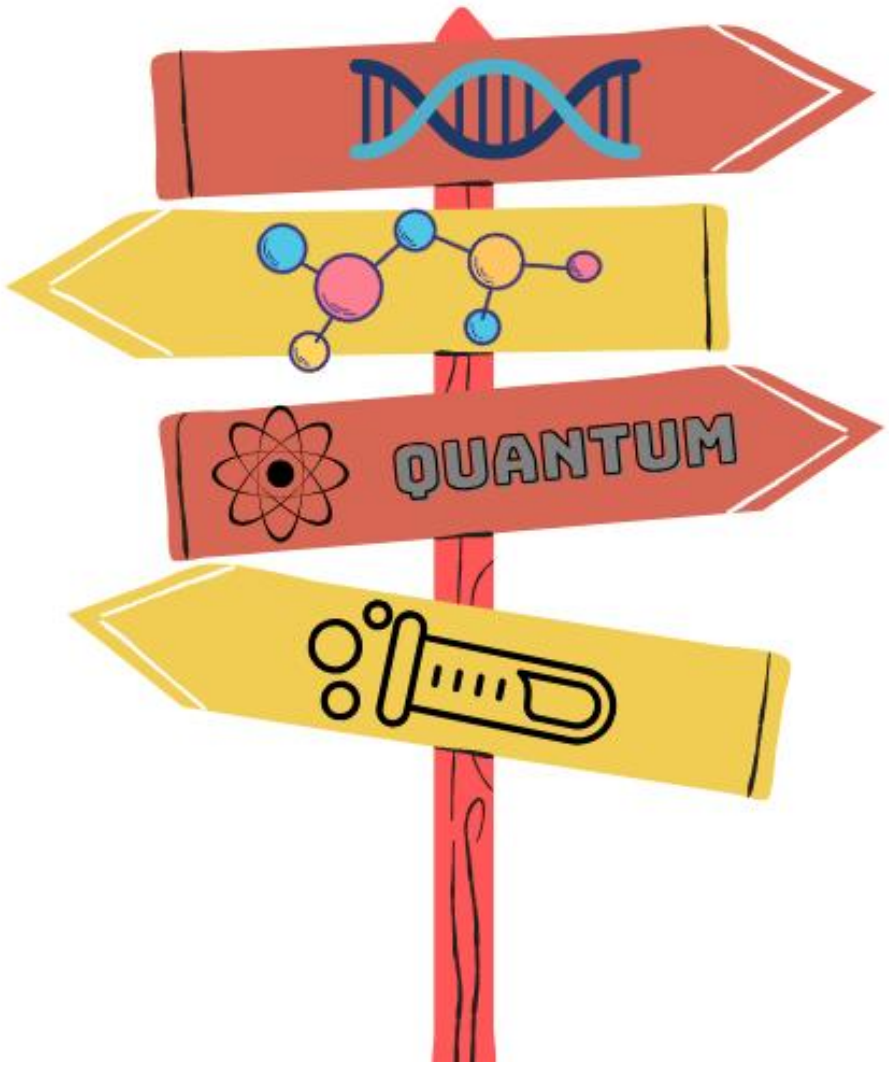


ORIENTATESI

Cdl in Chimica e Scienze Chimiche

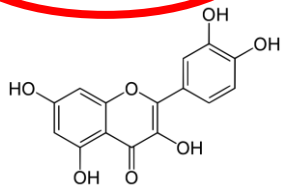
Scegli i tuoi esperimenti con...

METABOLITI

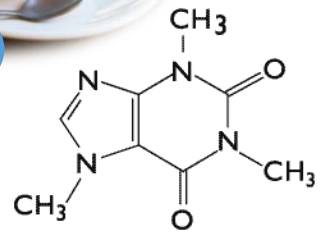
Phytochemicals

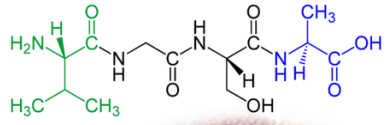
Lipidi

Polifenoli



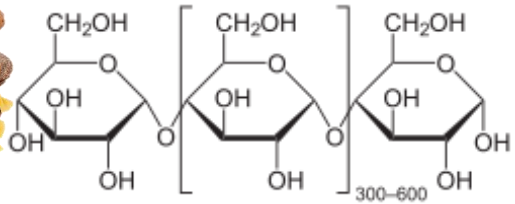
Alcaloidi





Amminoacidi e proteine

Carboidrati



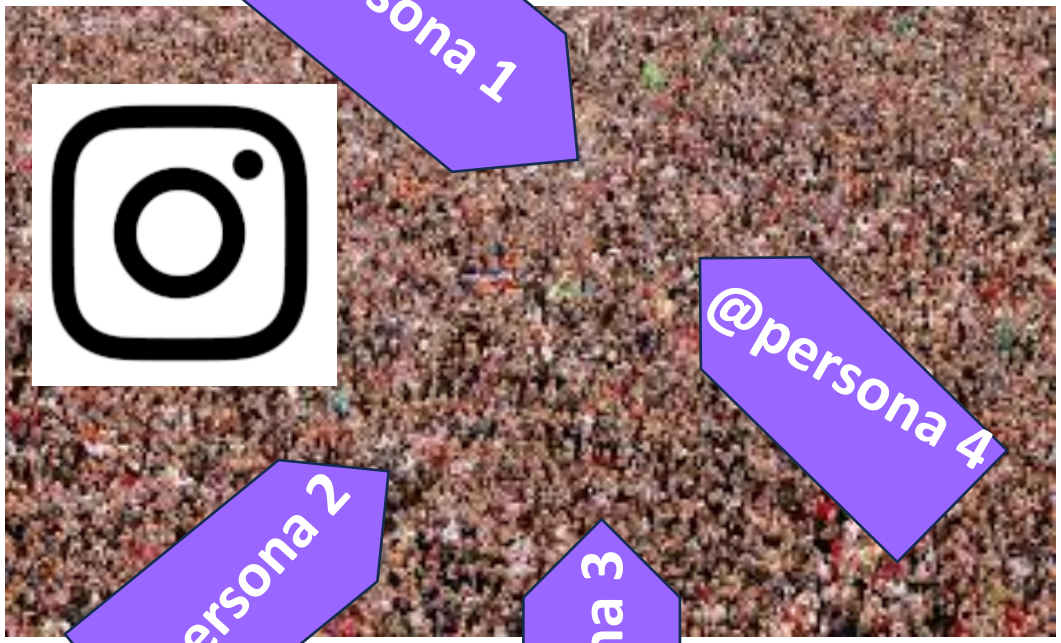
Madeleine Ernst, Denise Brentan Silva, Ricardo Roberto Silva, Ricardo Z. N. Vencio and Norberto Peporine Lopes, Nat. Prod. Rep., 2014, 31, 784

METABOLITI…..secondari

I metaboliti secondari sono una categorie di molecole bioattive che funzionano a basse concentrazioni e che vengono utilizzati principalmente per definire relazioni tra piante e altri organismi. Sono composti spesso cellula / tessuto o organo specifici che possono essere sintetizzati costitutivamente a livello basso ma che possono subire incrementi in seguito a risposte esterne come regolatori della crescita, condizioni di stress biotici o abiotici piuttosto che fasi di sviluppo e stagionalità.

Giuliana Bianco

UNTARGETED vs TARGETED



IMPRONTA DIGITALE

Informazione Unica per l'alimento

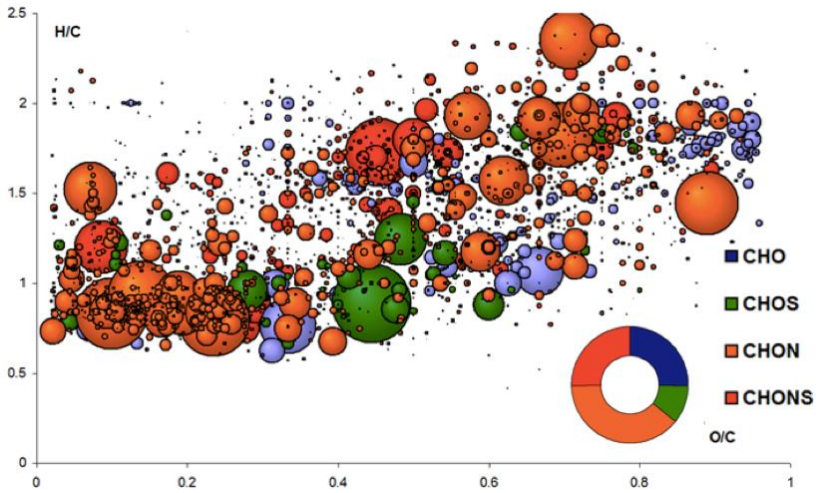
Utile per valutazione della qualità e dello stato di salute…

…e per la tracciabilità e la certificazione

IMPRONTA DIGITALE MOLECOLARE

INFORMAZIONI UNICHE PER L'ALIMENTO

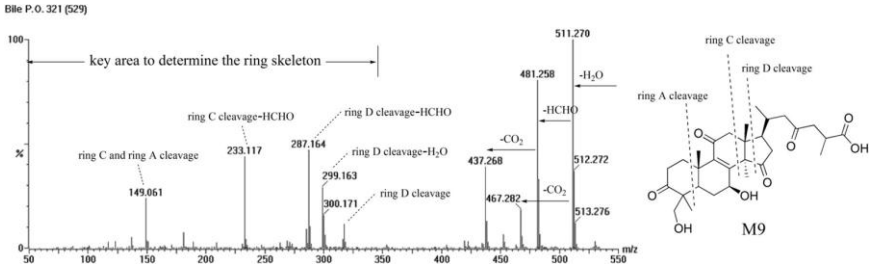
COSTRUZIONE DELL' IMPRONTA DIGITALE MOLECOLARE

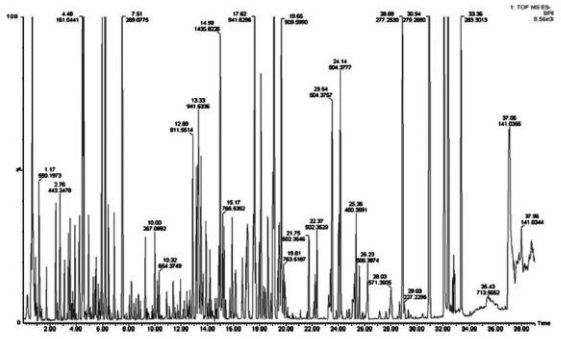


Spettrometria di massa

- E' la tecnica analitica che si basa sulla produzione di ioni da atomi o molecole *(sorgente)* i quali sono poi separati in accordo con il loro rapporto massa/carica (m/z) *(analizzatore)* e infine misurati *(rilevatore)*

MASS SPECTROMETRY

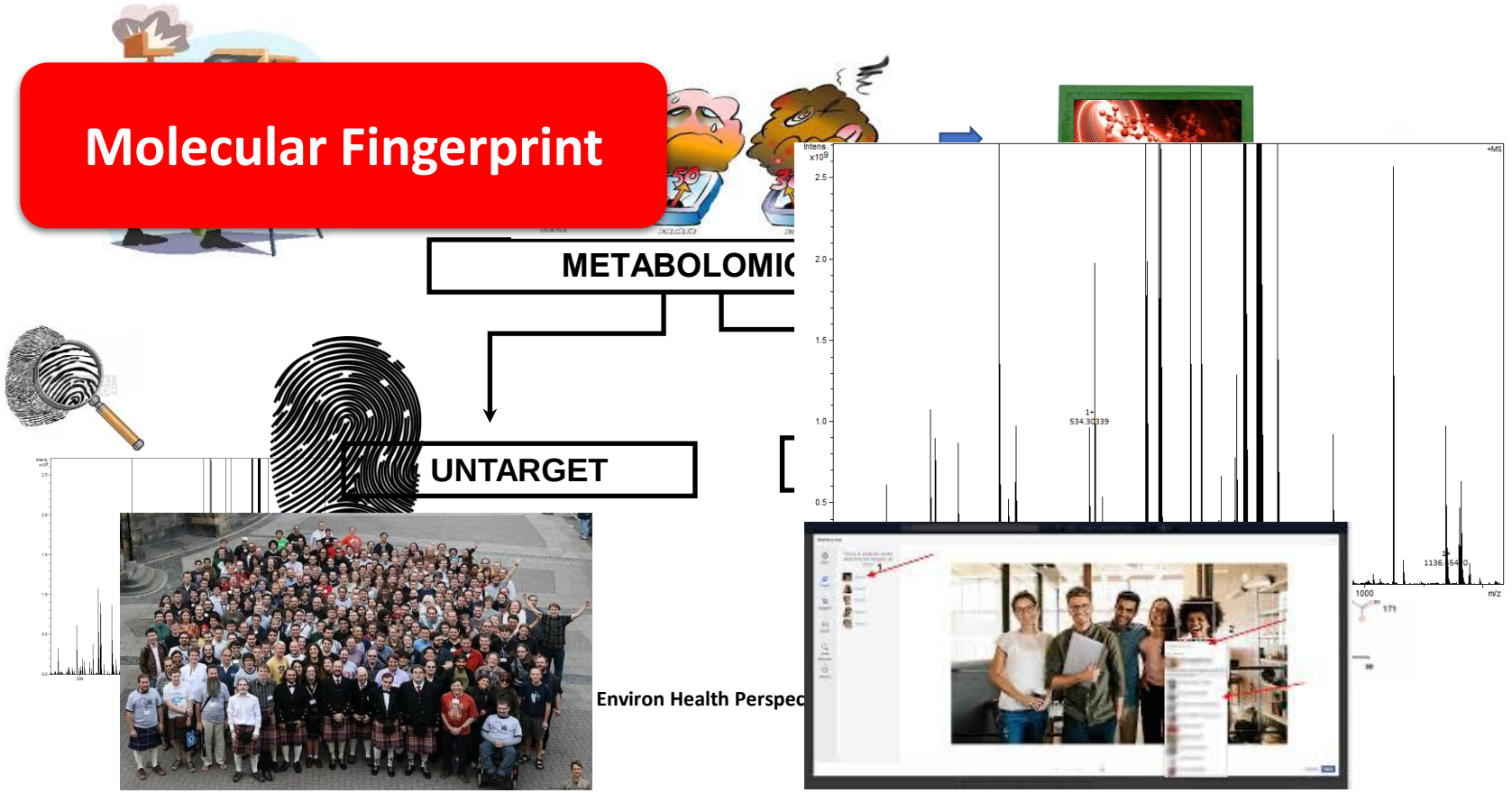




- Most common technique in Metabolomics
- High Specificity and Sensibility (~10^{-15} mol)
- Identification of different classes of Metabolites: **Untarget Analysis**
- Quantitative Analysis
- Coupling with Chromatographic techniques (GC-MS and LC-MS)

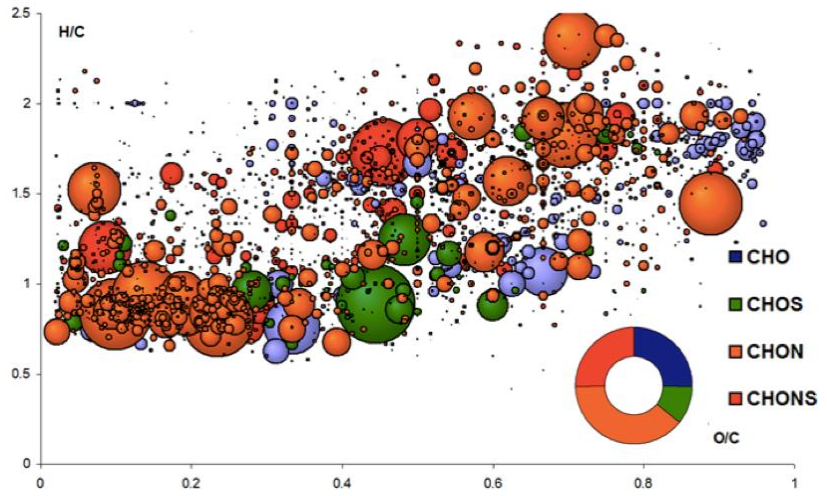
Zhentian Lei, David V. Huhman and Lloyd W. Sumner, *J. Biol. Chem.*
2011, 286, 25435-25442

METABOLOMICS



IMPRONTA DIGITALE MOLECOLARE

Composti	H/C	O/C
Acidi Grassi	1,4-2,3	0-0,3
Peptidi	1,0-2,4	0,2-0,8
Carboidrati	1,0-2,4	0,6-1,0
Polifenoli	0,4-1,4	0,2-0,7
Composti Condensati	0,5-1,2	0-0,4



Posizione dei punti = Formula Chimica
Atomi di Carbonio (C)
Atomi di Idrogeno (H)
Atomi di Ossigeno (O)

Kuhnert, N., Dairpoosh, F., Yassin, G., Golon, A., & Jaiswal, R. (2013). What is under the hump? Mass spectrometry based analysis of complex mixtures in processed food–lessons from the characterisation of black tea thearubigins, coffee melanoidines and caramel. *Food & function*, *4*(8), 1130-1147

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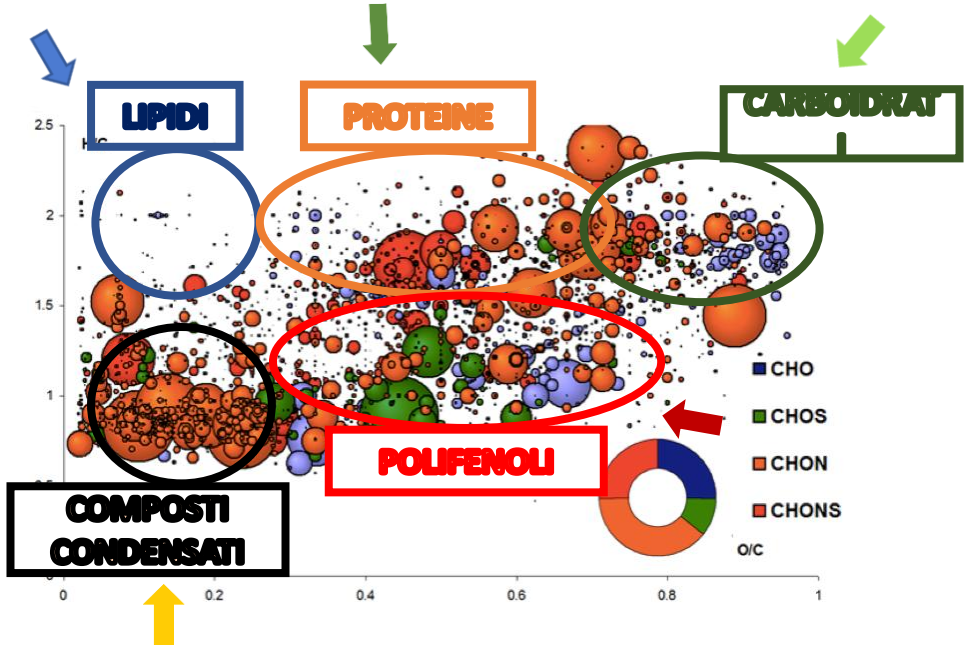
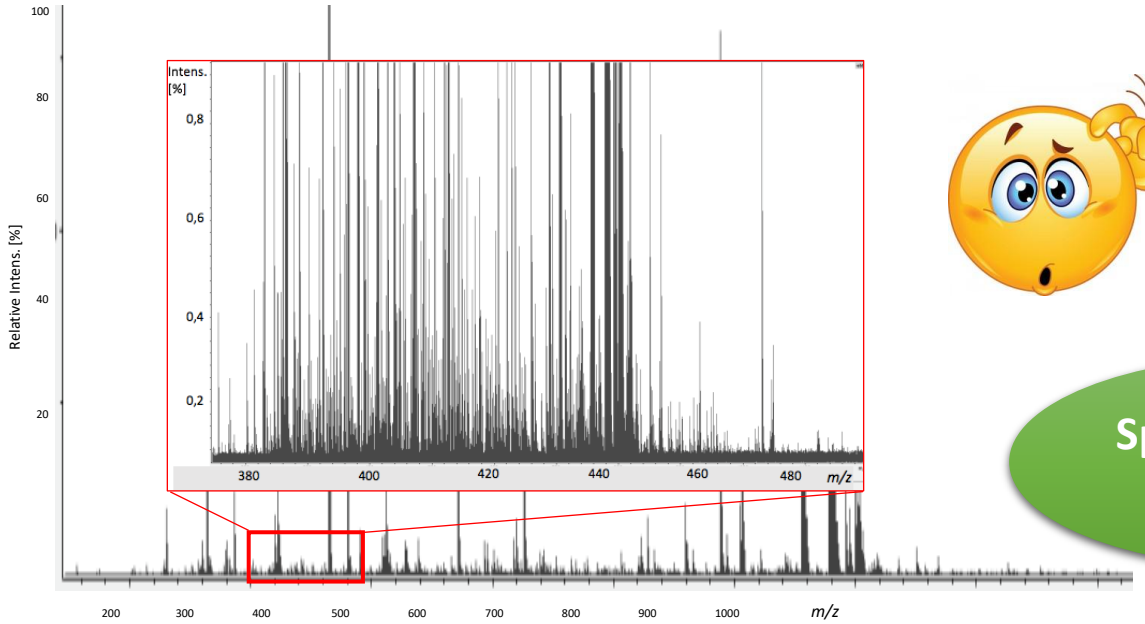


Kuhnert, N., Dairpoosh, F., Yassin, G., Golon, A., & Jaiswal, R. (2013). What is under the hump? Mass spectrometry based analysis of complex mixtures in processed food–lessons from the characterisation of black tea thearubigins, coffee melanoidines and caramel. *Food & function*, *4*(8), 1130-1147

ANALISI DEI METABOLITI



Spettrometro di Massa

Spettro di Massa ad Alta Risoluzione (HRMS)

Kuhnert, N., Dairpoosh, F., Yassin, G., Golon, A., & Jaiswal, R. (2013). What is under the hump? Mass spectrometry based analysis of complex mixtures in processed food–lessons from the characterisation of black tea thearubigins, coffee melanoidines and caramel. *Food & function*, *4*(8), 1130-1147

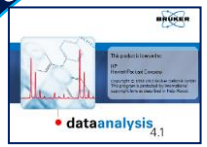
CALCOLO FORMULE CHIMICHE

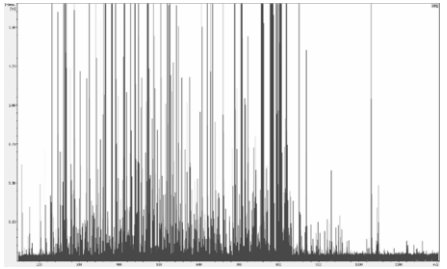
```
for(i in seq(1,length(Exp..m.z),1)){
  if(N[i]!=0 & S[i]!=0){
    x$HeteroClass[i]<-capture.output(cat(c("N",N[i],"S",S[i]), sep = ""))
  } else {
    if (N[i]!=0 & S[i]==0){
      x$HeteroClass[i]<-capture.output(cat(c("N",N[i]),sep = ""))
    } else {
      if (N[i]==0 & S[i]!=0){
        x$HeteroClass[i]<-capture.output(cat(c("S",S[i]),sep = ""))
      } else {
        if (N[i]==0 & S[i]==0){
          x$HeteroClass[i]<-c("CHO")
        }
      }
    }
```

```
vk_diagram<-function(z, manualcolors = c("blue","green","red", "yellow"), title =
                     gsize = FALSE, galpha = FALSE, widjitter = 0.1, xlabel = "O/
                     ylabel = "H/C", legend_title = "Type of Formula"){
  vkdiagram<-ggplot(data = z, aes(x = OC,y = HC))
  vkplot<-vkdiagram +
    geom_point(aes(color = Formula_type, size = Abundance, alpha = 0.5), position
    scale_colour_manual(legend_title, values = manualcolors) +
    scale_x_continuous(limits = c(0,1)) +
    scale_y_continuous(limits = c(0,2.5)) +
    scale_size(range = c(2,12), guide = gsize) +
    scale_alpha(guide = galpha) +
    theme_classic() +
    theme(axis.title.x = element_text(hjust = 1, face = "bold"),
          axis.title.y = element_text(hjust = 1, face = "bold")) +
    xlab(label = xlabel) +
    ylab(label = ylabel) +
    ggtitle(label = title)
```

```
for c in seq(1, maxC, 1){ #obviously our molecules contain at least 1 C and 1
    for h in seq(1, maxH, 1){ #Based on seven golden rules, a minimum/maximum
        hcrat = (h)/(c)
        if 0.2 < hcrat < 3.1:
            for p in seq(0, maxP, 1){
                for o in seq(1, maxO, 1){
                    ocrat = (o)/(c)
                    if ocrat < 1.2:
                        for n in seq(0, maxN, 1){
                            ncrat = (n)/(c)
                            if ncrat < 1.3:
                                for s in seq(0, maxS, 1){
                                    scrat = (s)/(c)
                                    rdbe = c - h/2 + n/2 + 1
                                    if (scrat < 0.8){
                                        if (rdbe > 0.5){ #Another constraint is a
                                            if (mode2 == "yes"){
```

Data analysis software

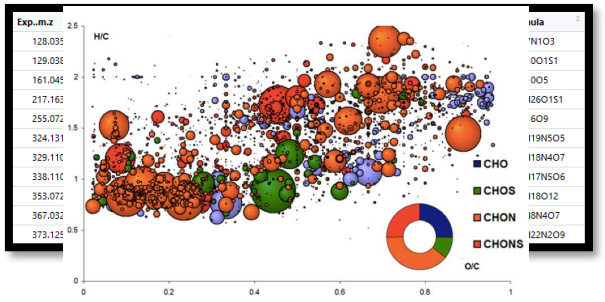




Spettro di massa ad Alta Risoluzione (HRMS)

R Studio

RStudio software



Kuhnert, N., Dairpoosh, F., Yassin, G., Golon, A., & Jaiswal, R. (2013). What is under the hump? Mass spectrometry based analysis of complex mixtures in processed food–lessons from the characterisation of black tea thearubigins, coffee melanoidines and caramel. *Food & function*, *4*(8), 1130-1147

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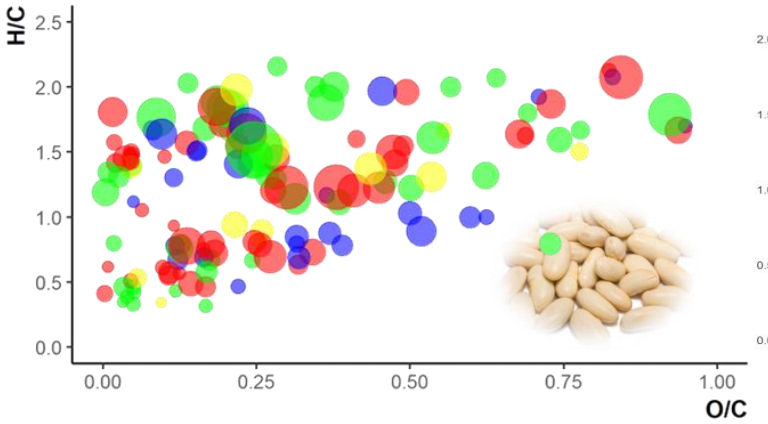
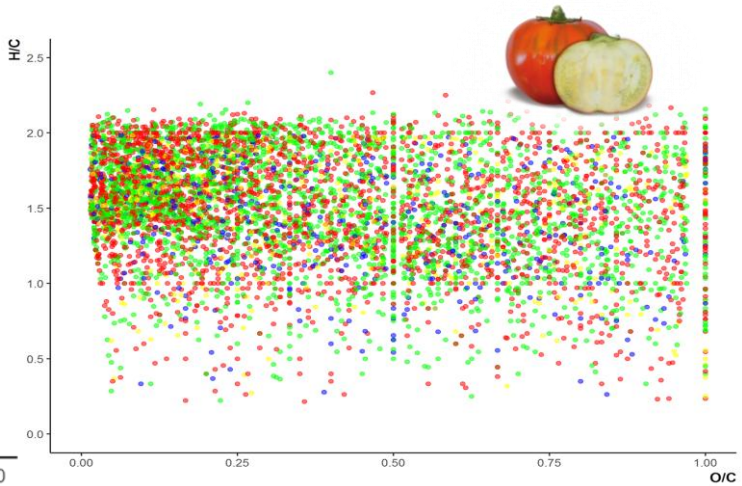
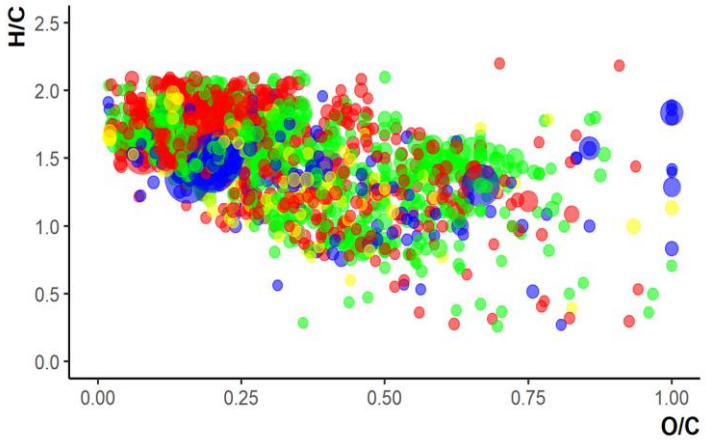
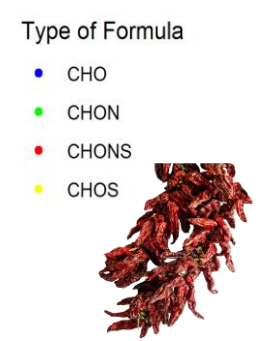
CARTOGRAFIA DEI PRODOTTI TIPICI LUCANI



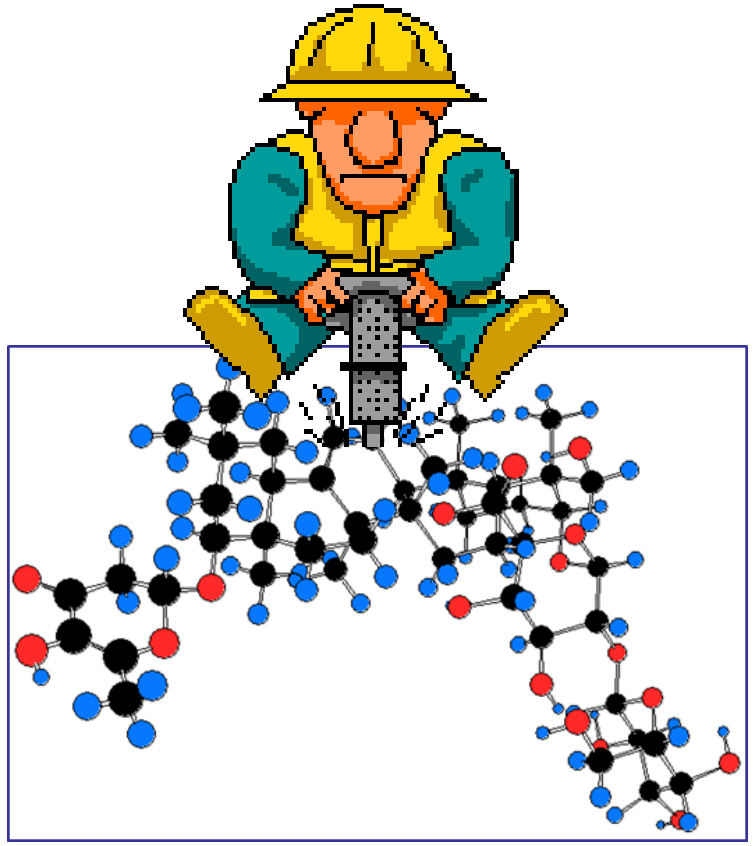


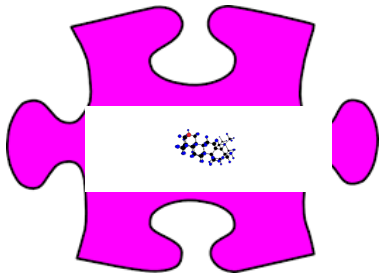


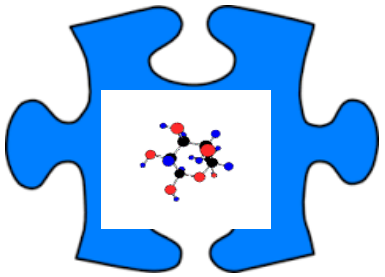


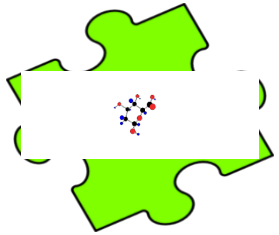
Kuhnert, N., Dairpoosh, F., Yassin, G., Golon, A., & Jaiswal, R. (2013). What is under the hump? Mass spectrometry based analysis of complex mixtures in processed food–lessons from the characterisation of black tea thearubigins, coffee melanoidines and caramel. *Food & function*, *4*(8), 1130-1147

Caratterizzazione strutturale TARGETED mediante MS/MS



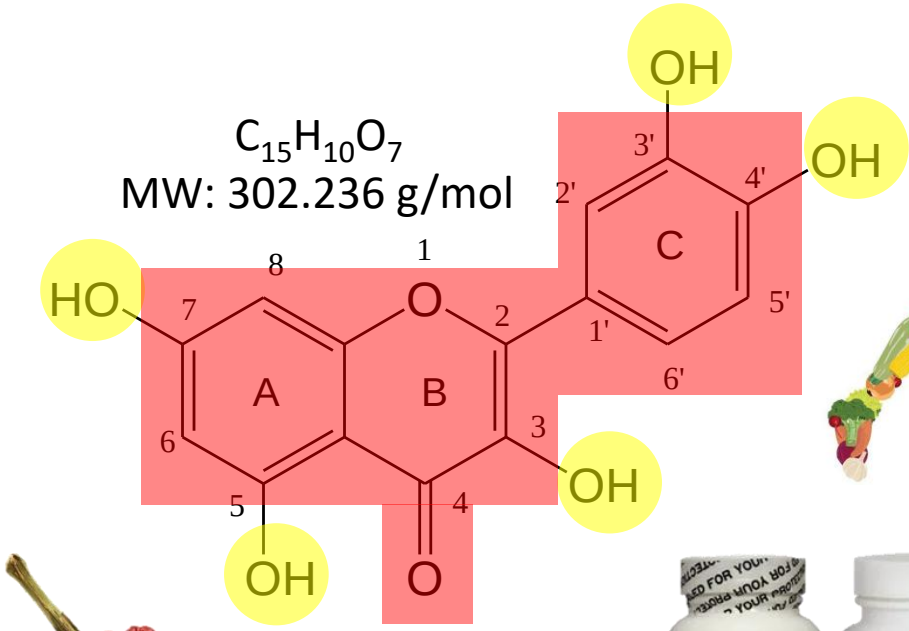


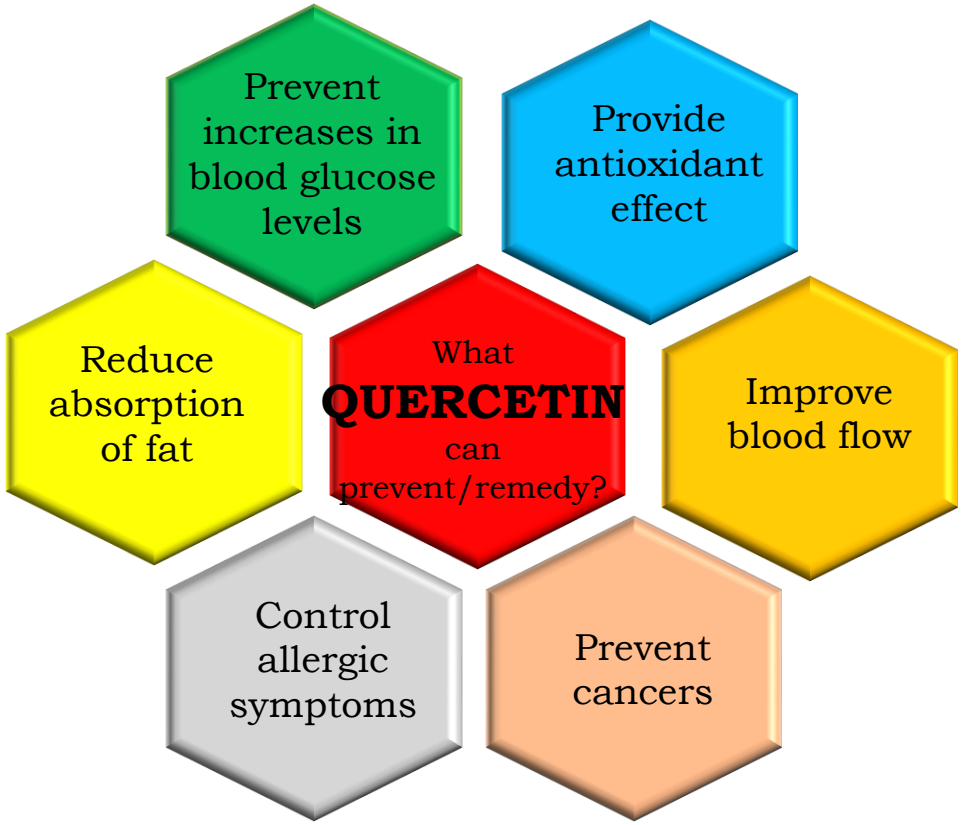




Giuliana Bianco

Identificazione TARGETED dei derivati della quercetina nei peperoni di Senise LC-ESI(-)-LTQ-MSMS





Giuliana Bianco

Identificazione TARGETED dei derivati della quercetina nei peperoni di Senise LC-ESI(-)-LTQ-MSMS

1.

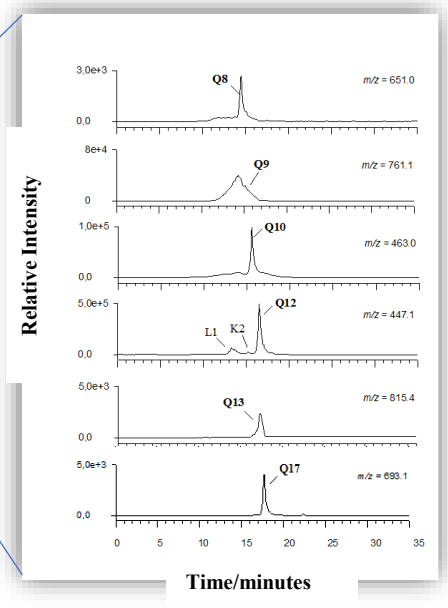
EXTRACTION

Extraction solvent:
MeOH 100%

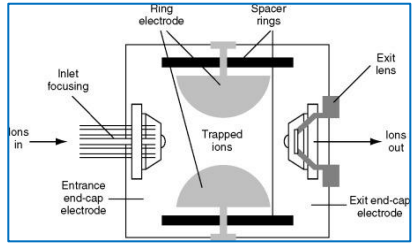
2.

LC SEPARATION

Luna-C18 (2) (150 × 4.6 mm, 3.0 µm)



3.

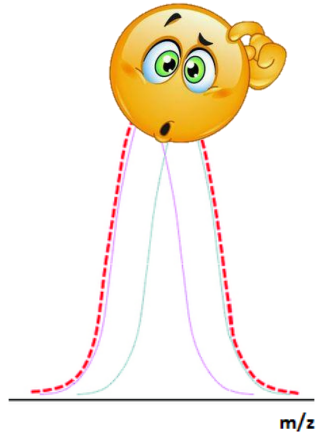


STRUCTURAL CHARACTERIZATION

ESI(-) Ionization
LTQ analyzer

Low-Resolution Mass spectrometry

- Resolving power < 10,000 at *m/z* 868.5
- Error > 5 ppm
- No accurate mass measurements



Pascale, R., Acquavia, M. A., Cataldi, T. R., Onzo, A., Coviello, D., Bufo, S. A., Bianco, G. (2020). Profiling of quercetin glycosides and acyl glycosides in sun-dried peperoni di Senise peppers (Capsicum annuum L.) by a combination of LC-ESI (-)-MS/MS and polarity prediction in reversed-phase separations. Analytical and Bioanalytical Chemistry, 1-11.

Giuliana Bianco