

# Foodomics, conceitos e perspectivas para alimentos e nutrição

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*Laboratório Multiusuário de Química de Produtos Naturais*

**Embrapa**



**SIAN**

Simpósio de Alimentos e Nutrição

**4ª EDIÇÃO**

Sustentabilidade e Inovação na Ciência dos Alimentos - Impacto na Bioeconomia

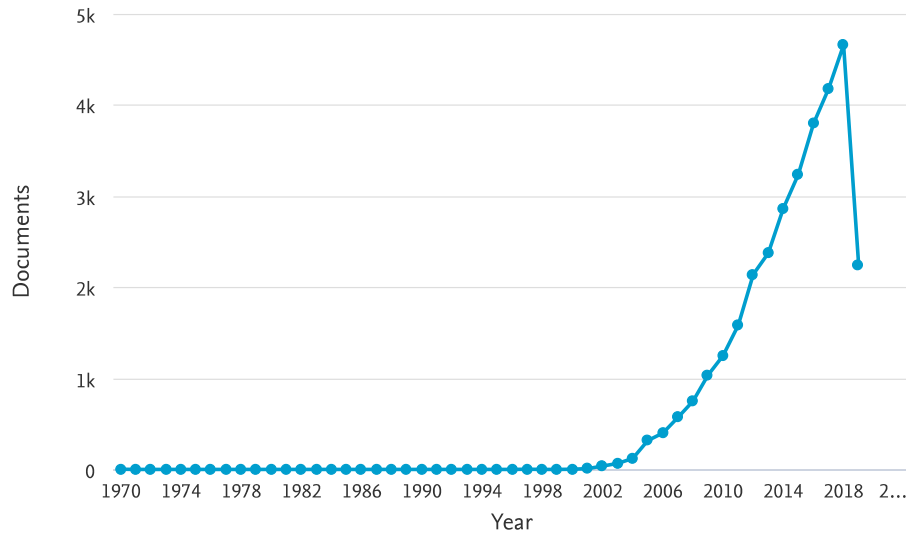
**17 E 18 DE JUNHO DE 2019**

# metabolomic

31,643 document results

Scopus junho 2019

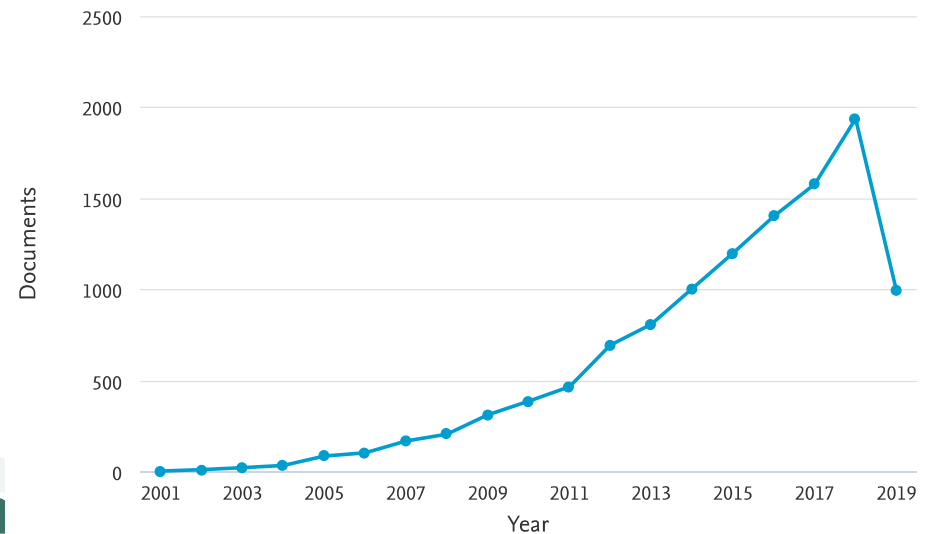
Documents by year



# metabolomic AND food

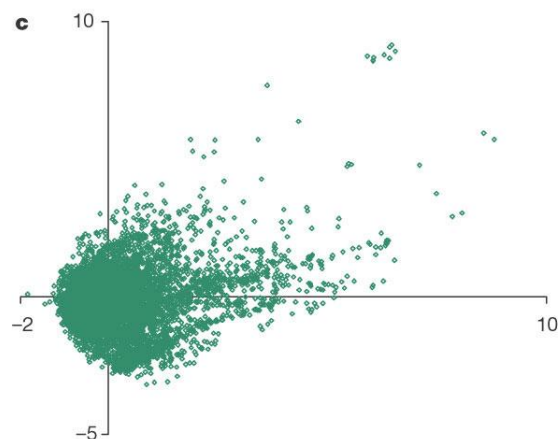
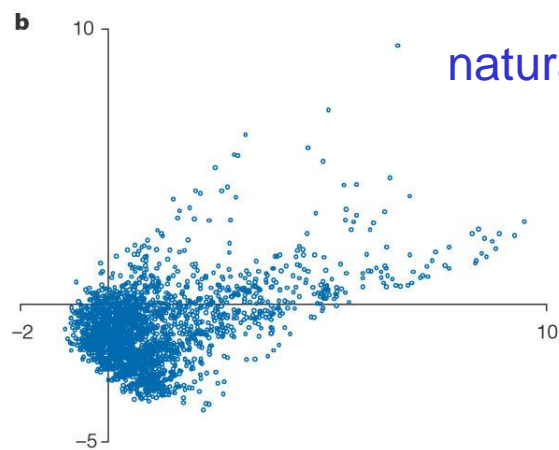
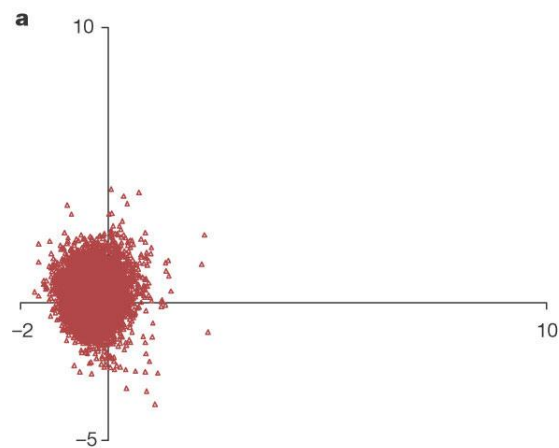
11,401 document results

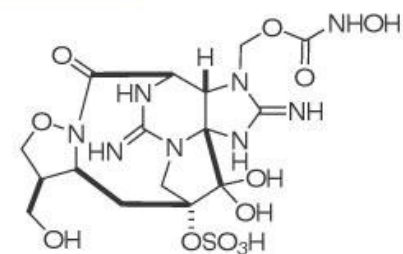
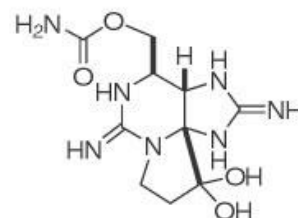
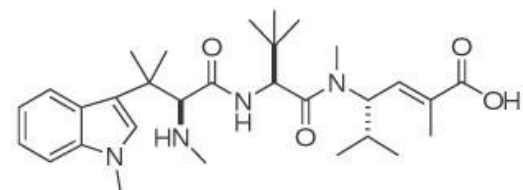
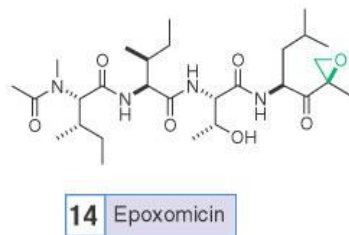
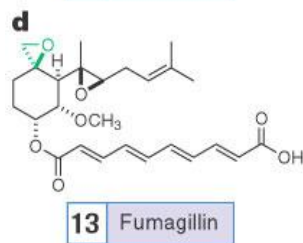
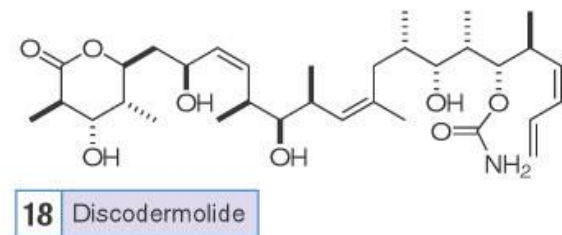
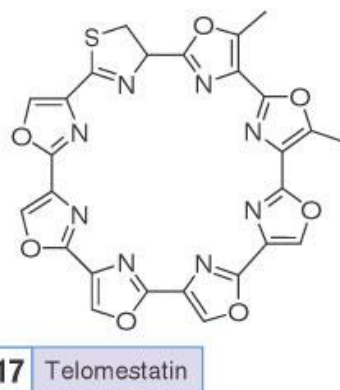
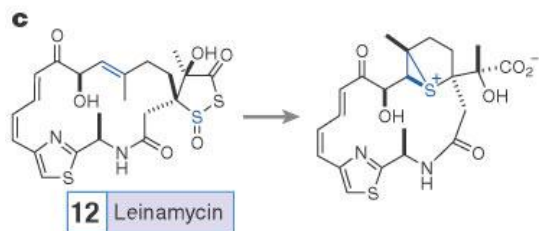
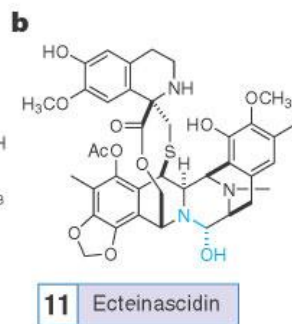
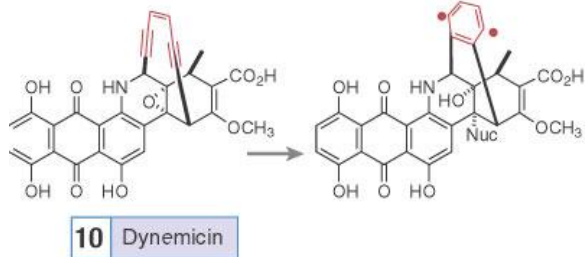
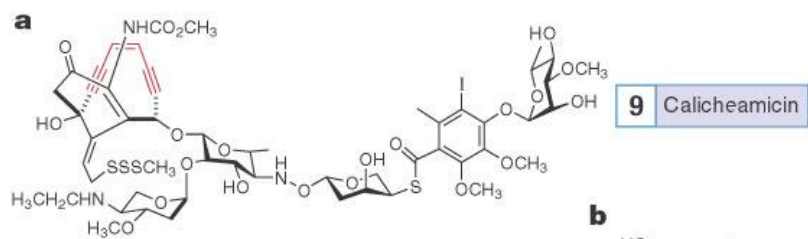
Documents by year



# Espaço Químico

basis of a variety of molecular properties





Molecular Plot

File



DATA SOURCES

Abbott kinase dataset

PLOTS

FLT1 vs FLT3

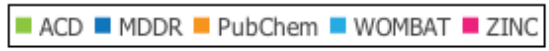
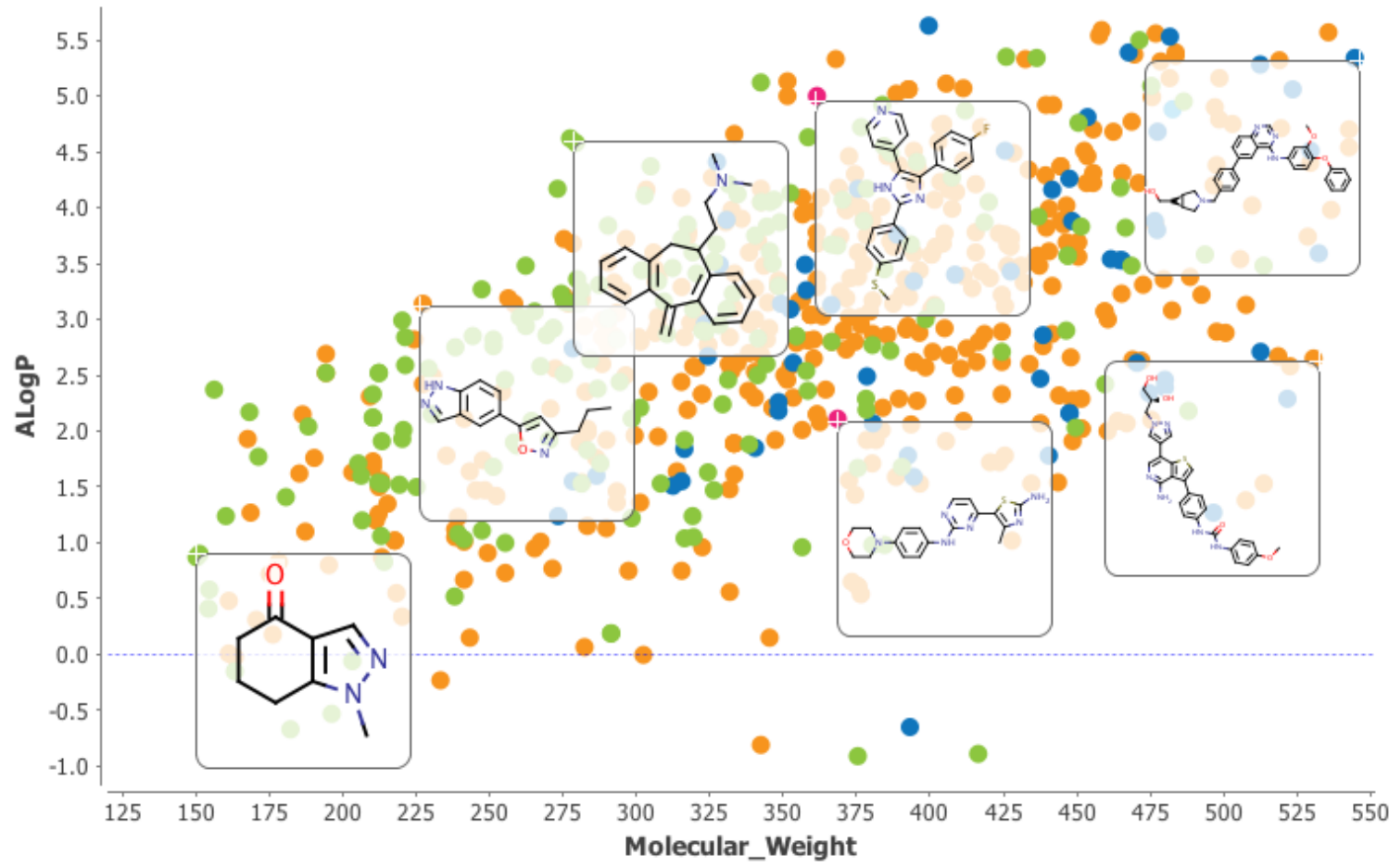
**AlogP vs MWT**

AKT1 vs AKT2

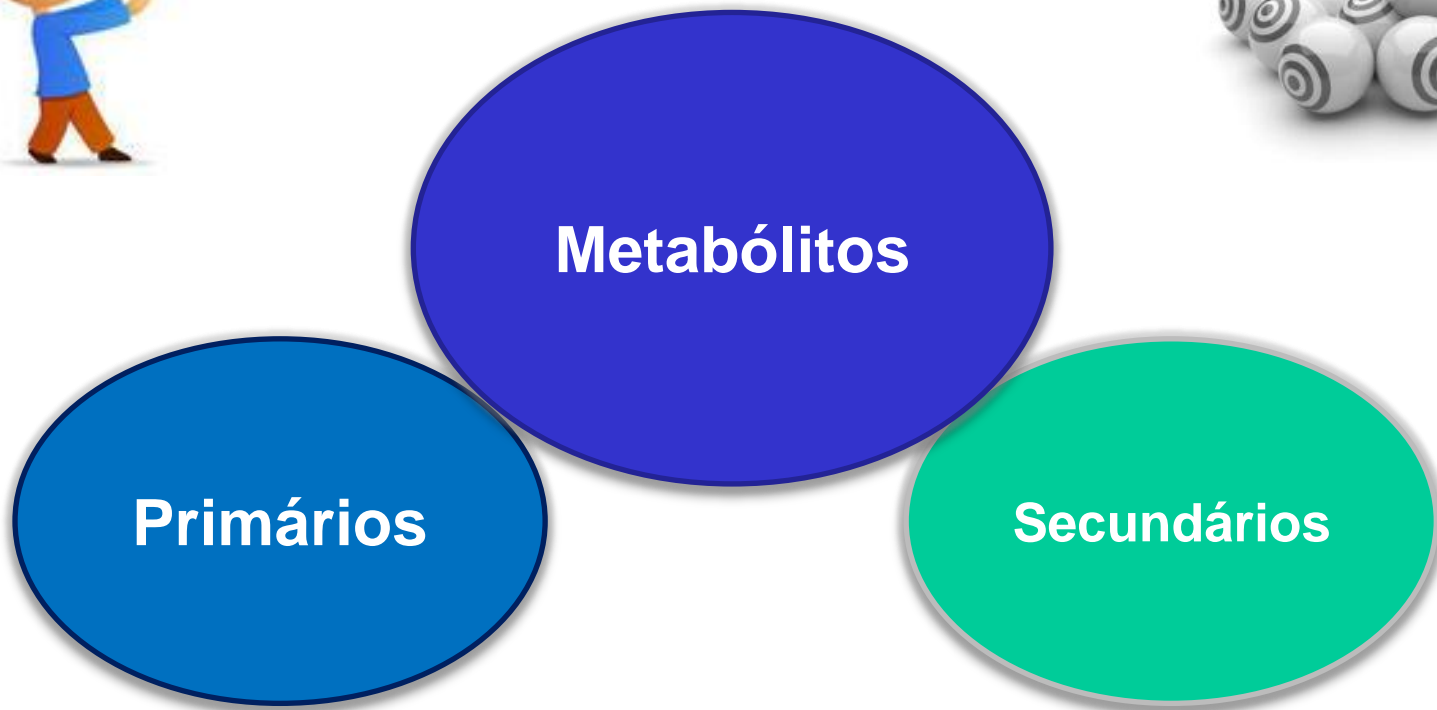
JAK2 vs JAK3

DYRK1A vs DYRK1B

**AlogP vs MWT**



# Metabolômica



Lipídeos, açúcares,  
Amino ácidos

Polifenóis, alcaloides,  
NRP, terpenos, etc





Metabolomica



*Foodomics*—a discipline that studies the food and nutrition domains through the application of advanced omics technologies to improve the consumer's well-being, health, and knowledge.

Cinfuentes, 2009





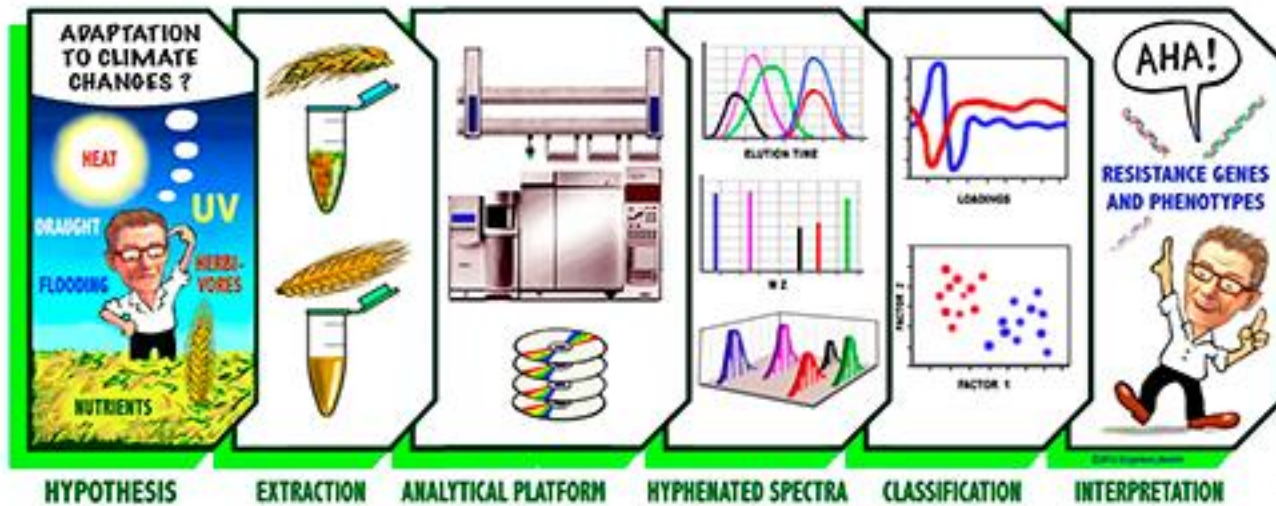
**Foodomics** é uma disciplina que **examina todo o conjunto de substâncias** presentes em nossos alimentos (foodome). A disciplina utiliza **plataformas analíticas avançadas** para investigar a composição do alimento e, assim, suas propriedades nutricionais e impacto na saúde.

As novas técnicas também fornecem uma imagem detalhada da **qualidade dos alimentos** e podem ser usadas para detectar fraudes em alimentos e encontrar **soluções** para outros **desafios** na produção de alimentos. Os resultados de pesquisas de foodomics têm um impacto direto sobre os consumidores, a indústria de alimentos e a sociedade.

Engelsen

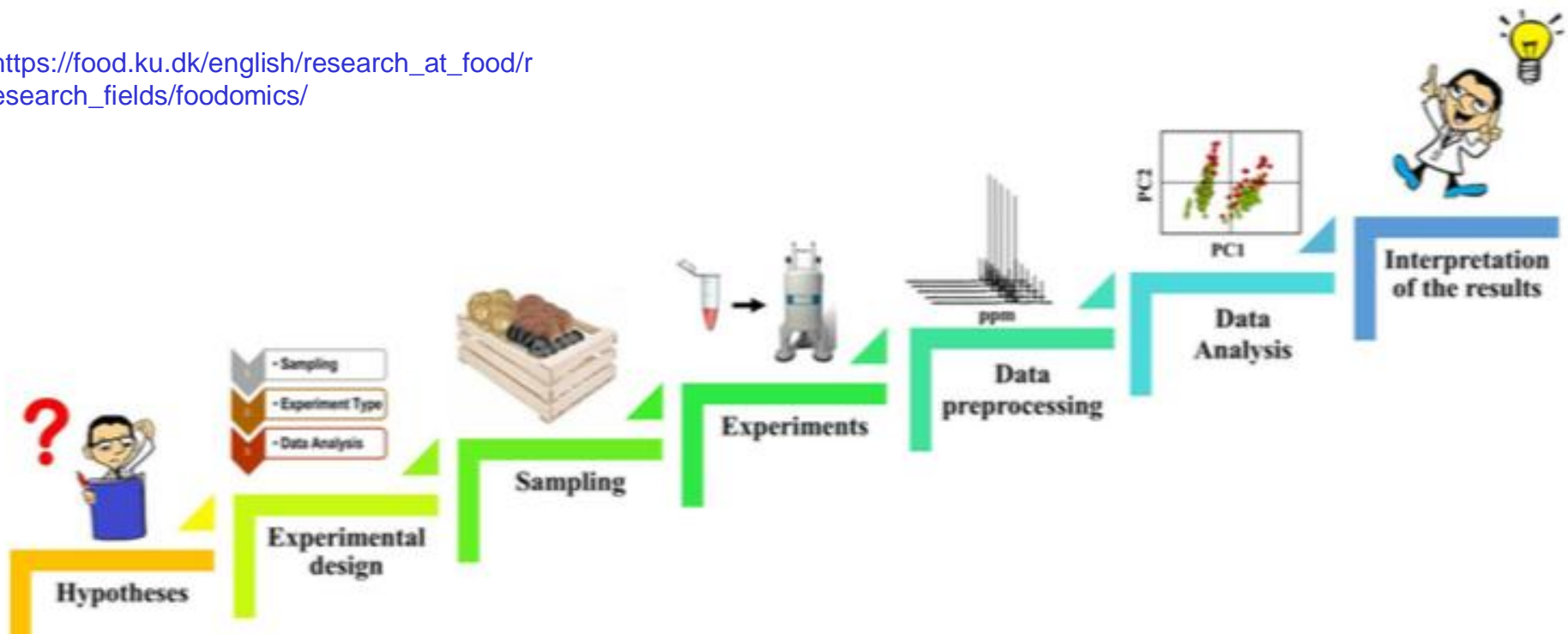
([https://food.ku.dk/english/research\\_at\\_food/research\\_fields/foodomics/](https://food.ku.dk/english/research_at_food/research_fields/foodomics/))





Foodomics. Illustration by Søren B. Engelsen and Tim Newlin ©

[https://food.ku.dk/english/research\\_at\\_food/research\\_fields/foodomics/](https://food.ku.dk/english/research_at_food/research_fields/foodomics/)





fingerprint



Metabolite Profile

© topendsports.com



**Table 1. Main Features of Most The Popular Techniques for Metabolomics**

technique	CE-MS	GC-MS	LC-MS	NMR 1D	NMR 2D
universality	++	+	+ / ++	+++	+++
accuracy	- / ++ <sup>a</sup>	- / ++ <sup>a</sup>	- / ++ <sup>a</sup>	+++	+++
reproducibility	++ / - <sup>a</sup>	++ / - <sup>a</sup>	++ / - <sup>a</sup>	+++	+++
sensitivity	+	++ / +++ <sup>a</sup>	+++	-	-
resolution	++	+++	+++	+	++
efficiency	++	-	+	++	++

<sup>a</sup>Accuracy, repeatability, and sensitivity mainly depend on the analyzer. GC-MS and LC-MS are usually performed either with a quadrupole or time-of-flight analyzer. “+” or “-” in front of and behind “/” represent quadrupole and time-of-flight analyzer, respectively.

ABORDAGEM?

COMPOSTOS

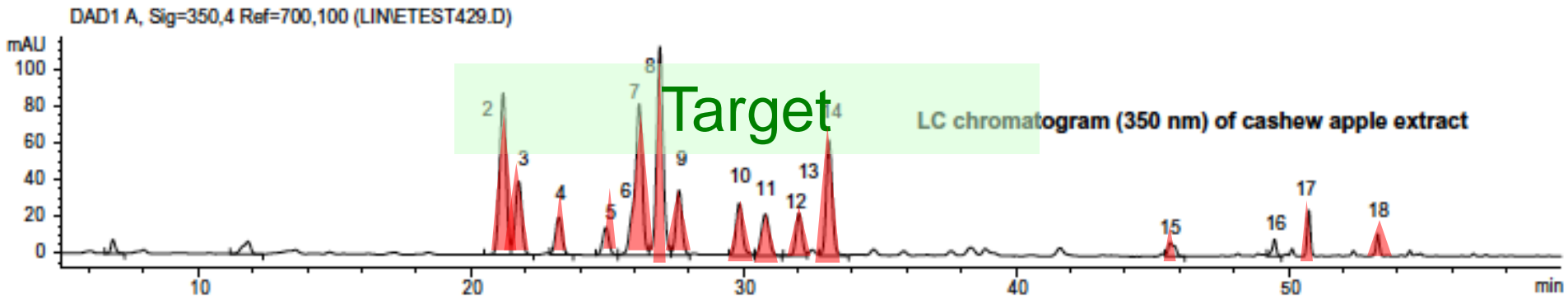
ALVO

NÃO ALVO

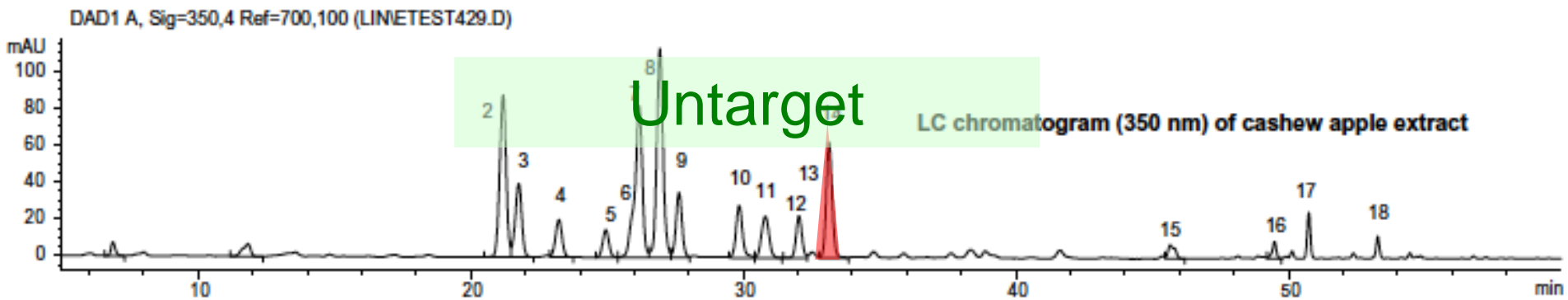




## Caracterização completa e quantificação



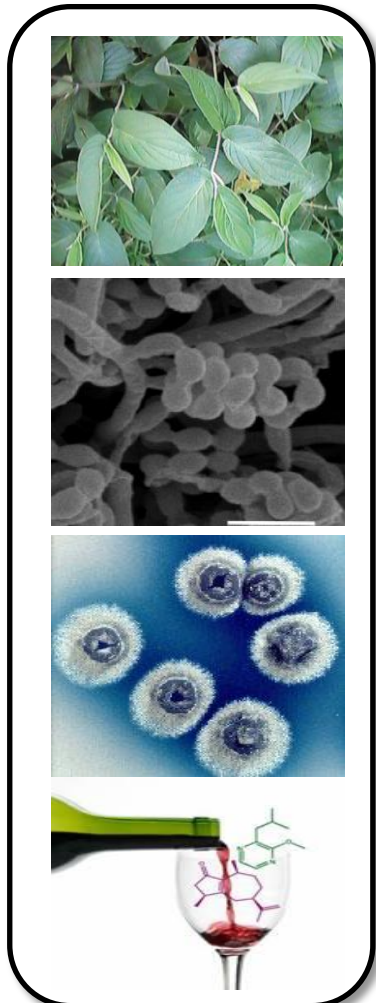
## Definição de marcadores e sua posterior quantificação



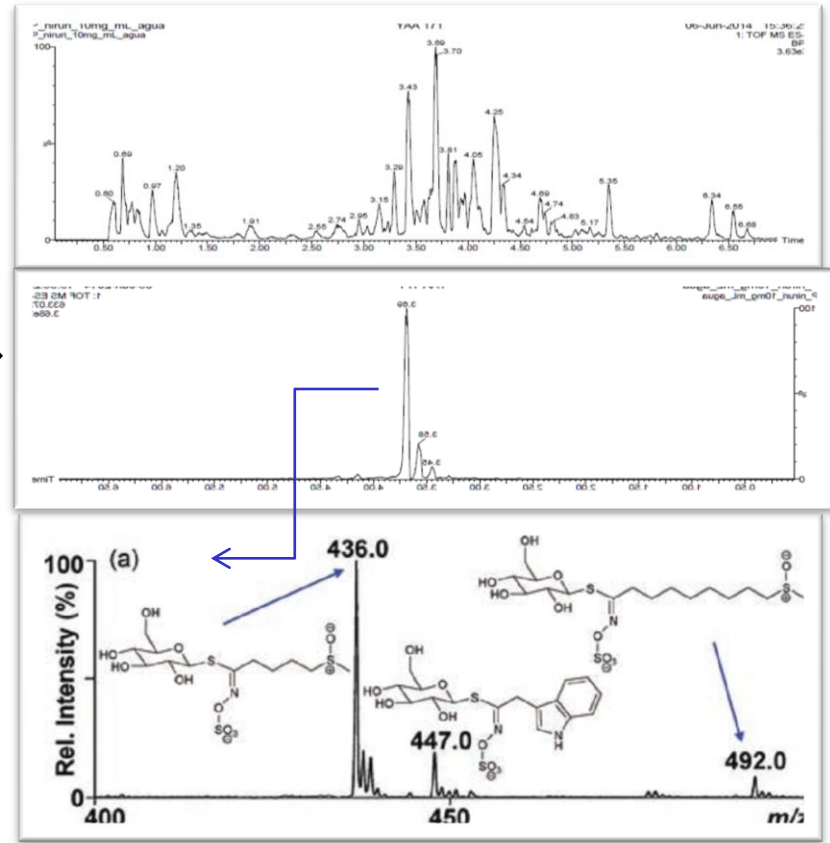
Como fazer? Plataformas analíticas + quimiometria



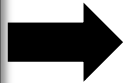
# Instrumentação: UPLC – QTOF – MS/MS



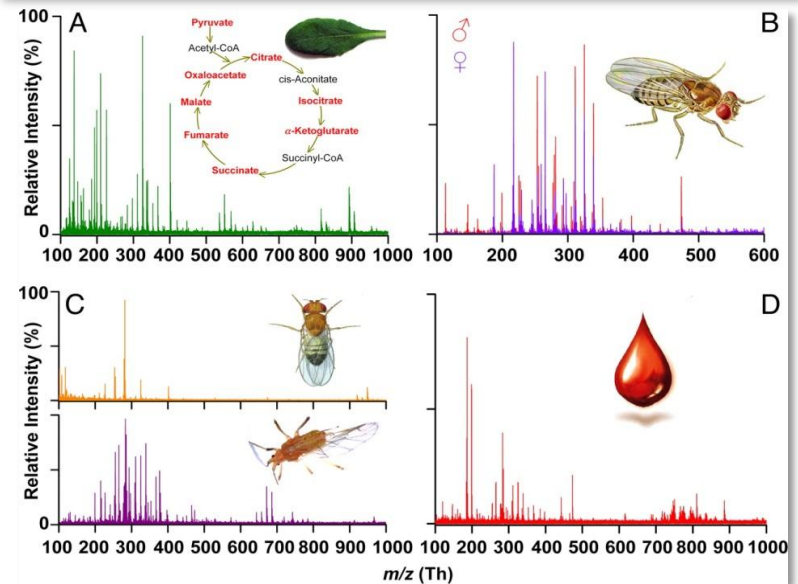
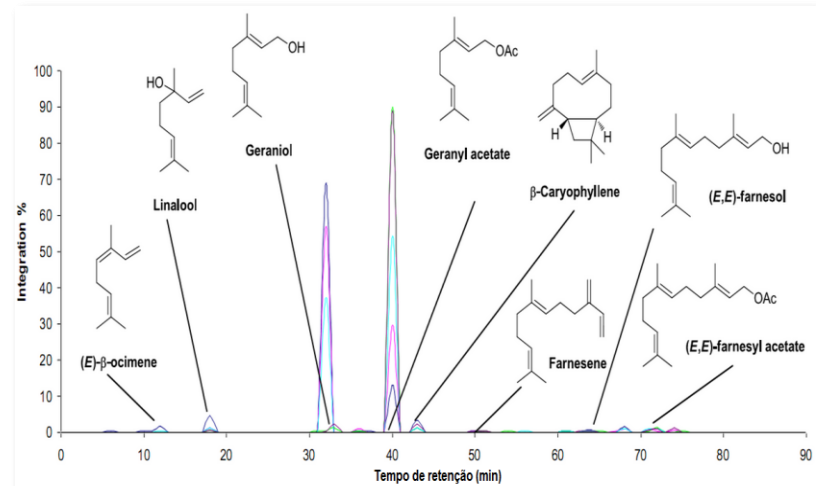
**Agumas aplicações:**  
**Produtos naturais -**  
**Insumos agroindustriais**  
**Determinação estrutural de**  
**substâncias de origem vegetal,**  
**animal e de microorganismos**



# Instrumentação: GC-MS/MS



**Algumas aplicações:**  
Análises de aromas de vinhos  
Óleos essenciais  
Feromônios  
Estudos de ecologia química



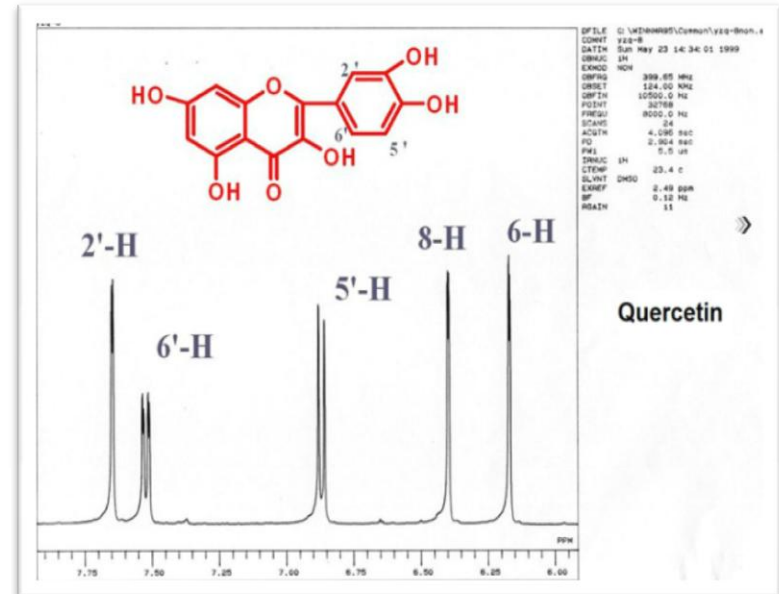
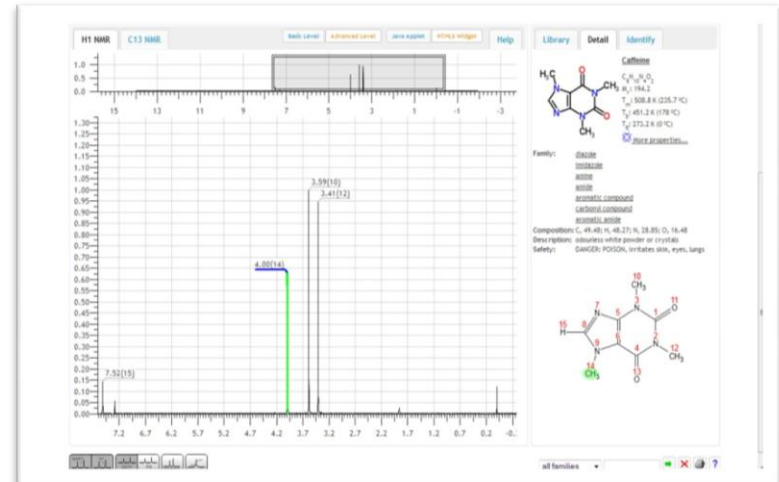
# Instrumentação: Ressonância Magnética Nuclear (RMN)



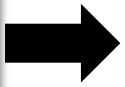
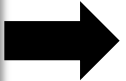
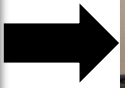
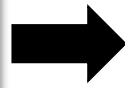
Sistema de detecção universal

Estudos de Metabolômica e Elucidação estrutural

Quantificação sem necessidade de padrões analíticos

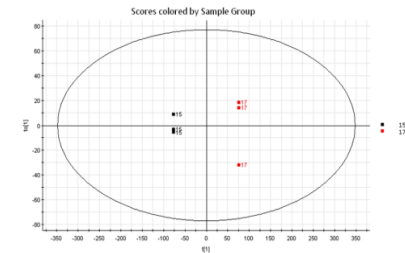






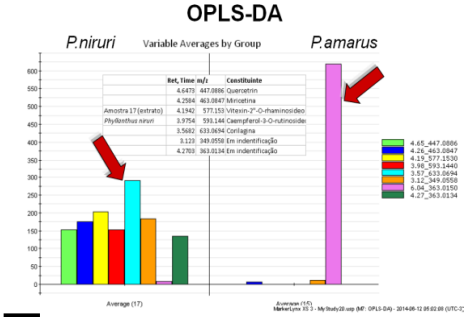
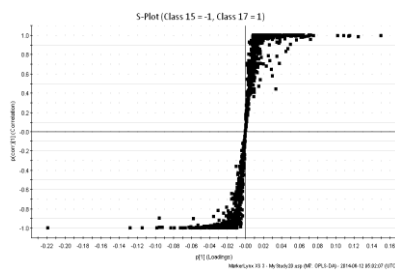
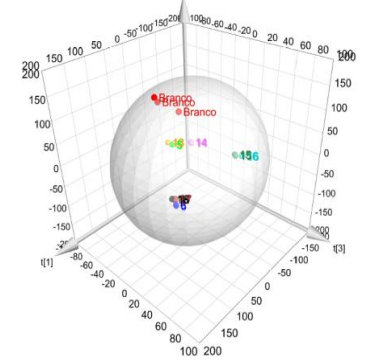
# Métodos Quimiométricos

## Análise de Componentes Principais (PCA)

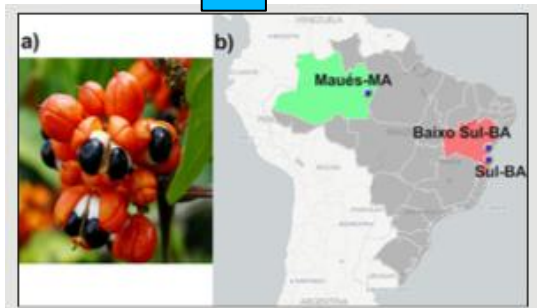


Amostra 17 - P.niruri, Exp. II 1 colheita (8 Hrs)  
Amostra 15 - P.amarus, Exp. II 1 colheita (8 Hrs)

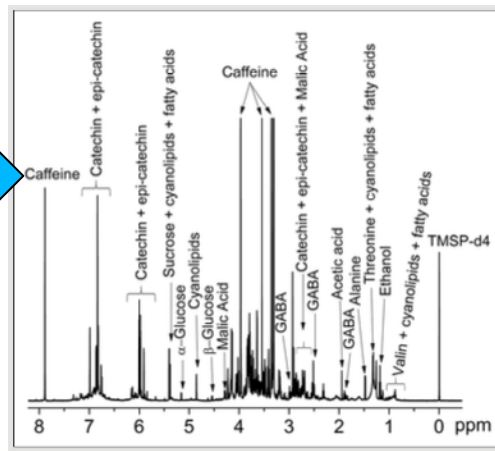
Scores Comp[1] vs. Comp[3] vs. Comp[2]. colored by Sample Group



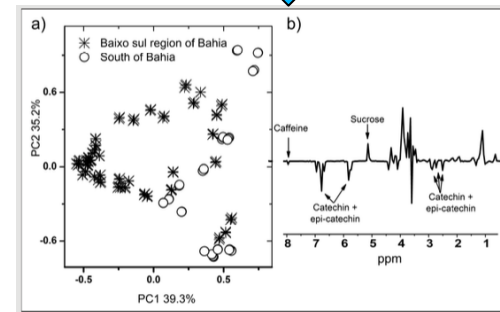
**Determinação de Biomarcadores**  
**Interpretação de grande volume de dados**



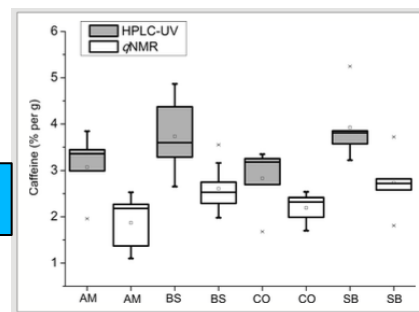
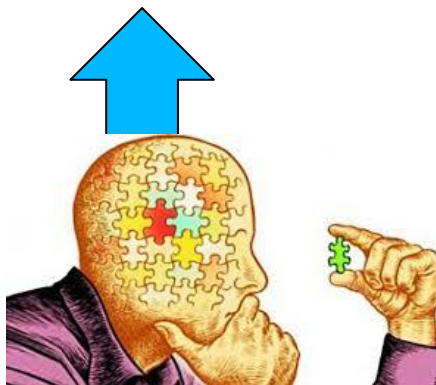
Sample set



fingerprint



chemometrics



quantitation

# Exemplos

**Processos:** térmicos e não térmicos

**Qualidade:** procedência geográfica, estágio de maturação

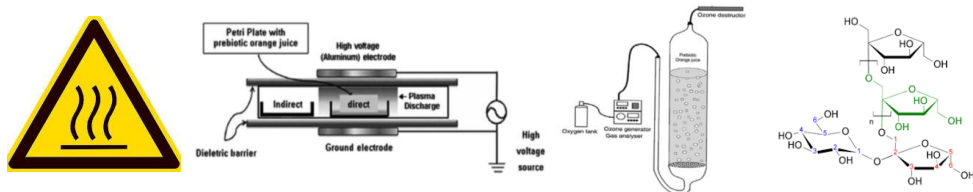
**Melhoramento genético:** feijão caupi, caju

**Nutrição:** fibra alimentar obesidade

**Amostra:** Sucos laranja, maracujá, melão, caju, acerola, água de coco



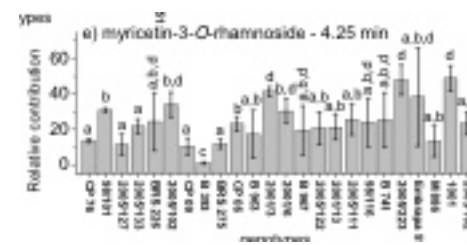
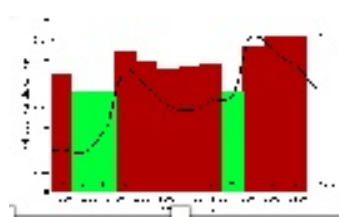
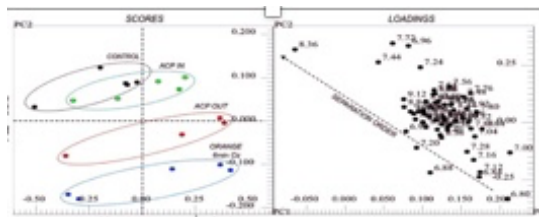
**Processamento:** térmicos (HTST e UHT), Plasma e O<sub>3</sub>, pré e probióticos



**Análise:** RMN <sup>1</sup>H, GC-MS, UPLC-MS, NIR



**Quimiometria:** PCA, OPLS-DA e quantificação (qNMR)

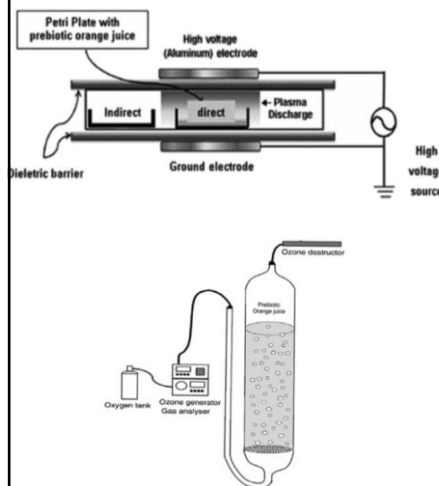


# Como os processos não térmicos afetam a composição do suco de laranja?

**Amostra:**  
Suco laranja



**Processamento:**  
Plasma e O<sub>3</sub>



**Plataforma:**  
GC-MS, RMN



**Quimiometria:**  
HCA + PCA

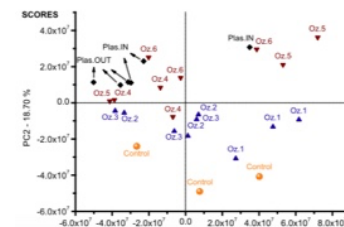
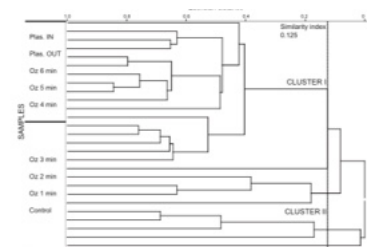
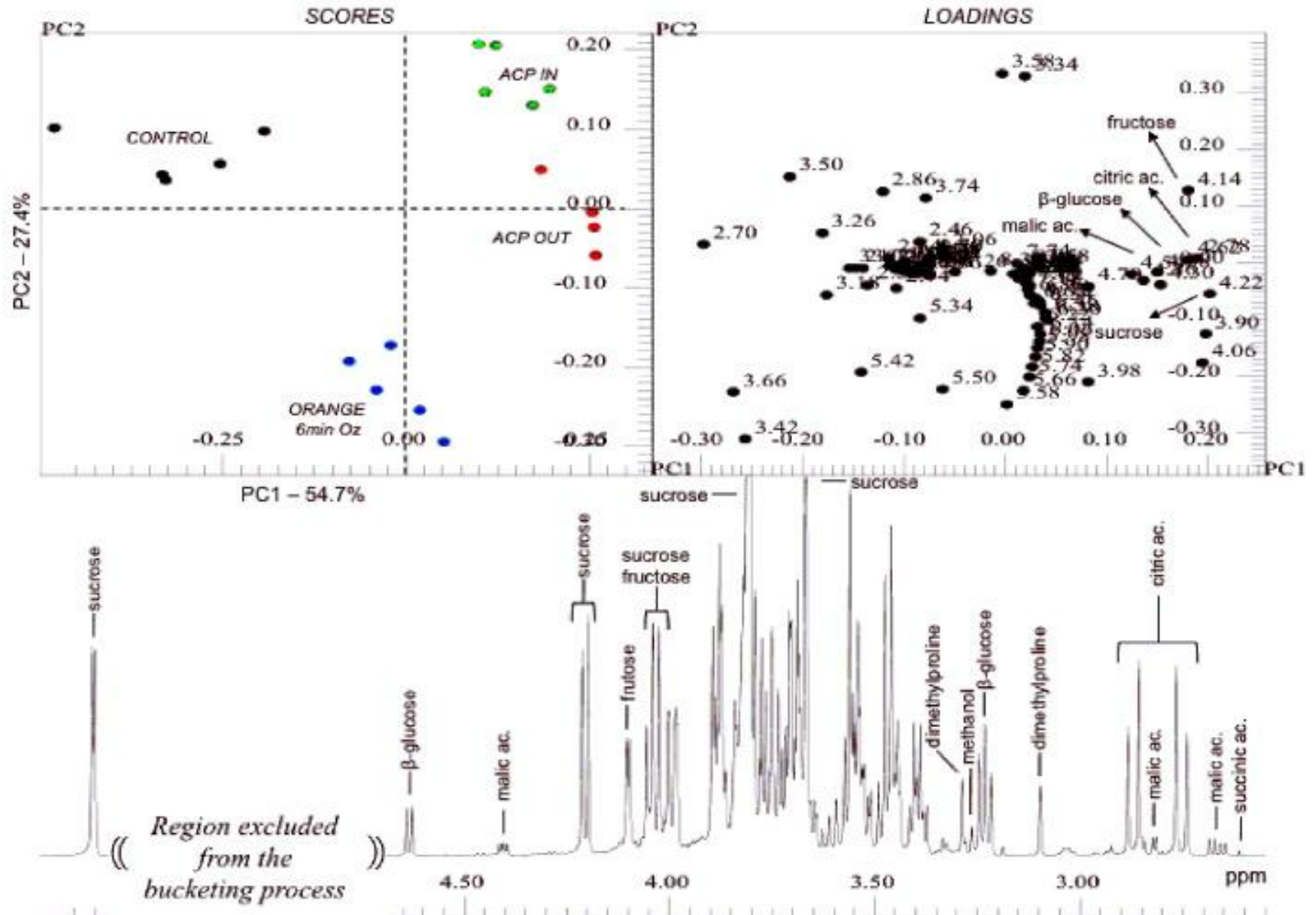
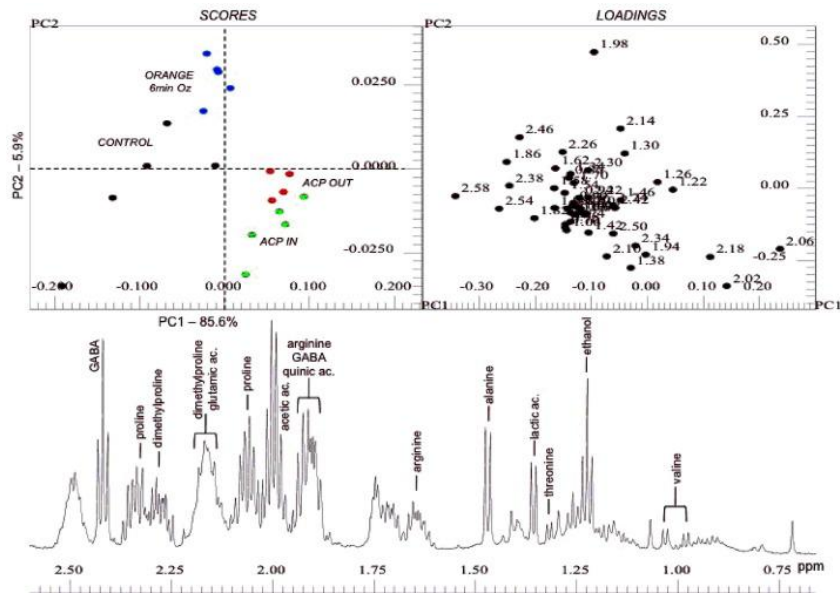




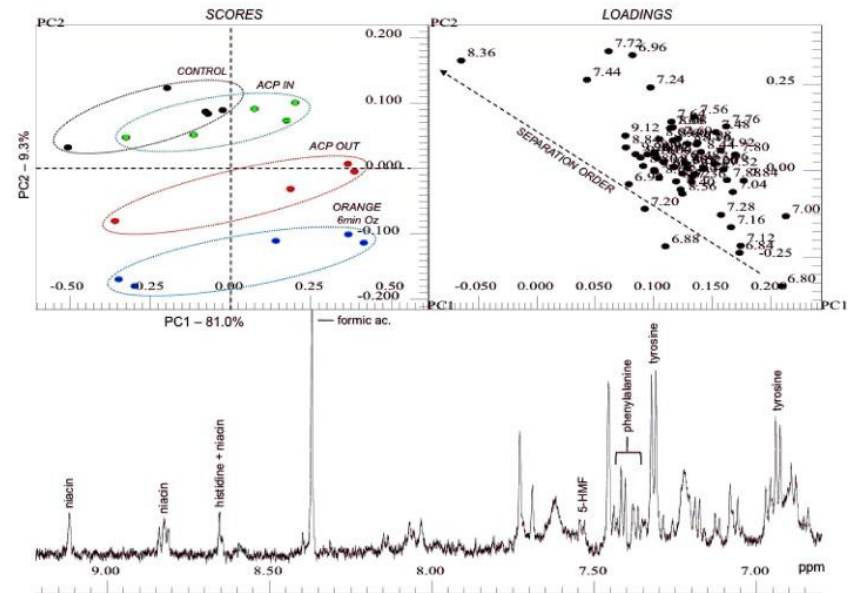
Fig. 1.  $^1\text{H}$  NMR spectrum (C), PC1 vs. PC2 scores (left side – A) and loadings (right side – B) coordinate system for the orange juice submitted to different processing: control – black; 0.230 mg  $\text{O}_3 \text{ mL}^{-1}$  – blue; ACP IN – green; ACP OUT – red

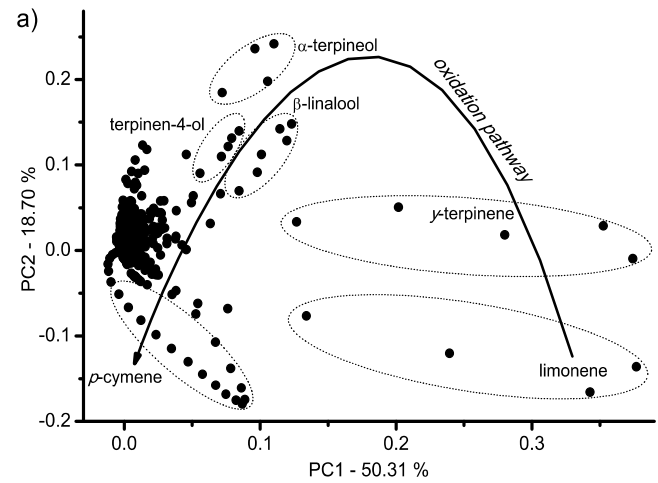
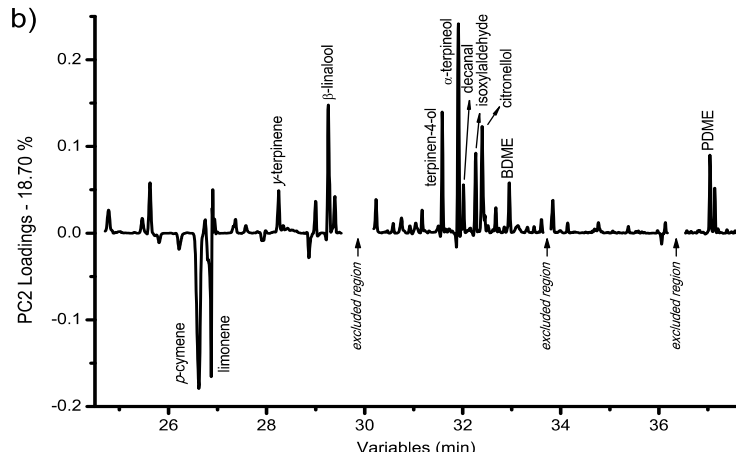
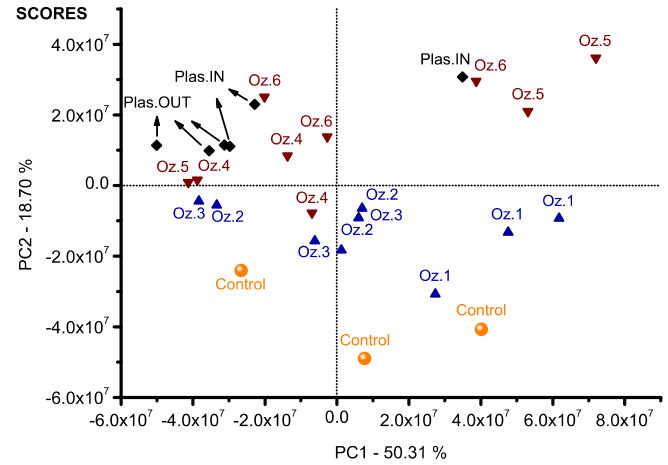
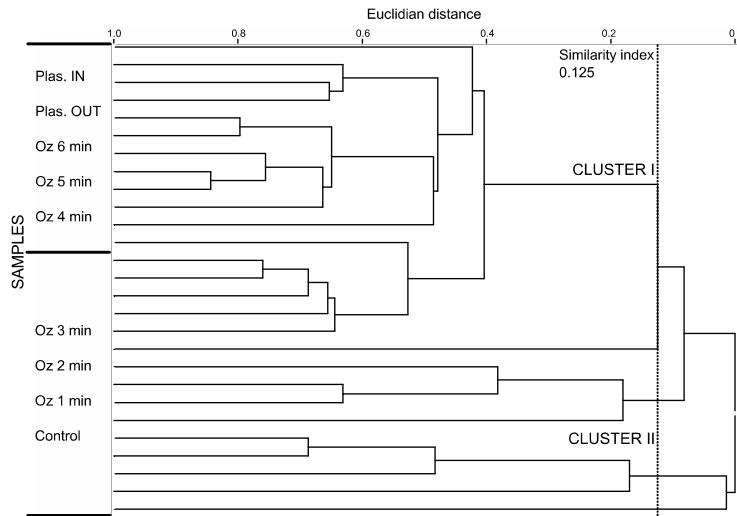


## Região alifáticos



## Região aromáticos



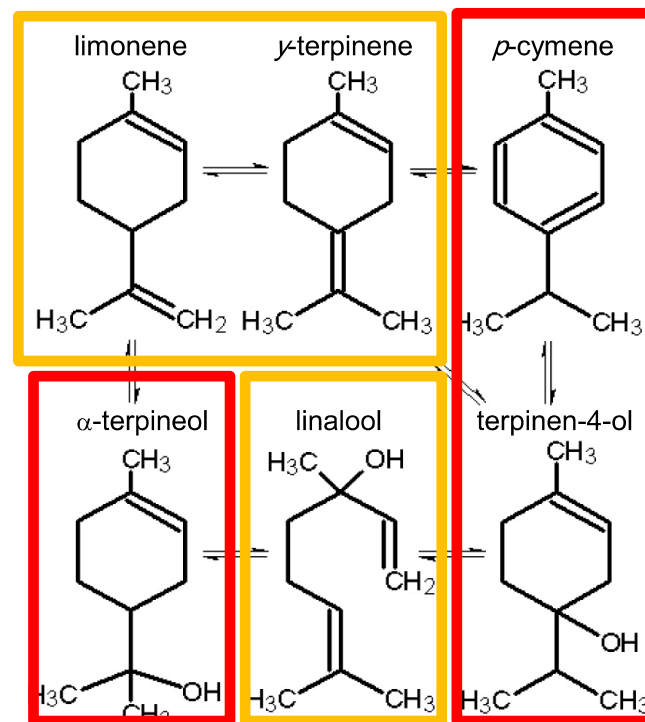


**Table 2**

Variations in the concentrations of the volatile compounds after different non-thermal processing of orange juices (Cluster I: 1 to 3 min of ozone); Cluster II (4 to 6 min of ozone, and plasma IN and OUT).

Volatile compounds	Cluster I	Cluster II	Characteristic marker	References
Limonene	- 0.1	- 12.5	Flavor	(Silva et al., 2012)
<i>p</i> -Cymene	- 36.0	- 60.5	Off-flavor	(Perez-Cacho & Rouseff, 2008)
$\gamma$ -Terpinene	+ 25.1	+ 14.5	Flavor	(Moshonas & Shaw, 1994)
Linalool	+ 40.7	+ 64.8	Flavor	(Högnadóttir & Rouseff, 2003)
$\alpha$ -Terpineol	+ 54.9	+ 113.5	Off-flavor	(Selli et al., 2004)
Terpinen-4-ol	+ 53.4	+ 99.4	Off-flavor	(Schieberle & Grosch, 1988)
Decanal	+ 144.5	+ 265.0	Flavor	(Arena et al., 2006)

\* Symbol “+” represent “increase”; and “-” represent “decrease”.



**Fig. 5.** Proposed oxidation, hydrolysis and reduction of terpenes under plasma and ozone processing of orange juice.



- **Conclusões**

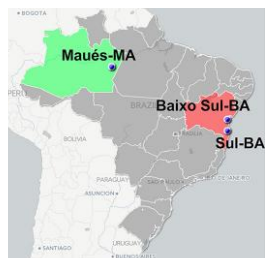
- Os processos tiveram pequeno efeito na composição do suco.
- As variações não resultaram em mudanças significativas na composição.
- Plasma e ozônio afetaram o perfil de voláteis do suco de laranja.
- A oxidação de limoneno,  $\gamma$ -terpineno e linalool levaram a  $\alpha$ -terpineol e terpinen-4-ol (off-flavors).
- Terpenos podem ser usados como marcadores para a avaliação de processos não térmicos.

# Existe diferença na composição do guaraná provenientes da BA e do AM?

**Amostra:**  
Guaraná



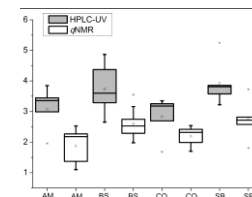
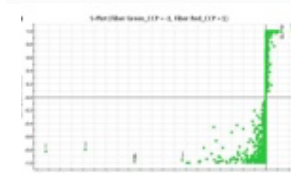
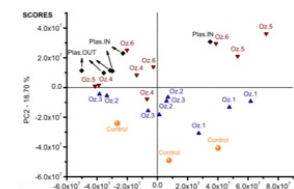
**Origem:**  
BA e AM



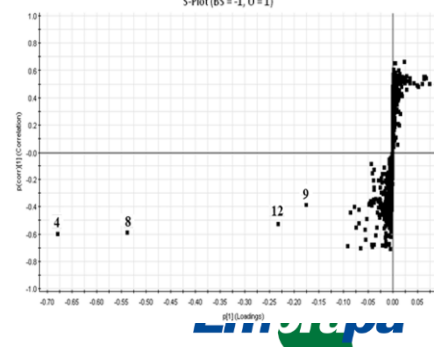
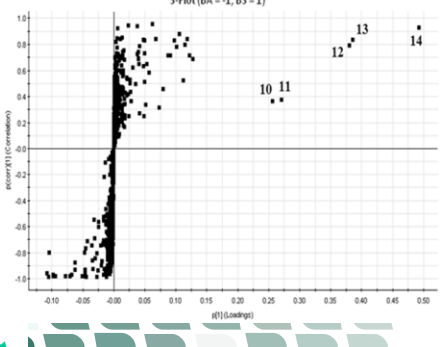
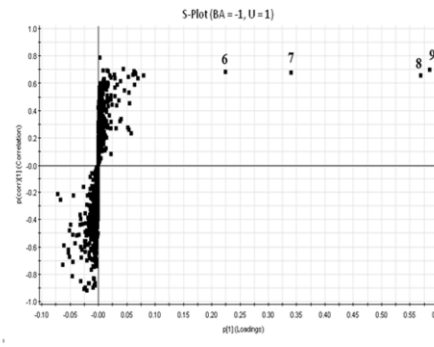
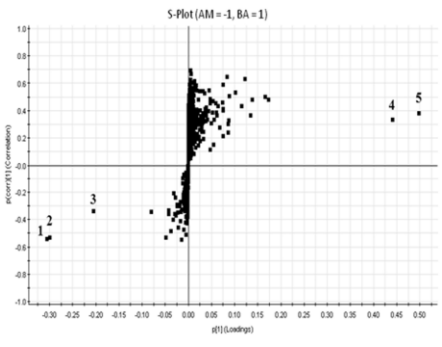
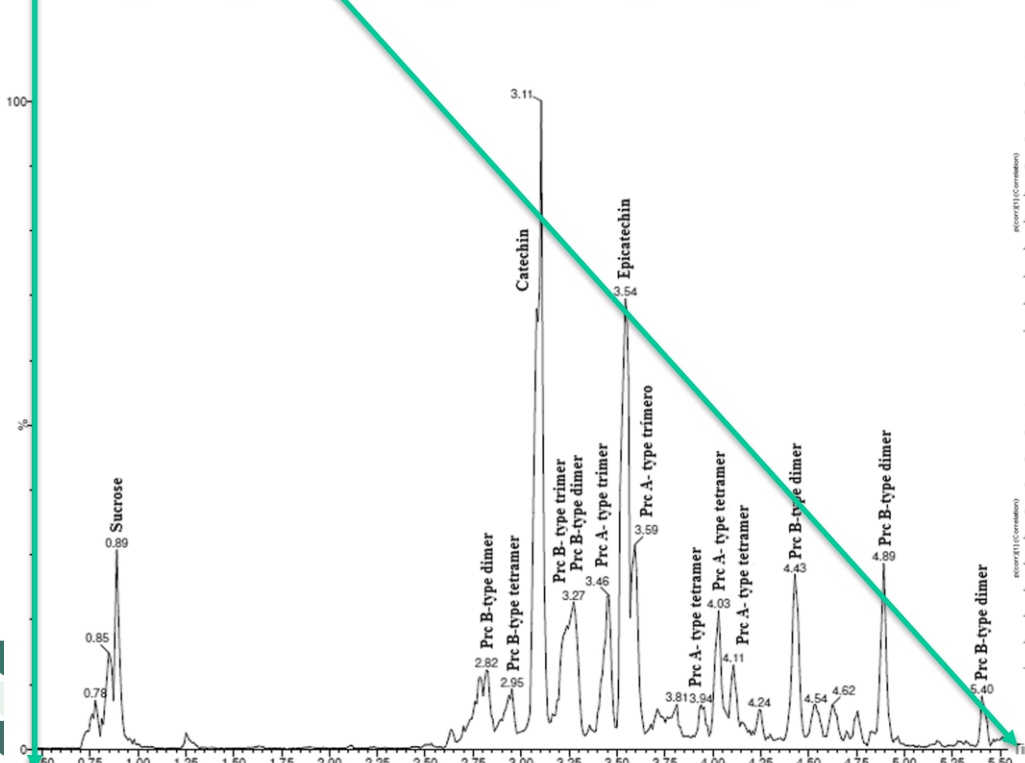
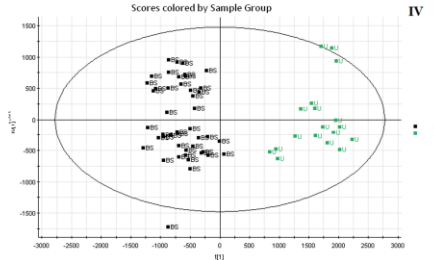
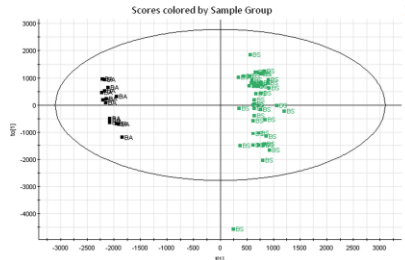
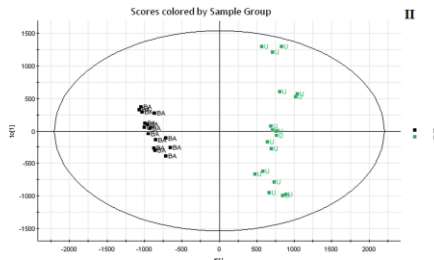
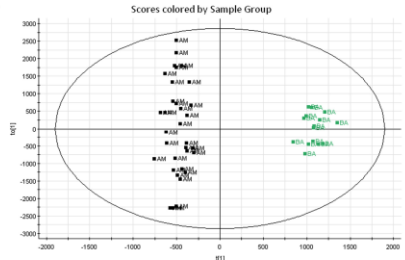
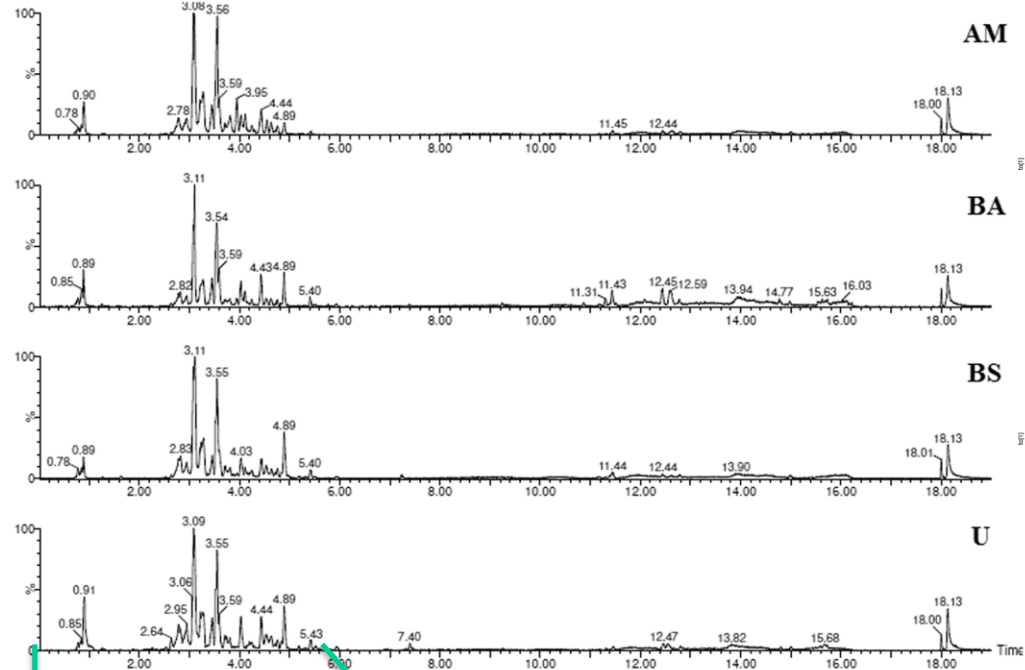
**Plataforma:**  
LC-MS, RMN

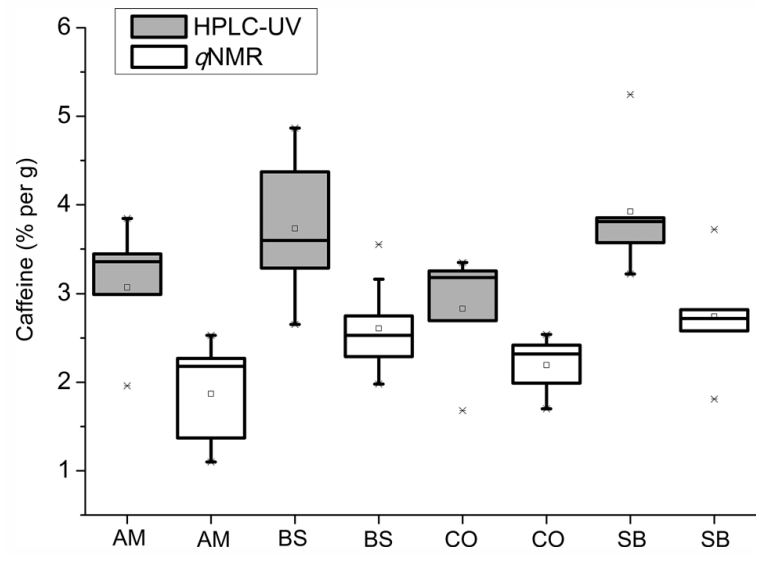
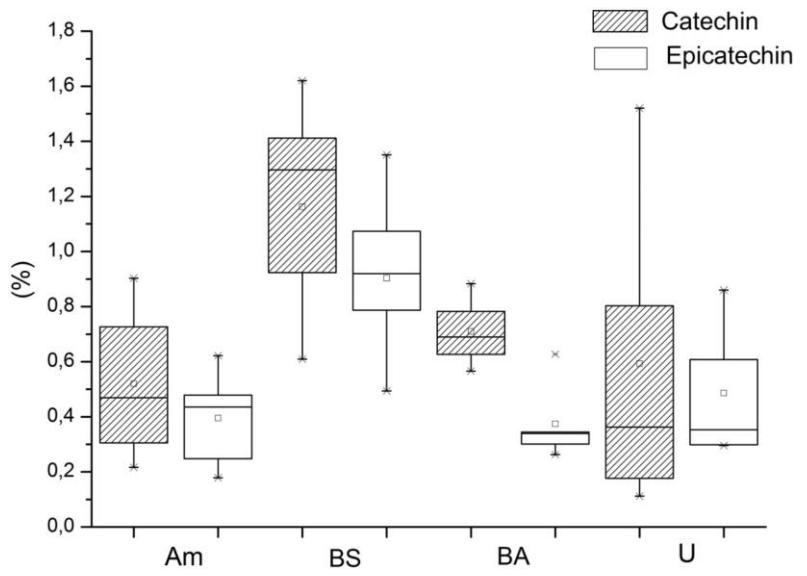
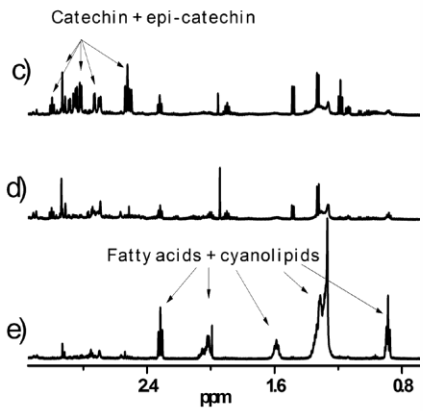
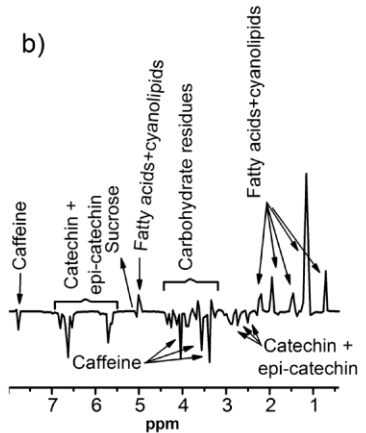
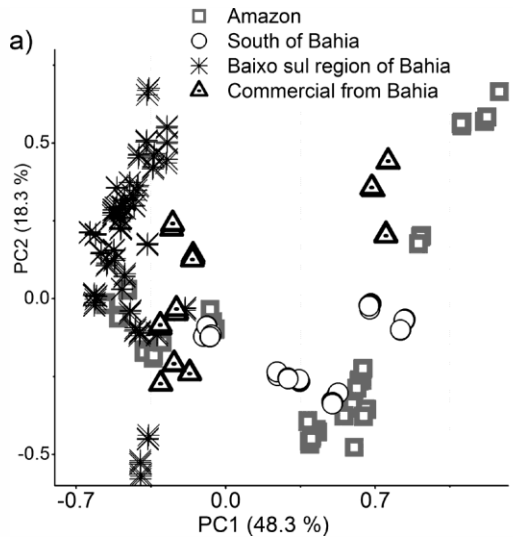


**Quimiometria:**  
PCA, OPLS-DA  
e quant









- **Conclusões**

- Catequina e epi-catequina foram os principais metabólitos responsáveis pela discriminação das amostras, tanto por LC-MS quanto por RMN.
- Amostras da BA apresentaram os maiores teores de fenólicos (catequina e epi-catequina).
- Amostras do AM apresentaram os maiores teores de ácidos graxos.
- O perfil de fenólicos indicou a origem geográfica das amostras de guaraná.

# Quais os metabólitos que diferenciam diferentes genótipos de feijão fradinho?

## Amostra:

*Vigna unguiculata*



## Origem:

Banco de germoplasma (UFC)



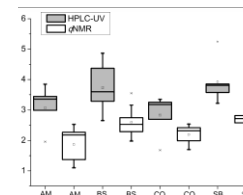
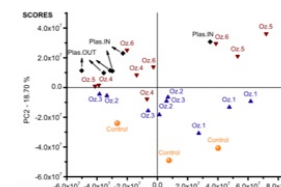
## Plataforma:

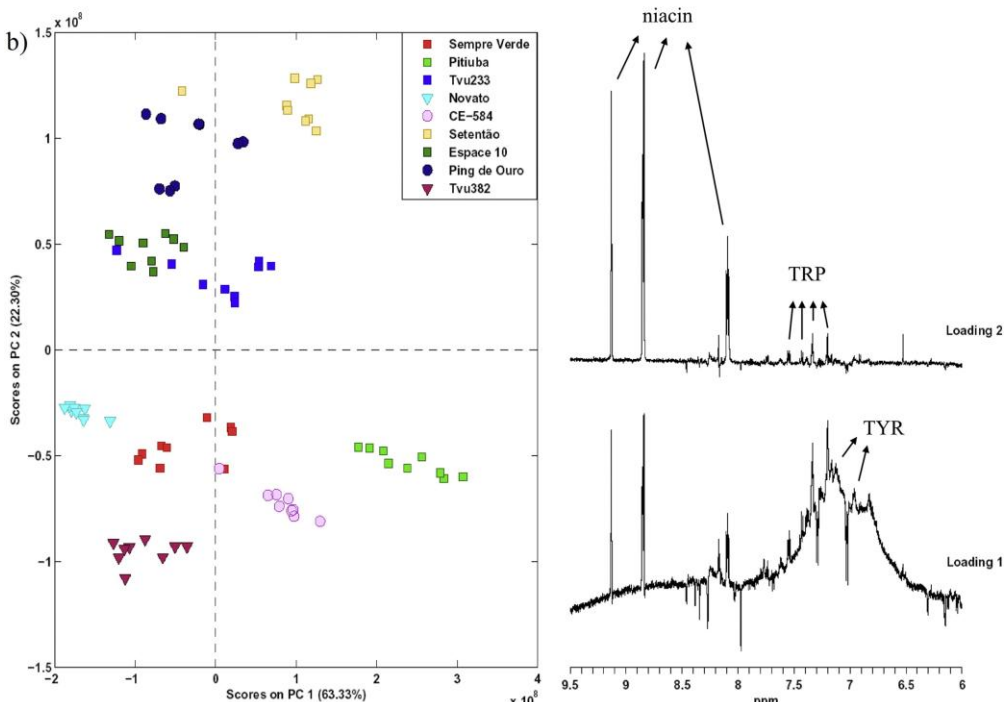
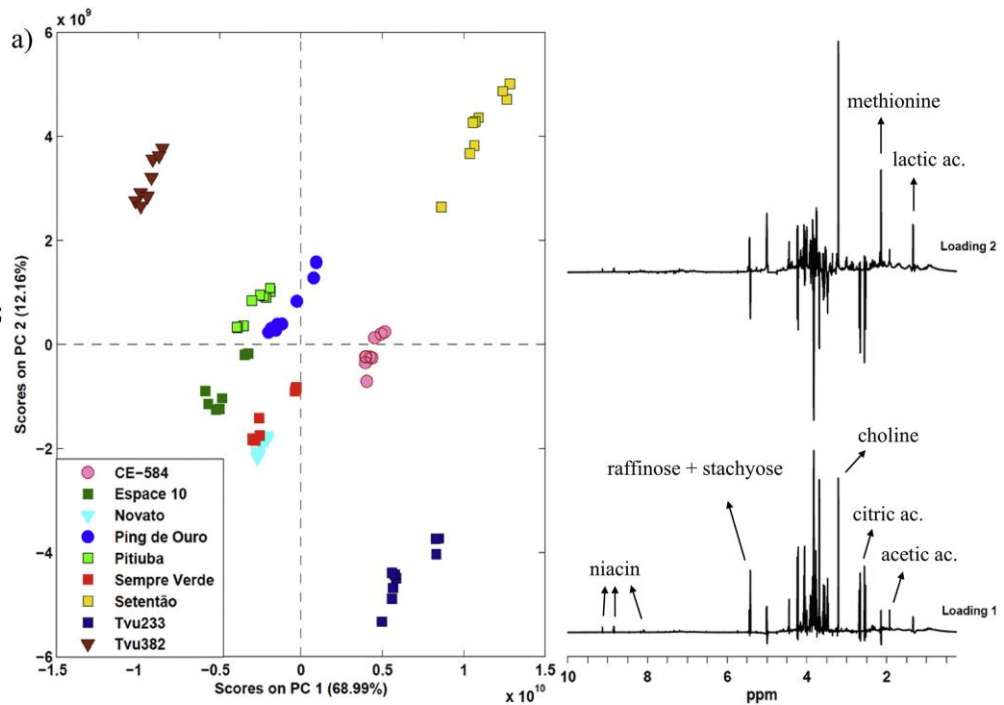
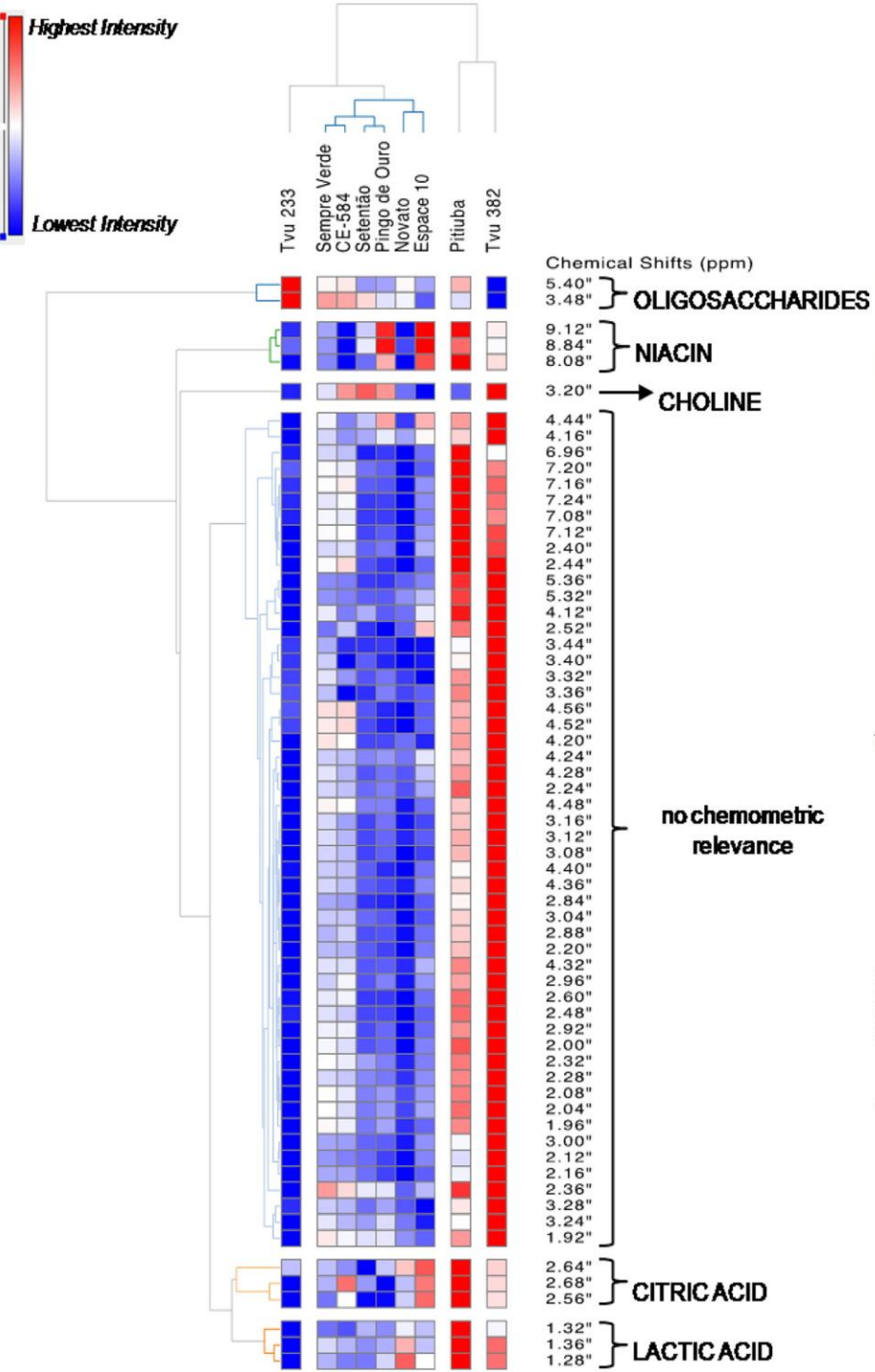
RMN

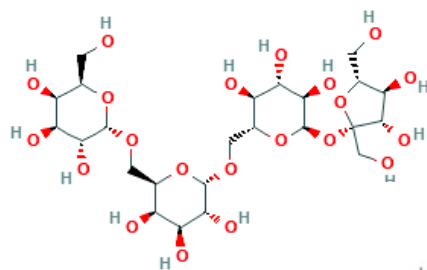
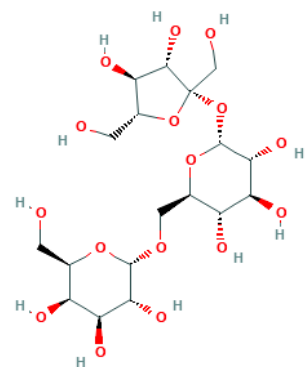


## Quimiometria:

PCA e qNMR

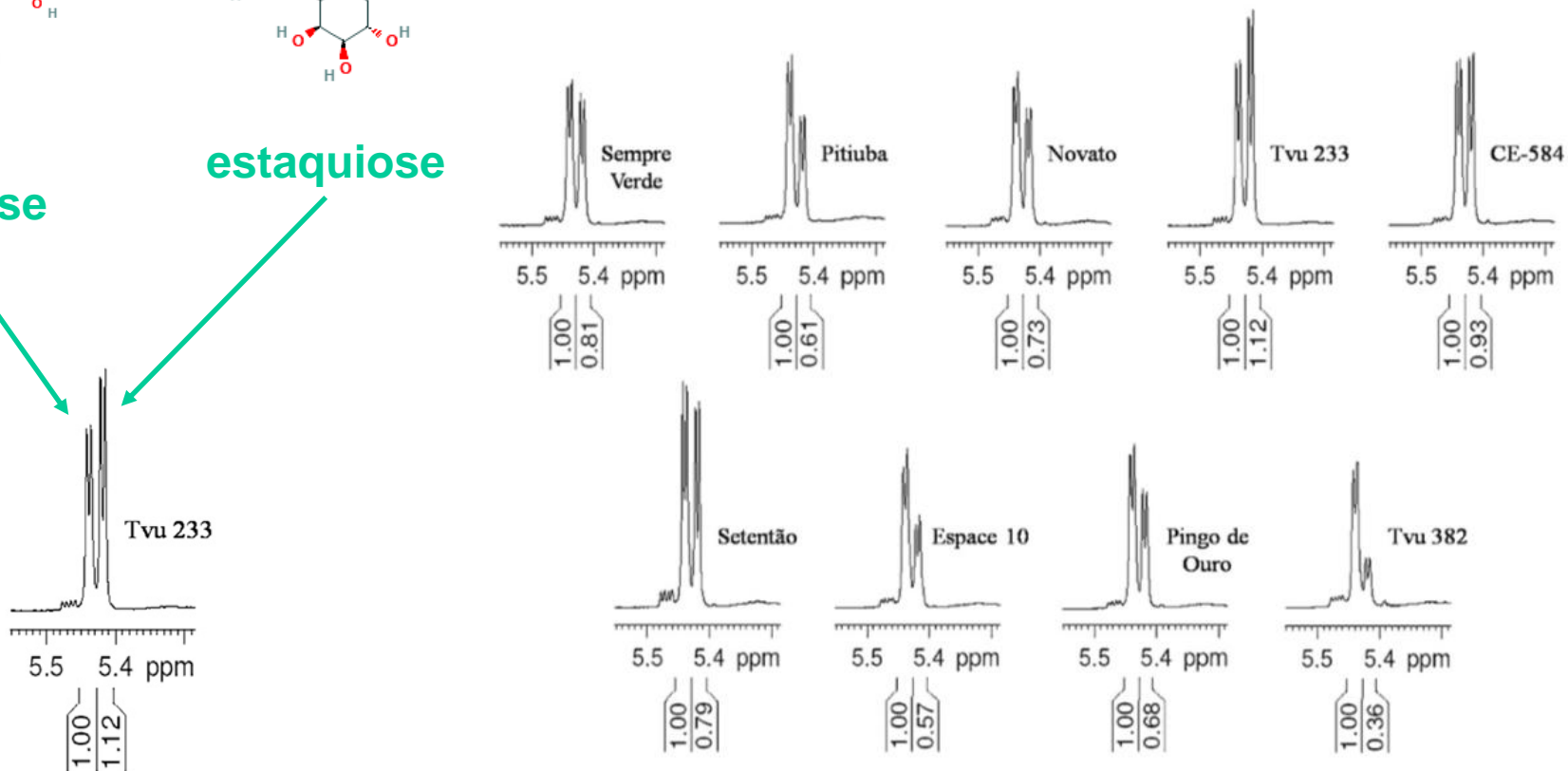






rafinose

estachiose



**Table 1**

Means and standard deviation of the concentrations of niacin, raffinose, and stachyose ( $\text{mg} \cdot \text{g}^{-1}$  of cotyledon) in the different genotypes of cowpea seeds. The values within the lines of concentrations with different superscript letters were significantly different at 0.05 of significance level as identified using a one-way ANOVA and Tukey Test.

Compounds	Genotype									
	Sempre Verde	Pitiuba	Novato	Tvu 233	CE-584	Setentão	Epace 10	Pingo de Ouro	Tvu 382	
Niacin	1.0 <sup>a</sup> ± 0.1	1.2 <sup>b</sup> ± 0.1	0.9 <sup>a</sup> ± 0.0	1.2 <sup>b</sup> ;	0.0	1.5 <sup>c</sup> ± 0.0	1.2 <sup>b</sup> ± 0.0	1.3 <sup>d</sup> ± 0.0	0.8 <sup>e</sup> ± 0.0	
Raffinose	26.0 <sup>a</sup> ± 0.5	21.8 <sup>b</sup> ± 0.5	24.4 <sup>c</sup> ± 0.5	38.6 <sup>d</sup> ;	0.2	34.2 <sup>f</sup> ± 0.7	19.8 <sup>g</sup> ± 0.4	24.5 <sup>c</sup> ± 0.6	11.4 <sup>h</sup> ± 0.8	
Stachyose	41.9 <sup>a</sup> ± 0.5	47.0 <sup>b</sup> ± 0.8	45.6 <sup>c</sup> ± 0.6	45.0 <sup>c</sup> ;	0.5	56.9 <sup>d</sup> ± 0.9	46.5 <sup>bc</sup> ± 0.6	47.4 <sup>bc</sup> ± 1.4	44.6 <sup>bc</sup> ± 1.3	
Total Oligosac.	67.9 ± 1.0	68.8 ± 1.3	70.0 ± 1.1	83.6	0.7	91.1 ± 1.6	66.3 ± 1.0	71.9 ± 2.0	56.0 ± 2.1	

40%



- **Conclusões**

- Oligosacarídeos, niacina, ácido cítrico e ácido láctico variaram de acordo com o genótipo.

- qNMR permitiu a quantificação de forma rápida o teor de rafinose e estaquiose no feijão fradinho e adiferenciação entre genótipos.

# Quais os metabólitos que diferenciam diferentes genótipos de feijão fradinho?

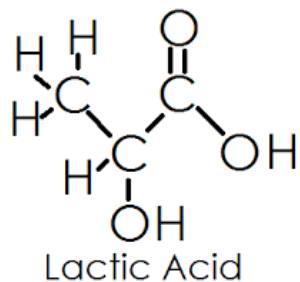
## Amostra:

Sucos de caju  
e melão



## Origem:

Fermentação  
lática



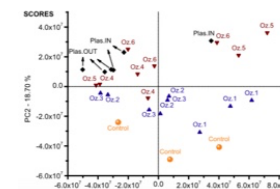
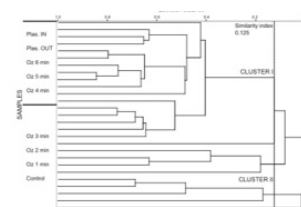
## Plataforma:

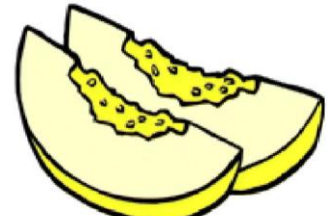
GC-MS



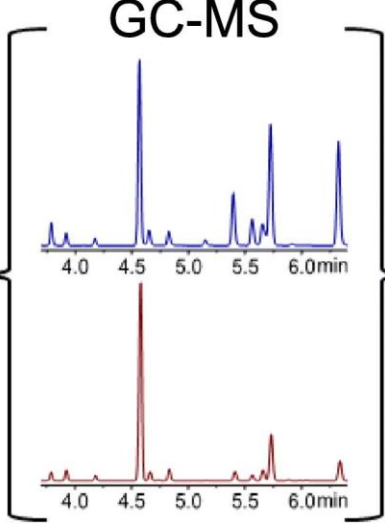
## Quimiometria:

HCA e PCA

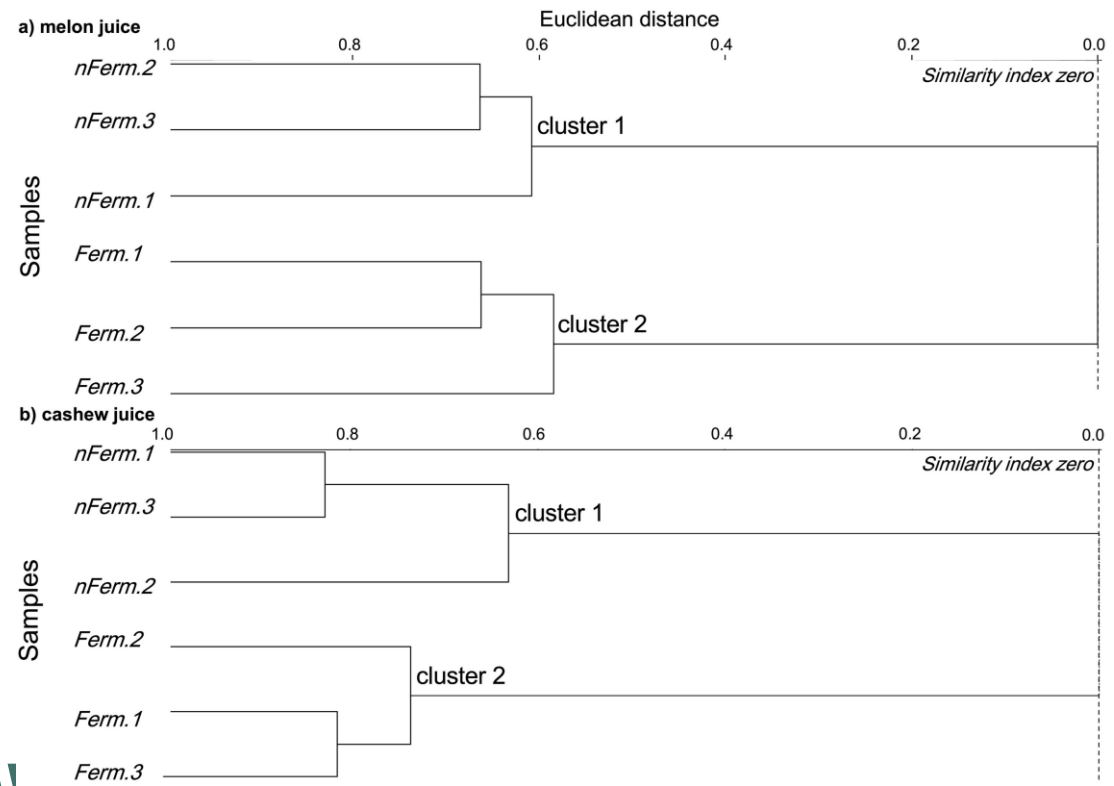
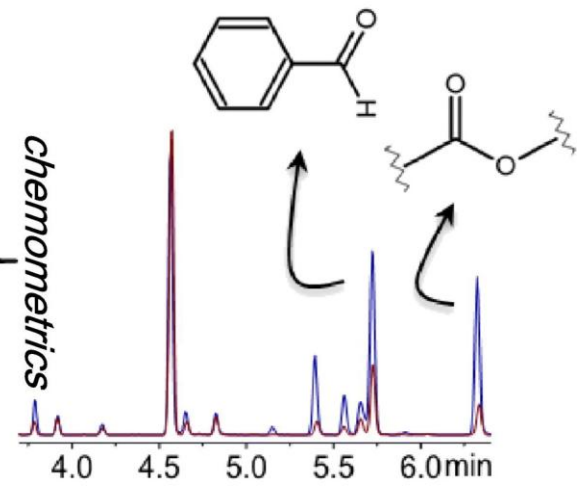


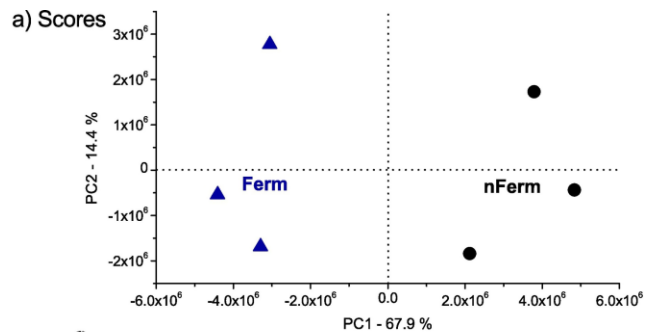


*Lactobacillus casei*

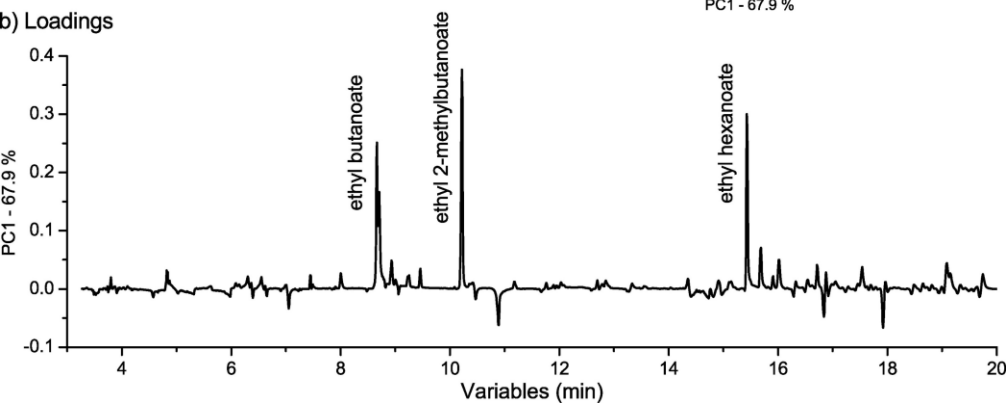


*chemometrics*

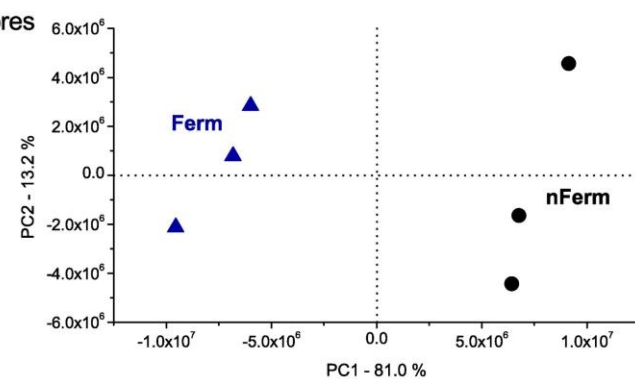




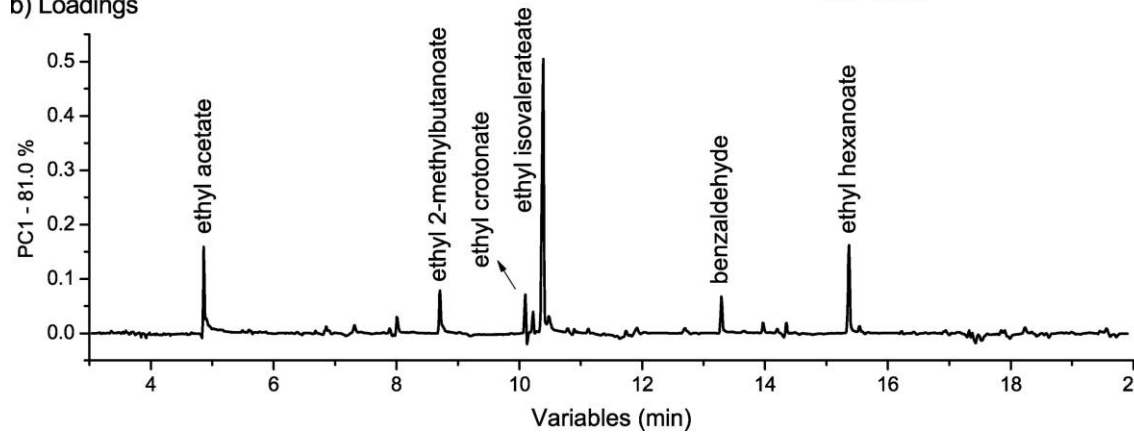
b) Loadings

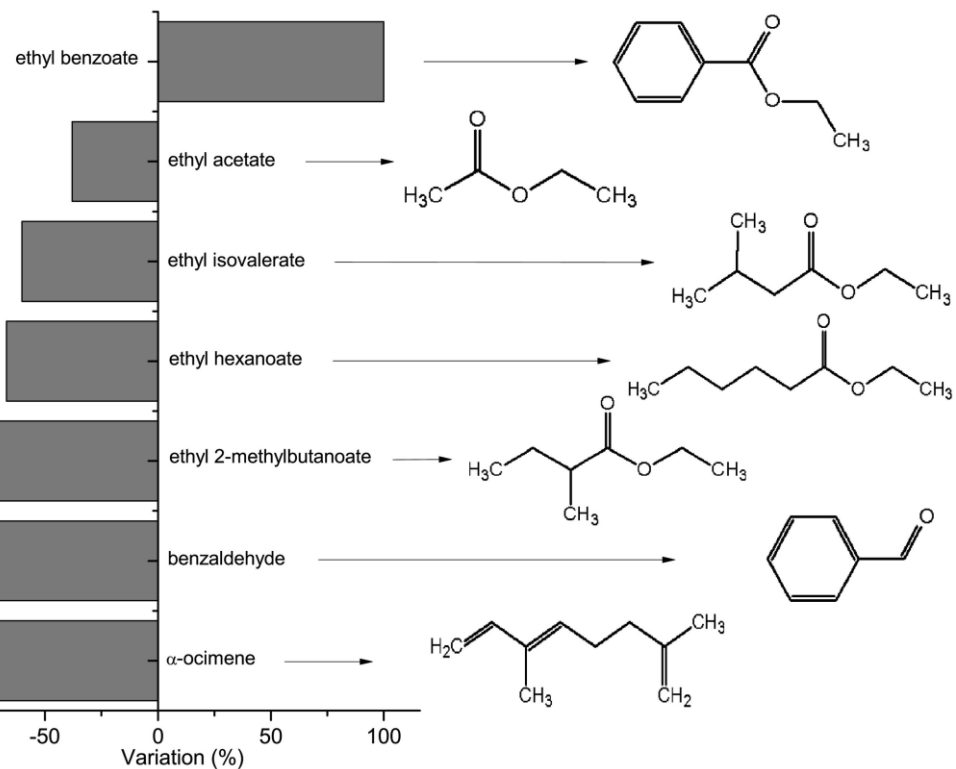
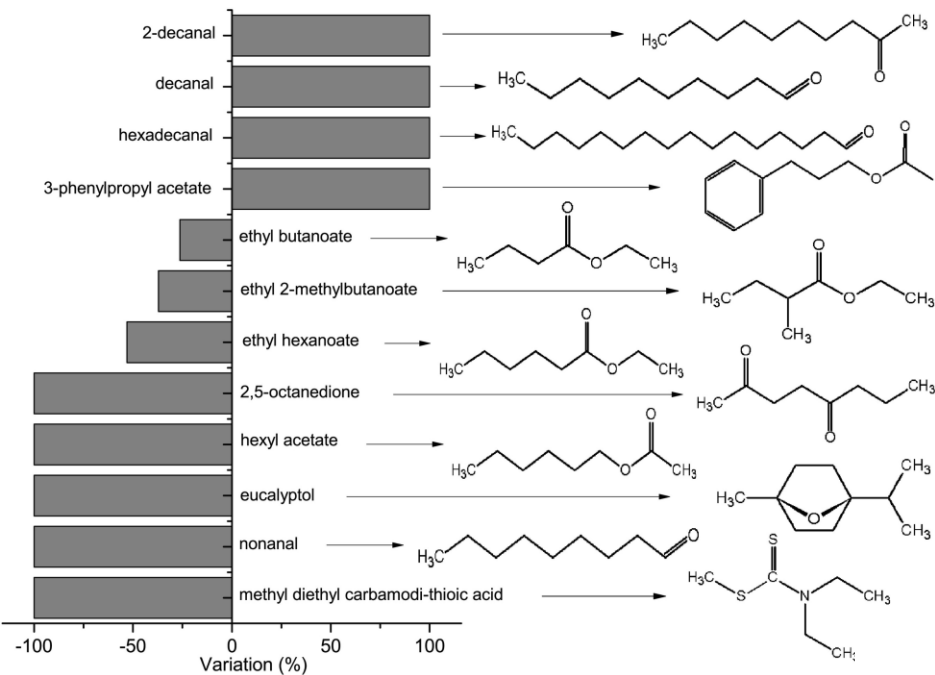


a) Scores



b) Loadings





- **Conclusões**

- Os sucos de caju e de melão fermentados não apresentaram compostos relacionados com off-flavors.

- O aroma característico das frutas foi mantido após a fermentação.

- Não foram encontrados compostos relacionados com o aroma de iogurte em concentrações significativas.



# Como a fibra do caju influencia o metabolismo de animais obesos?

**Amostra:**



**Origem:**

Dieta hipercalórica



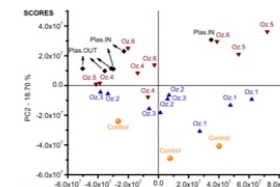
**Plataforma:**

RMN



**Quimiometria:**

PCA, bioquímica



# Preparação da ração dos camundongos

Metabolismo normal



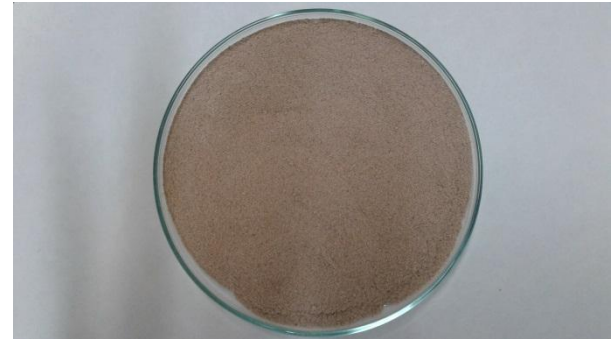
FcI (10%)



Dieta Normal (ND)  
– Ração comercial



ND-FcI



FcSM (10%)



Dieta Normal (ND)  
– Ração comercial



ND-FcSM

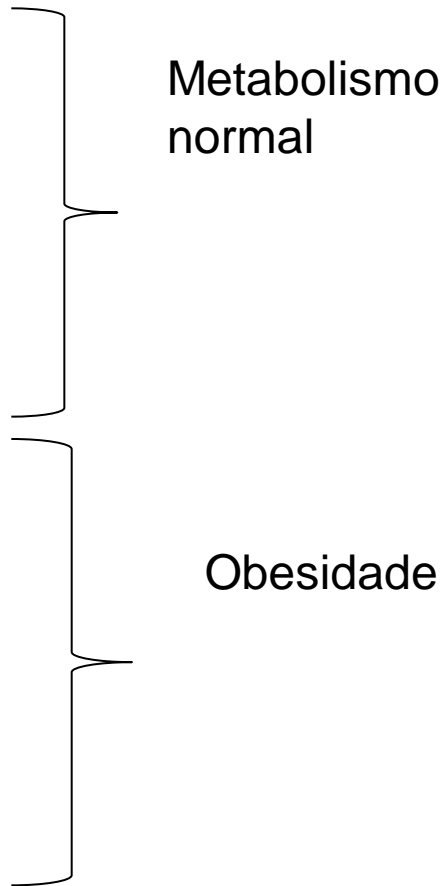




(p:19-25g)  
(CEPA/UFC 21/15)

Dietas

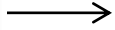
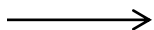
- Dieta Normal (ND)  
n=10
- ND-FcI (10%)  
n=10
- ND-FcSM (10%)  
n=10
- Dieta Normal (ND)  
n=10
- HFD  
n=10
- HFD-FcSM (10%)  
n=10



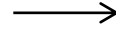
Alimentados durante 15 semanas; ração e água *ad libidum*

Peso animal  
Consumo de ração e água  
2x/semana





Soro



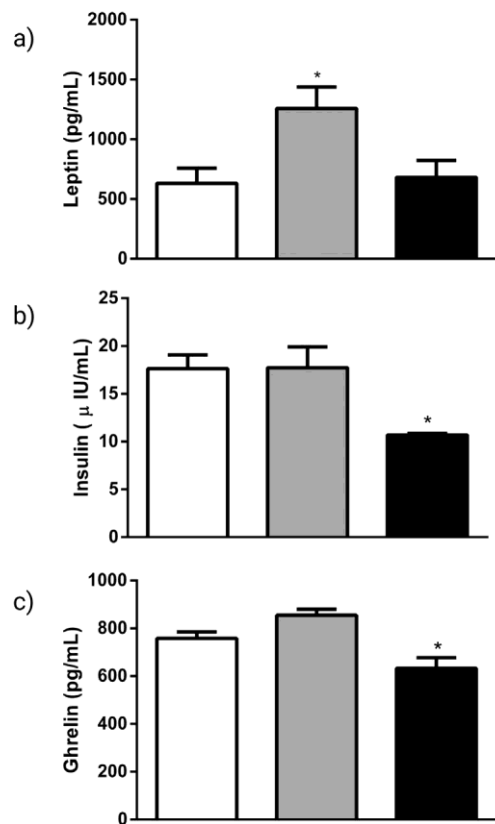
- Glicose
- Colesterol total, HDL, LDL, triglicerídeos
- Enzimas hepáticas (AST, ALT)
- Enzimas digestivas (amilase, lipase)
- Hormônios (Insulina, leptina, grelina)
- Citocinas (IL-6 e TNF- $\alpha$ , adiponectina)



- Peso
- MDA
- NP-SH
- Colesterol
- Histologia

Peso



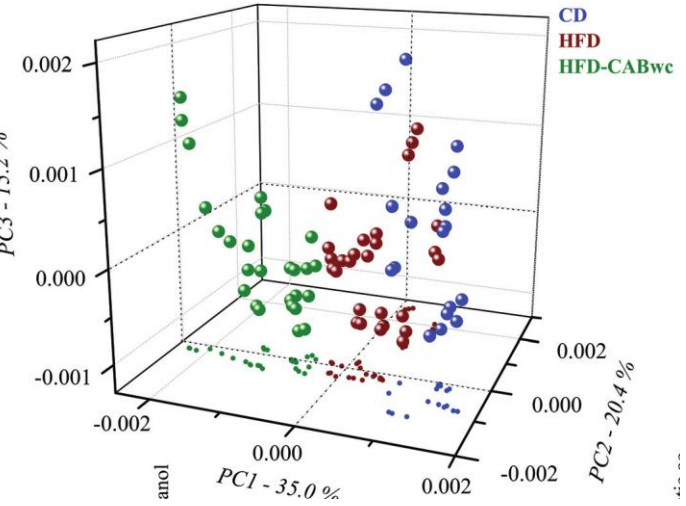
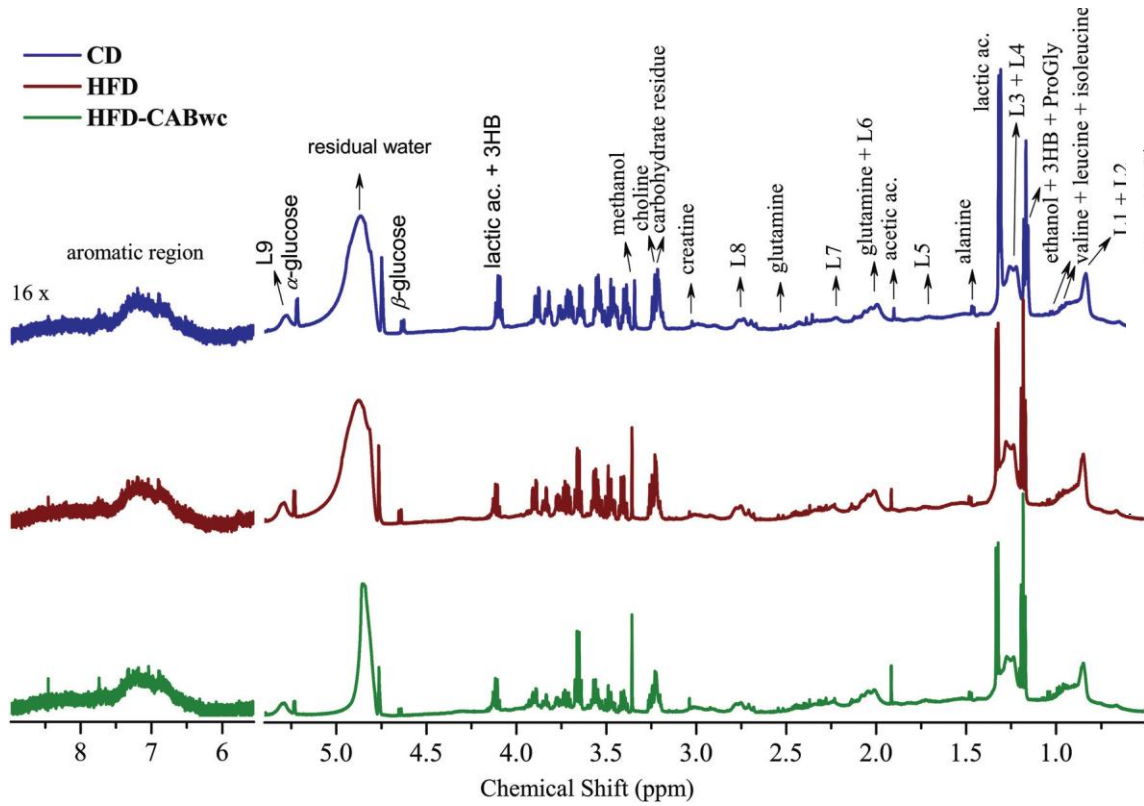


**Table 2** Effects of CABwc on serum and hepatic parameters in mice fed with experimental diets for 15 weeks

Parameters	CD	HFD	HFD-CABwc
Amylase (U L <sup>-1</sup> )	401.10 ± 20.36	494.80 ± 17.23 <sup>a</sup>	333.50 ± 36.47 <sup>b</sup>
Lipase (U L <sup>-1</sup> )	26.10 ± 1.30	33.65 ± 1.56 <sup>c</sup>	27.42 ± 1.61 <sup>d</sup>
ALT (U L <sup>-1</sup> )	37.40 ± 2.29	64.40 ± 10.45 <sup>a</sup>	38.83 ± 3.54 <sup>d</sup>
AST (U L <sup>-1</sup> )	102.00 ± 5.53	130.00 ± 7.60 <sup>a</sup>	82.10 ± 4.53 <sup>b</sup>
Glucose (mg dL <sup>-1</sup> )	115.20 ± 6.08	192.90 ± 10.45 <sup>e</sup>	138.70 ± 5.02 <sup>b</sup>
Insulin (ng mL <sup>-1</sup> )	1.35 ± 0.31	4.03 ± 0.79 <sup>c</sup>	1.50 ± 0.37 <sup>f</sup>
HOMA-IR	6.28 ± 0.97	29.05 ± 4.38 <sup>e</sup>	8.88 ± 1.89 <sup>b</sup>
Total cholesterol (mg dL <sup>-1</sup> )	92.68 ± 3.81	141.70 ± 8.06 <sup>e</sup>	134.40 ± 2.52 <sup>e</sup>
Triglycerides (md dL <sup>-1</sup> )	72.80 ± 3.92	90.20 ± 3.21 <sup>c</sup>	68.50 ± 2.79 <sup>f</sup>
HDL (mg dL <sup>-1</sup> )	92.48 ± 3.18	108.7 ± 3.43 <sup>c</sup>	128.20 ± 2.04 <sup>b,e</sup>
LDL (mg dL <sup>-1</sup> )	11.2 ± 0.56	19.68 ± 1.13 <sup>e</sup>	21.94 ± 1.00 <sup>e</sup>
Liver total cholesterol (mg g <sup>-1</sup> )	0.5 ± 0.02	0.6 ± 0.02 <sup>a</sup>	0.58 ± 0.00
Liver MDA (nmol g <sup>-1</sup> )	12.64 ± 0.92	17.47 ± 0.42 <sup>c</sup>	14.54 ± 0.72 <sup>d</sup>
Liver NP-SH (μg mg <sup>-1</sup> )	0.13 ± 0.01	0.14 ± 0.00	0.20 ± 0.02 <sup>a,d</sup>

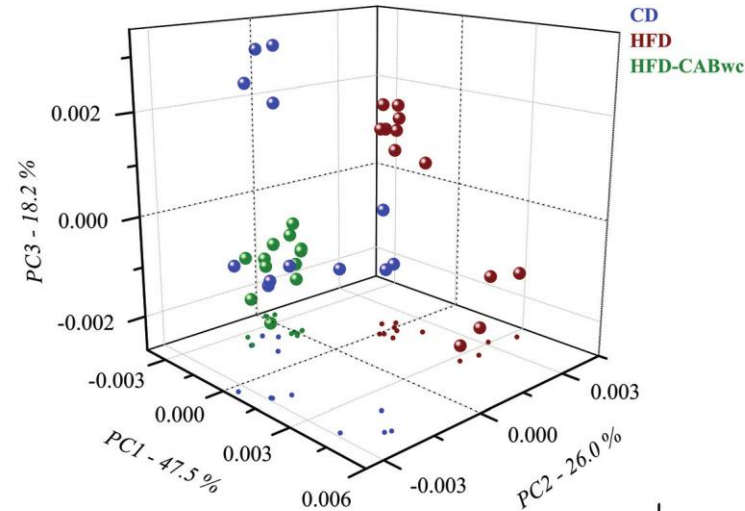
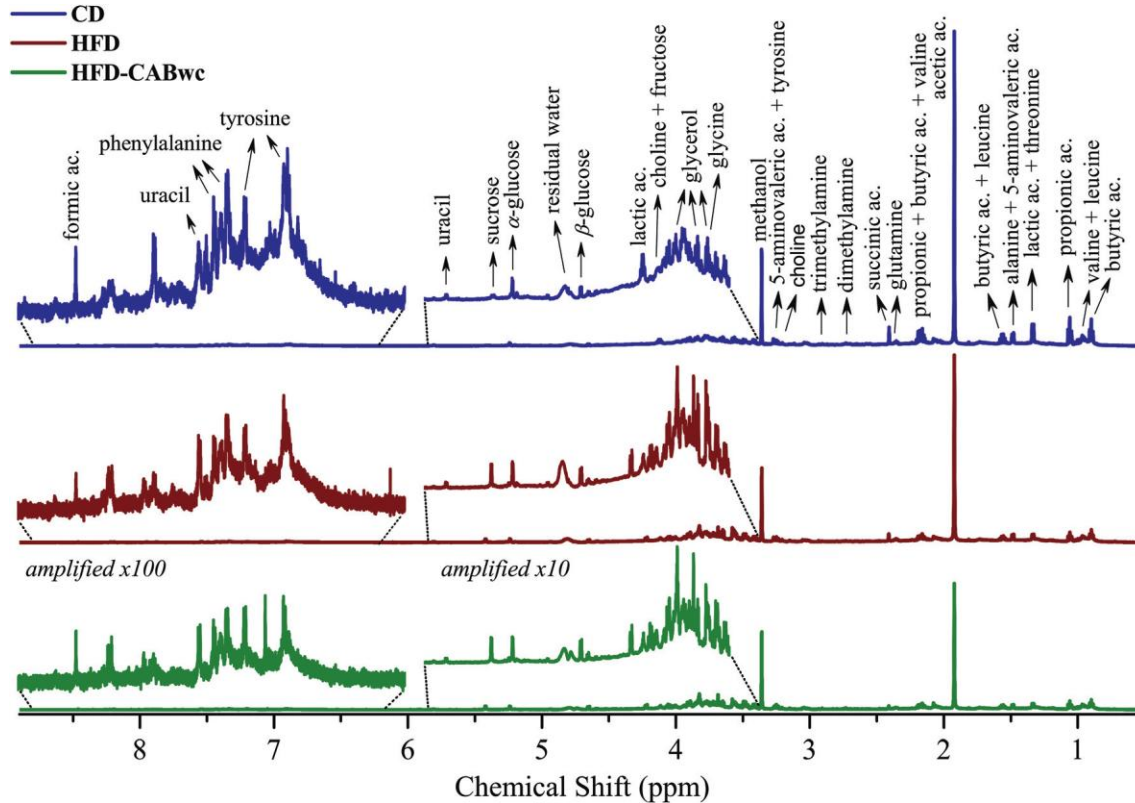
Results are expressed as the mean ± SEM. <sup>a</sup>  $P < 0.05$  when compared to CD. <sup>b</sup>  $P < 0.001$  when compared to HFD. <sup>c</sup>  $P < 0.01$  when compared to CD. <sup>d</sup>  $P < 0.05$  when compared to HFD. <sup>e</sup>  $P < 0.001$  when compared to CD. <sup>f</sup>  $P < 0.01$  when compared to HFD (ANOVA followed by Tukey's test). CD = chow diet, HFD = high fat diet, HFD-CABwc = HFD supplemented with cashew apple fiber without low molecular weight metabolites.

soro





fezes



A comparação entre os espectros mostrou que as fezes são principalmente compostos de **ácidos orgânicos de cadeia curta** (acético, propiônico, butírico, láctico, succínico e fórmico), **aminoácidos** (leucina, alanina, uracila, tirosina e fenilalanina), **açúcares** (sacarose, glicose e frutose) e **metanol**.

- **Conclusões**

- A fibra de caju promoveu a saciedade em ratos alimentados com uma dieta hipercalórica, melhorando o metabolismo da glicose e dos lipídios.

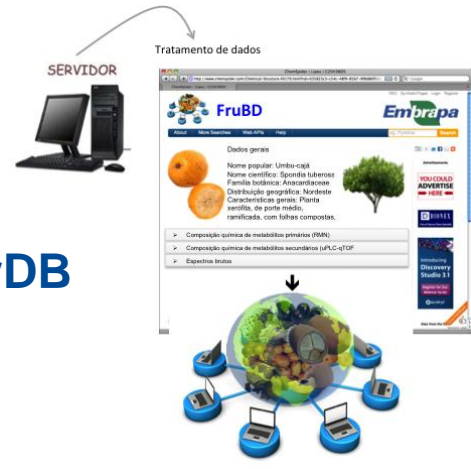
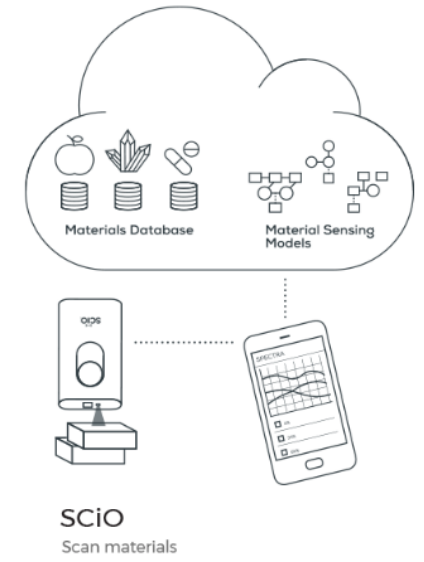
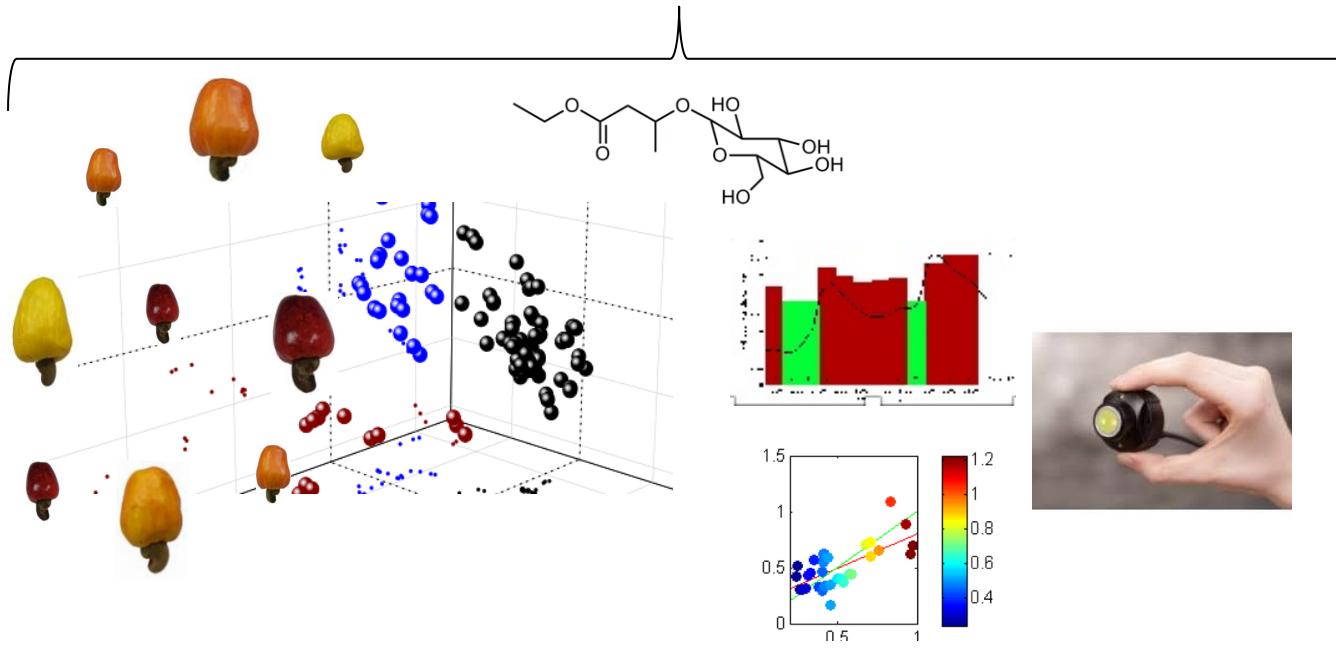
- Os efeitos positivos podem estar associados com a produção de SCFA.



# • Perspectivas

- Associação com métodos rápidos não destrutivos (ex. NIR).

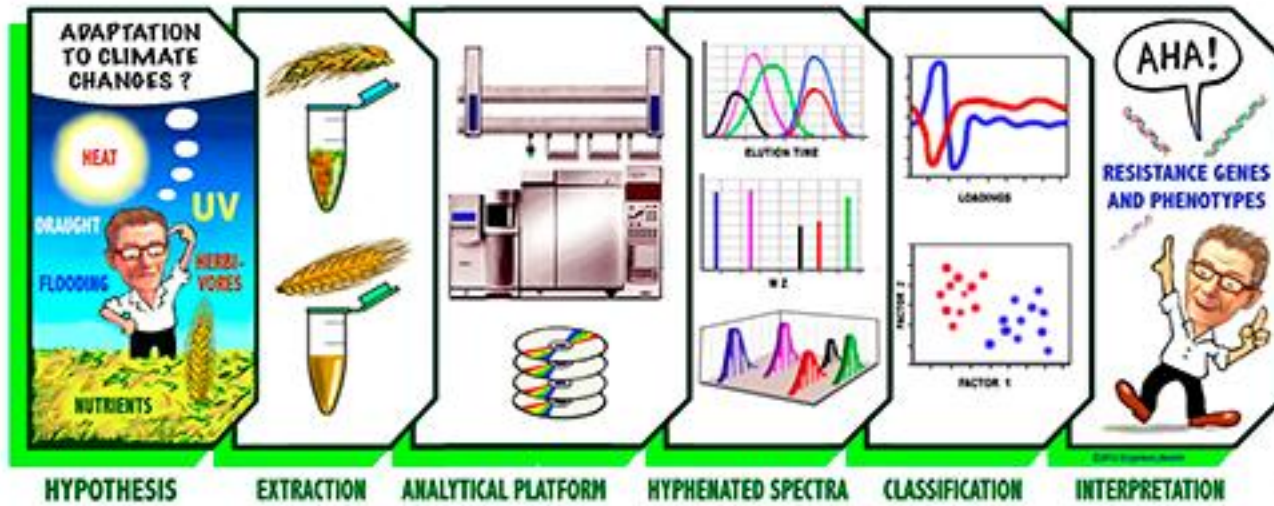
2014-2019



FruBrDB



?



!

Foodomics. Illustration by Søren B. Engelsen and Tim Newlin ©



**Foodomics** é uma disciplina que **examina todo o conjunto de substâncias** presentes em nossos alimentos (foodome). A disciplina utiliza **plataformas analíticas avançadas** para investigar a composição do alimento e, assim, suas propriedades nutricionais e impacto na saúde.

As novas técnicas também fornecem uma imagem detalhada da **qualidade dos alimentos** e podem ser usadas para detectar fraudes em alimentos e encontrar **soluções** para outros **desafios** na produção de alimentos.

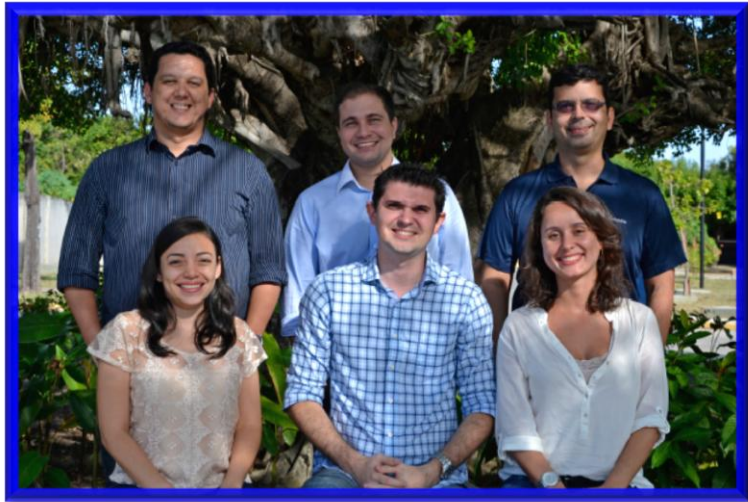
Os resultados de pesquisas de foodomics têm um **impacto** direto sobre os **consumidores**, a **indústria** de alimentos e a **sociedade**.

Engelsen ([https://food.ku.dk/english/research\\_at\\_food/research\\_fields/foodomics/](https://food.ku.dk/english/research_at_food/research_fields/foodomics/))





# Agradecimentos



# Agradecimentos

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Prof Dr Elenilson G. Alves Filho

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Prof Flemming H Larsen

## UESC

Prof Dr Raildo M Jesus

## Dublin Inst Tech

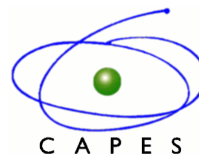
P.J. Cullen



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Departamento de Engenharia Química



UNIVERSITY OF COPENHAGEN







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MINISTÉRIO DA  
AGRICULTURA, PECUÁRIA  
E ABASTECIMENTO

