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## Relationship between a technofunctional property of food product and the physico-chemical and structural characteristics of peptides: An in silico approach

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AGRO  
CAMPUS  
OUEST



# Relationship between a techno-functional property of cheese and milk protein derived peptides

*In silico* approach

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15<sup>th</sup> Food Colloid Conference  
April 13-16, 2014





Science & Technology  
of Milk & Egg

78 standing fellow workers  
25 PhD students

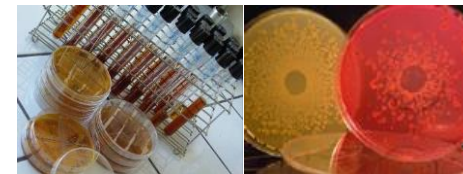


A multidisciplinary and multiscale approach,  
reinforced by two high-calibre facilities:

Dairy Platform



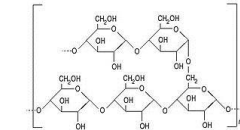
Biological Resource Centre



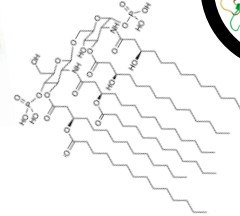
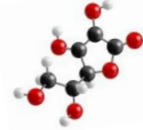
- ❑ **Structuration / destructuration mechanisms of food matrix:**  
*from structural characterization to digestion*
- ❑ **Dairy processing and cheese making:**  
*toward sustainable dairy systems*
- ❑ **Microbial interaction:**  
*food matrix and host cell*

# Context

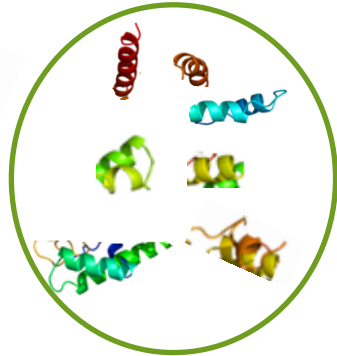
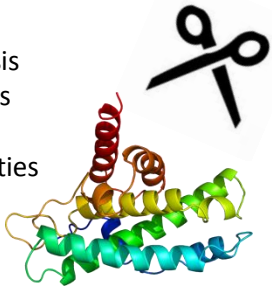
Food products have a complex composition



Evolution of the composition



Proteolysis enhances protein functionalities



Food protein properties  $\blacktriangleup$ :  
emulsifying / foaming / gelling / texture

**Relationship between a DH and functionality**

Relationship between peptide characteristics (pHi, size, hydrophathy, charges, secondary structure) and functionality?

## Aim & Strategy

Stretchability



Texture quality of cheese

The stretchability of cheese depends on its gross composition, pH, mineralisation and **proteolysis**.

**What are the physico-chemical and structural characteristics of peptides involved in the stretchability of cheese?**



→ From the identification of peptides in the aqueous extract of cheese:



1/ Calculation of their size, charges, hydrophathy, aliphatic index, pHi, secondary structure



2/ Establish the relationship between these characteristics and the stretchability of cheese

# In silico approach

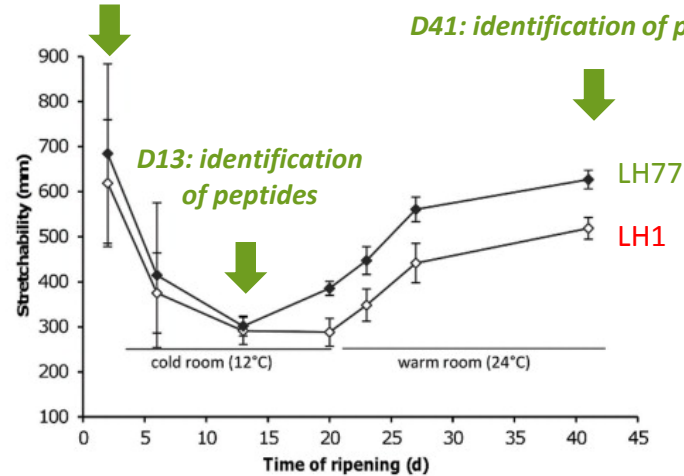
Swiss-type cheeses



LH1 or LH77



D1: identification of peptides

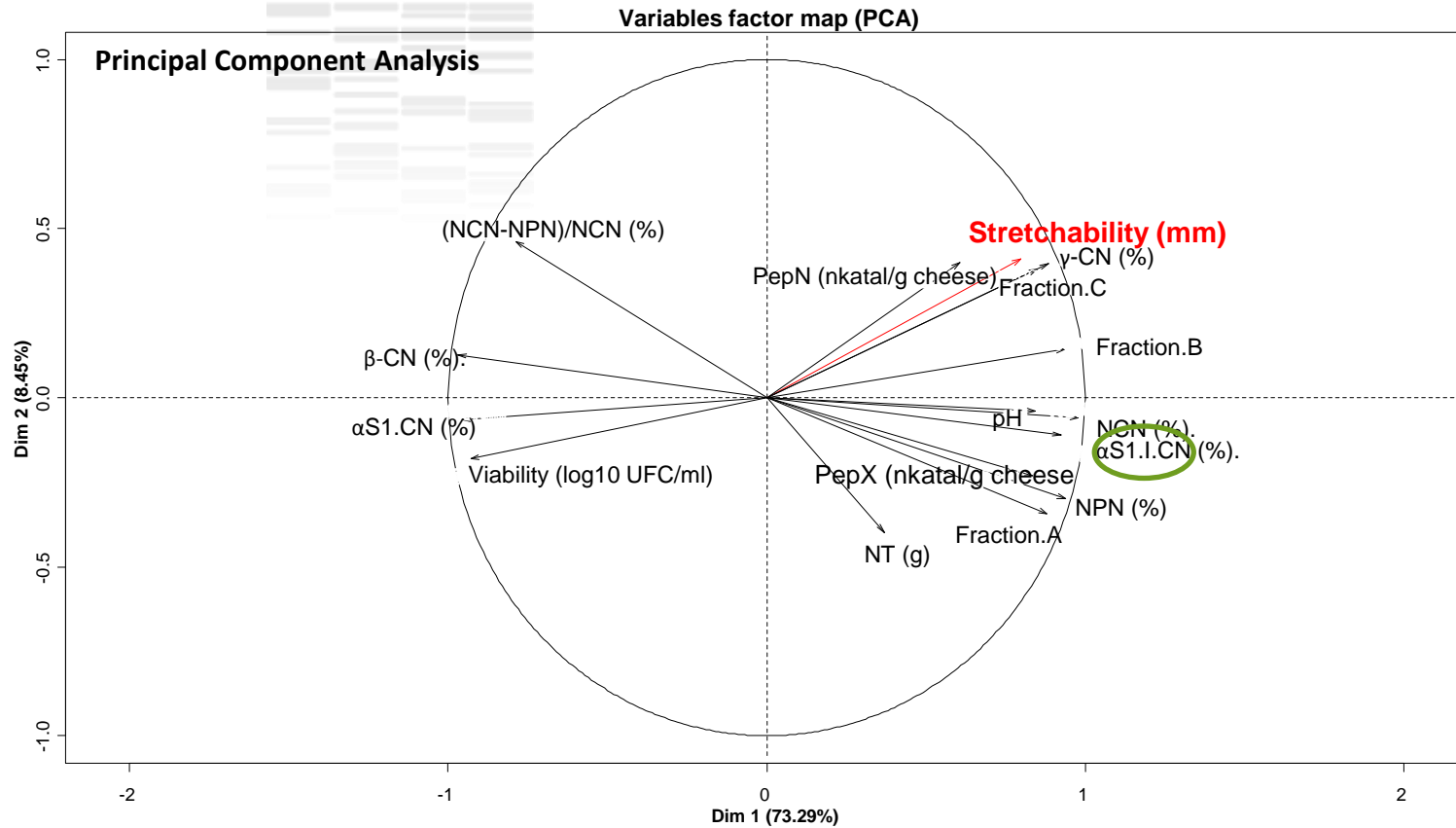


Proteolytic activities:  
LH1 > LH77

6 cheeses

LH1-D1	LH77-D1
LH1-D13	LH77-D13
LH1-D41	LH77-D41

(Sadat-Mekmene et al., 2013)



## Cheese characteristics

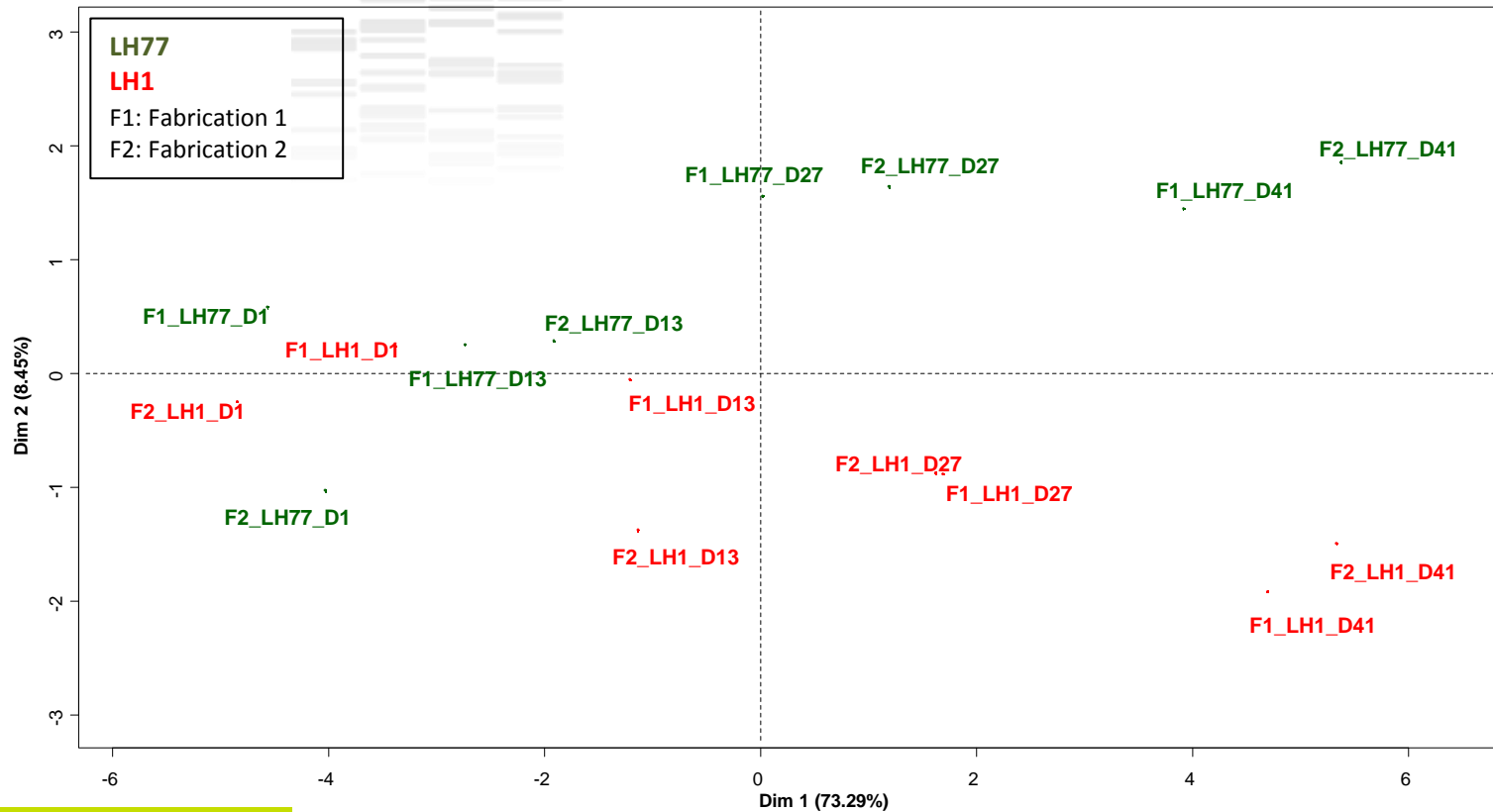
(microbiological, biochemical and technofunctional)

The **stretchability** is correlated with the **proteolysis** of caseins.

Casein  $\alpha$ 1-(f24-199) has softening properties (Borsting et al. 2012, Brickley et al. 2007, Creamer et Olson 1982).

(Sadat-Mekmene et al., 2013)

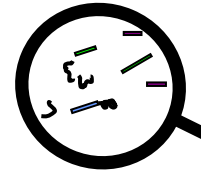
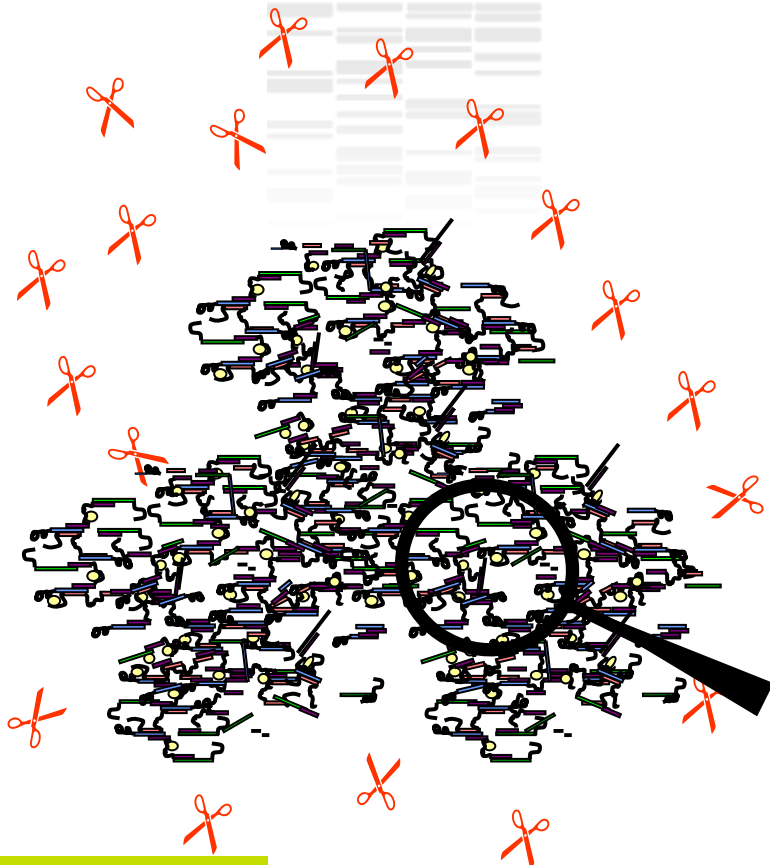
Individuals factor map (PCA)



Proteolysis rate and protease's nature affect the stretchability of cheese.

LH77-D41 generates the best stretchability.



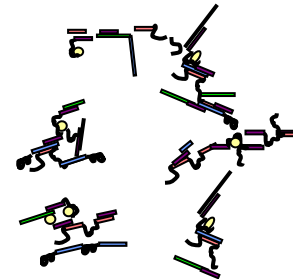
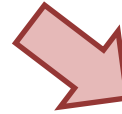
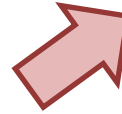


*Aqueous extract of cheese matrix*



Identification of peptides

Peptides in aqueous extract are more accessible to our identification technique and are a part of information on the stretchability of the cheeses.



*Solid extract =  
Cheese matrix after extraction of  
aqueous extract*

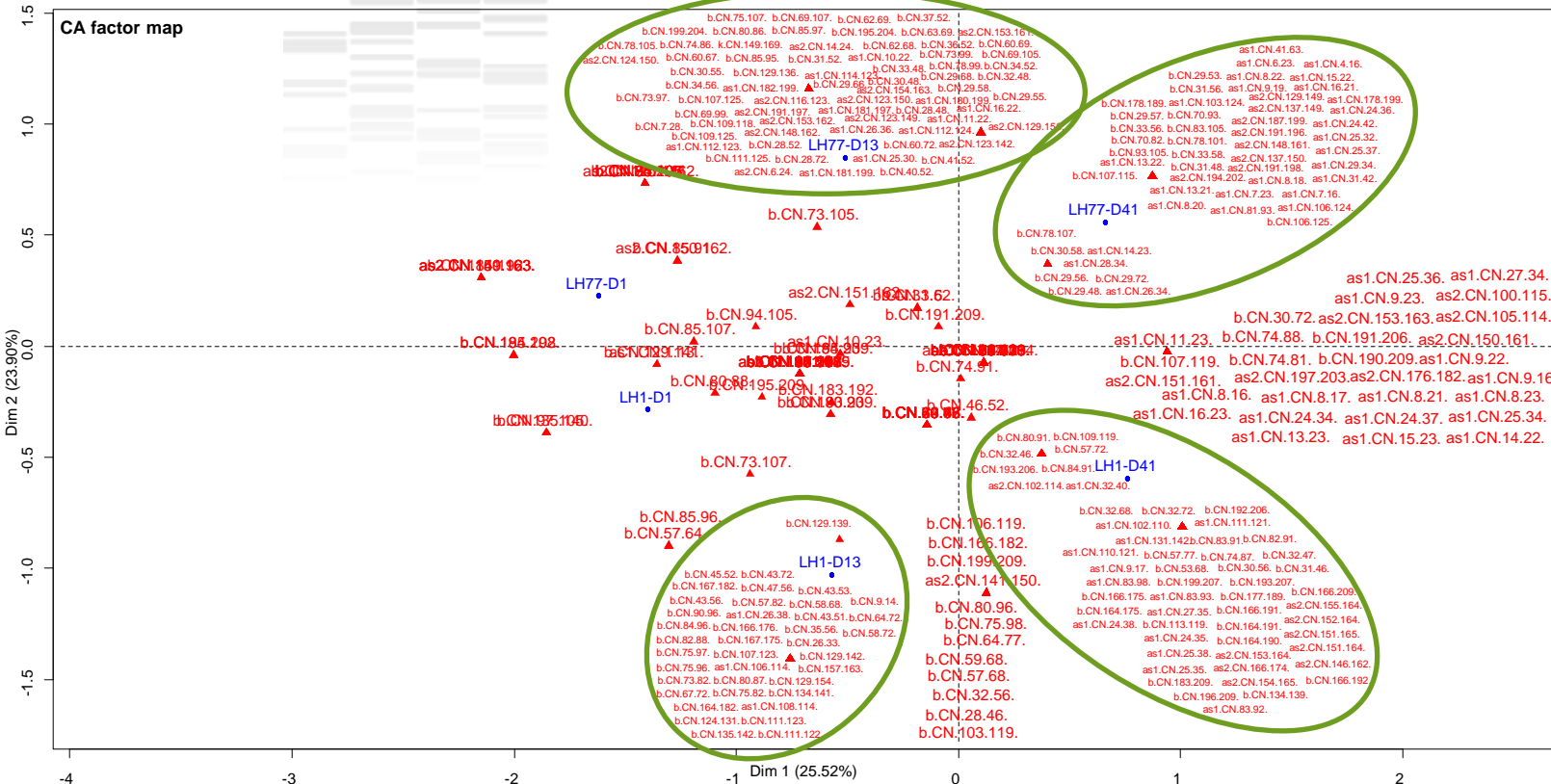


Deduction of cleavage sites



Deduction of peptides that can be produced

## Peptides in aqueous extract of cheese



Each cheese has a unique profile of peptides.

Several peptides are common to 2 or more cheeses.

*Analysis of the peptides present in aqueous extract for each time*

**D1**  
 b.CN.84.93.=0  
 b.CN.74.82.=0  
 b.CN.53.72.=0  
 b.CN.35.52.=0  
 b.CN.32.52.=0  
 b.CN.30.52.=0  
 b.CN.29.52.=0  
 b.CN.195.206.=0  
 b.CN.194.208.=1  
 b.CN.185.192.=1  
 b.CN.111.119.=0  
 b.CN.103.113.=0  
 as2.CN.101.114.=0  
 as1.CN.24.30.=0  
 as1.CN.17.23.=0

**D13**  
 b.CN.80.90.=1  
 b.CN.47.52.=1  
 b.CN.32.58.=1  
 b.CN.195.207.=1  
 b.CN.195.202.=1  
 b.CN.194.207.=1  
 b.CN.194.206.=1  
 b.CN.167.176.=1  
 b.CN.135.141.=1  
 b.CN.126.133.=1  
 as2.CN.101.115.=1  
 as1.CN.181.189.=1  
 as1.CN.10.23.=0

**D41**  
 b.CN.74.88.=1  
 b.CN.74.81.=1  
 b.CN.30.72.=1  
 b.CN.191.206.=1  
 b.CN.190.209.=1  
 b.CN.129.141.=0  
 b.CN.107.119.=1  
 as2.CN.197.203.=1  
 as2.CN.176.182.=1  
 as2.CN.153.163.=1  
 as2.CN.151.161.=1  
 as2.CN.150.161.=1  
 as2.CN.105.114.=1  
 as2.CN.100.115.=1

**D41**  
 as1.CN.9.23.=1  
 as1.CN.9.22.=1  
 as1.CN.9.16.=1  
 as1.CN.8.23.=1  
 as1.CN.8.21.=1  
 as1.CN.8.17.=1  
 as1.CN.8.16.=1  
 as1.CN.27.34.=1  
 as1.CN.25.36.=1  
 as1.CN.25.34.=1  
 as1.CN.24.37.=1  
 as1.CN.24.34.=1  
 as1.CN.16.23.=1  
 as1.CN.15.23.=1  
 as1.CN.14.22.=1  
 as1.CN.13.23.=1  
 as1.CN.1.13.=0  
 as1.CN.11.23.=1

1 = peptide presents only at this time  
 0 = peptide absents only at this time

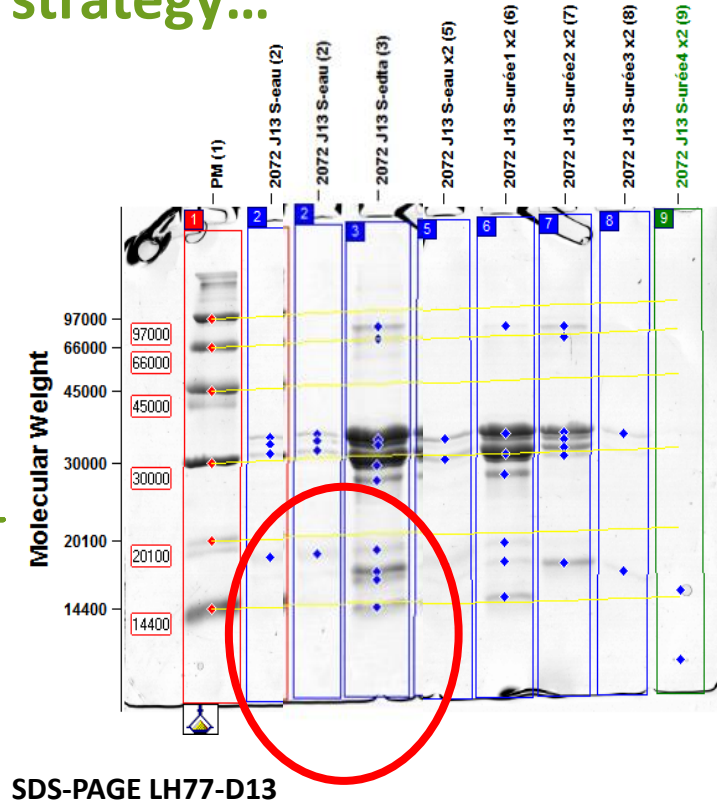
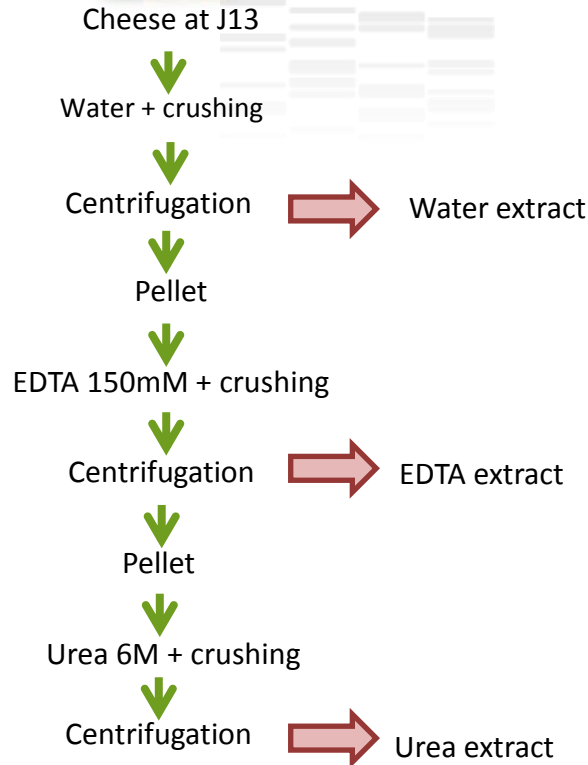
=> Only peptides that are different between the days of ripening.

Peptides are significantly different at D1, D13 and D41.

Proteolysis is the main factor which modulate the stretchability.



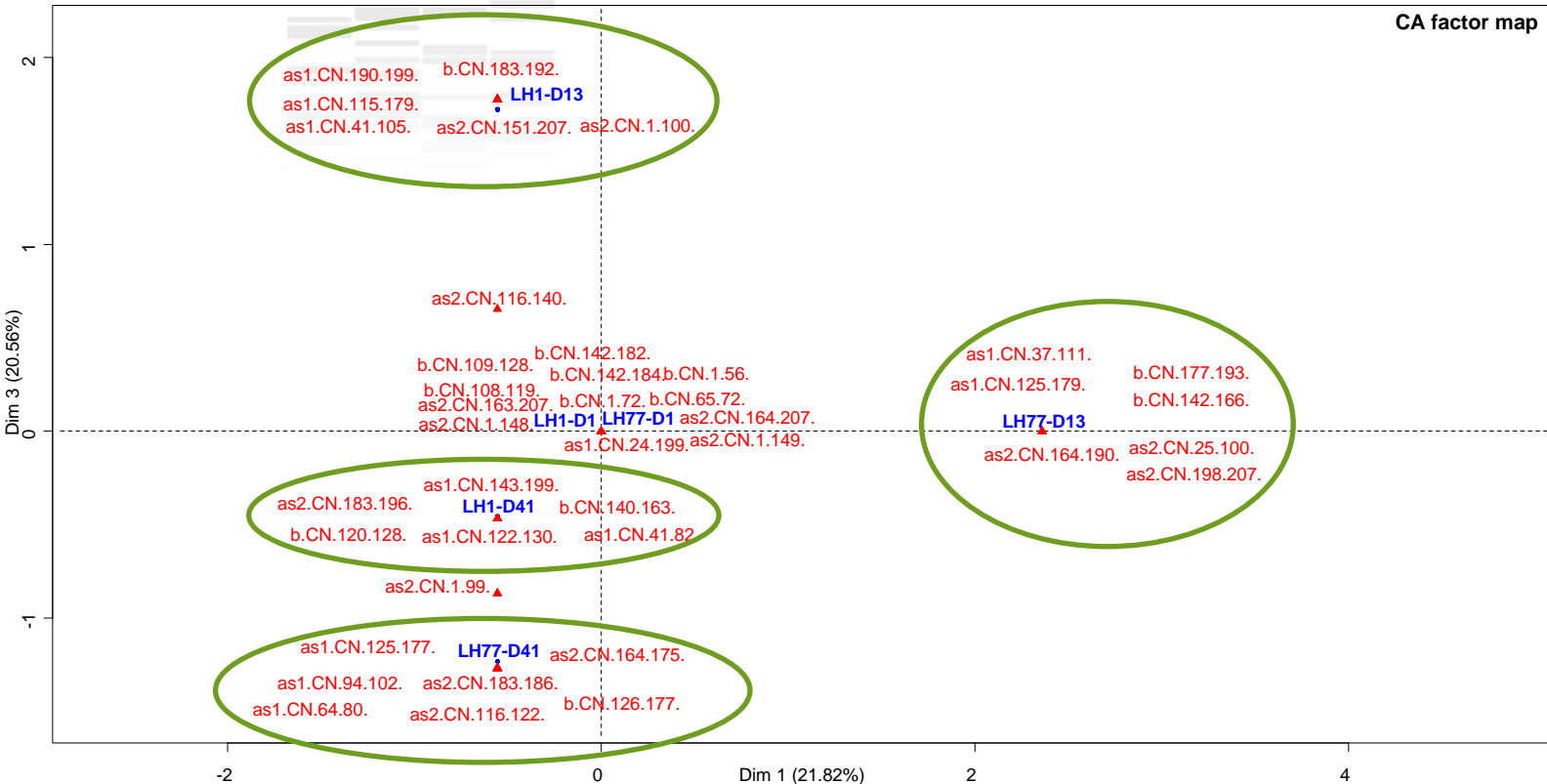
## To verify our strategy...



A lot of peptides are not extracted by water and are trapped in the «cheese matrix».

Casein  $\alpha$ 1-(f24-199) possesses some texture properties (Borsting et al. 2012, Brickley et al. 2007, Creamer et Olson 1982).

## From the cleavage sites: deduction of peptides into the cheese matrix



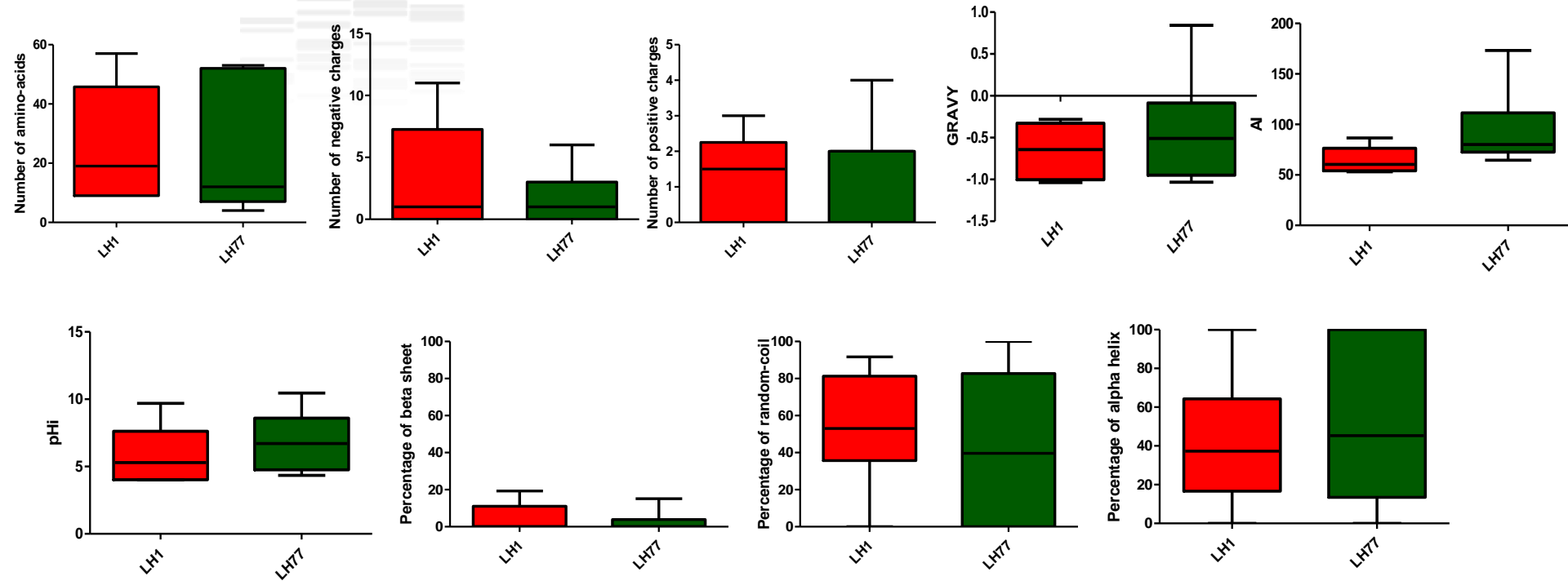
Each cheese possesses a different peptide profile.

At D1, the peptide profiles are similar.

At D41, the majority of peptides is derived from  $\alpha$ 1-casein and  $\alpha$ 2-casein.


LH1 LH77

## Relationship between cheese stretchability and peptide characteristics (D41)



# Advantages / Disadvantages



- ✓ From the peptide identification  to establish a relationship between proteolysis and the enhancement of the functional properties of protein.
- ✓ To have information on peptide profile that can be involved on the stretchability of cheese.
- ✓ To have a comprehensive view of data already obtained.



- ✓ The study lacks the quantification of peptides in the aqueous extract.
- ✓ No information on the distribution of peptides between aqueous extract and cheese matrix.

# Conclusion & Perspectives

## To recap:

Identification of peptides in aqueous extract of cheese



Identification of cleavage sites



Deduction of peptides in cheese matrix



Multivariate analysis



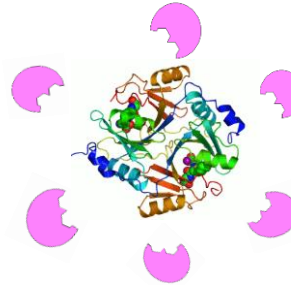
pools of peptides related to stretchability



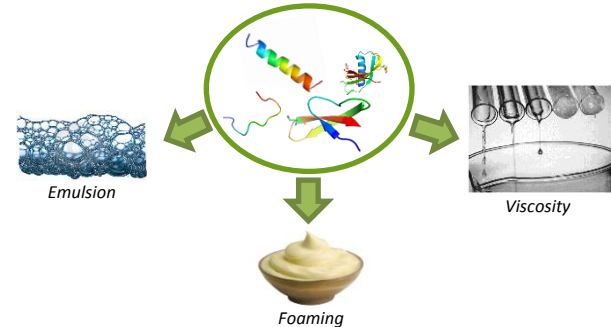
Calculate the peptide characteristics in each pool to connect these characteristics with the stretchability of cheese

Potential of this approach to establish the relationship between characteristics of peptides and their functionality in complex matrices

To select enzymes to produce peptides related to the targeted functionality



Can be applied to other types of peptides and others functionalities







***MERCI***



***THANK YOU FOR  
YOUR ATTENTION***

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