Pattern recognition



Computer Vision



Artificial Intelligence smelling



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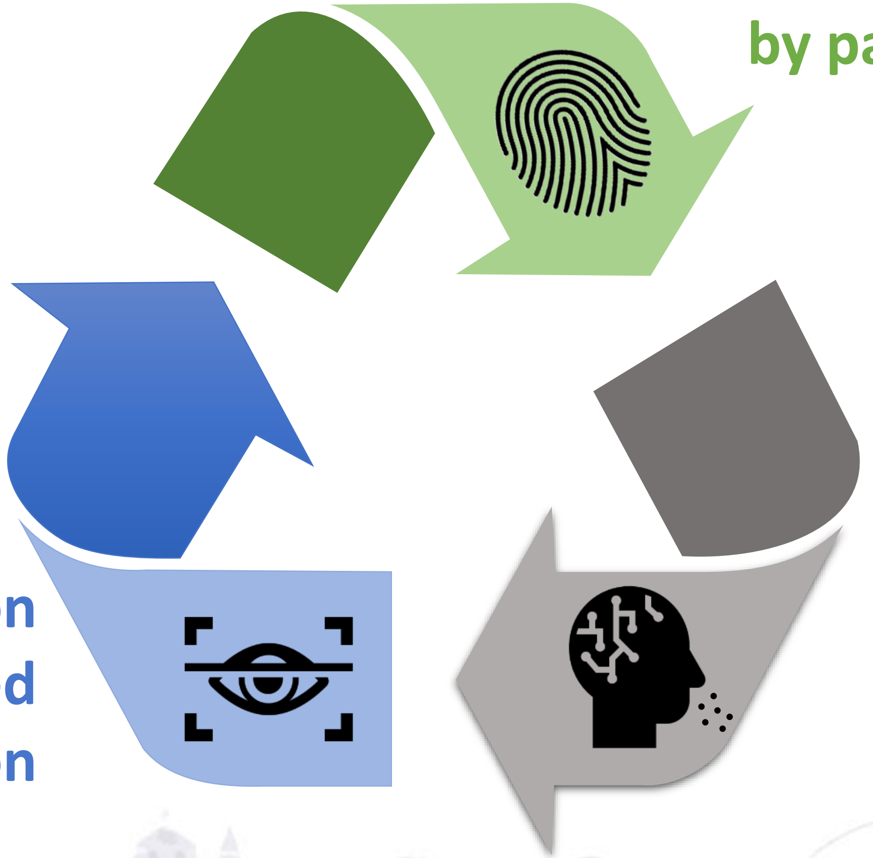
GESTALT

GESTALT

noun \ gə-ˈstält

understanding the whole, not merely the sum of its parts.

Fingerprinting/profiling by pattern recognition



Computer Vision and Augmented Visualization

Artificial Intelligence smelling machine molecular resolution tool

Thank you for your attention

Acknowledgments

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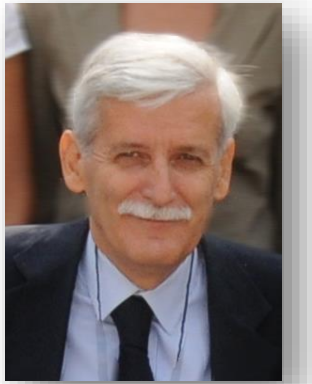
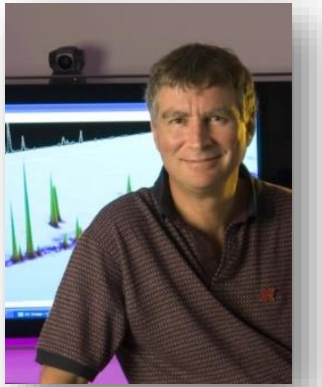
UNIVERSITY OF Nebraska Lincoln

GC Image
Software for Multidimensional Chromatography



Prof. Carlo Bicchi



Prof. Stephen E. Reichenbach

Dr. Qingping Tao

Dr. Andrea Caratti

Dr. Simone Squara

Dr. Angelica Fina

GC Image
Software for Multidimensional Chromatography

Agilent
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ANALYTICAL SOLUTIONS

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Gruppo FERRERO