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

*In silico* approach

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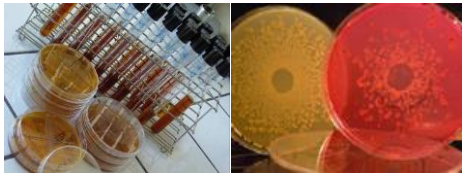
15th Food Colloid Conference
April 13–16, 2014

STLO

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

Dairy Platform

Biological Resource Centre



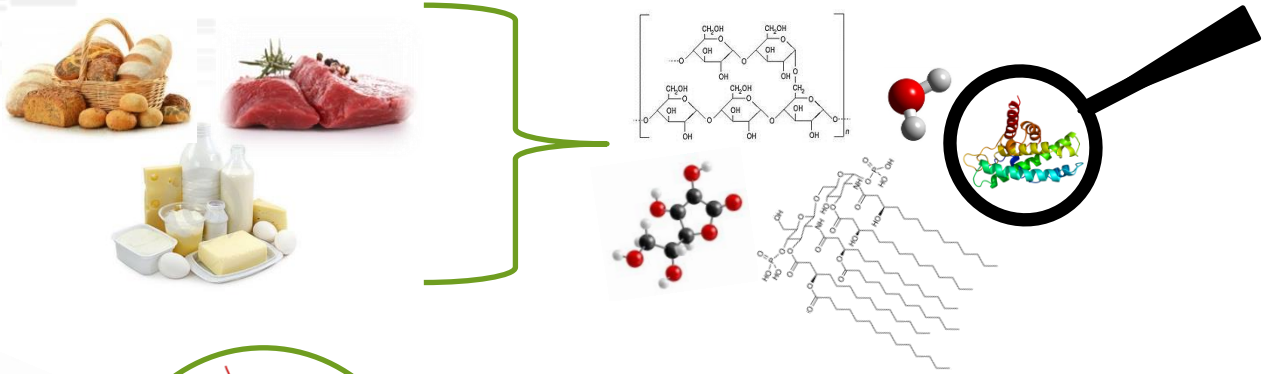
- **Structuration / destructuration mechanisms of food matrix:**
  *from structural characterization to digestion*
- **Dairy processing and cheese making:**
  *toward sustainable dairy systems*
- **Microbial interaction:**
  *food matrix and host cell*



**Please visit http://www6.rennes.inra.fr/stlo_eng**

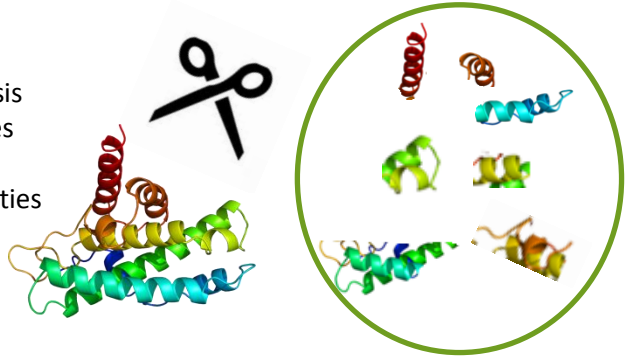
# Context

Food products have a complex composition



Evolution of the composition

Proteolysis enhances protein functionalities



Food protein properties ↗:
emulsifying / foaming / gelling / texture

**Relationship between a DH and functionality**

Relationship between peptide characteristics (pHi, size, hydropathy, 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?**

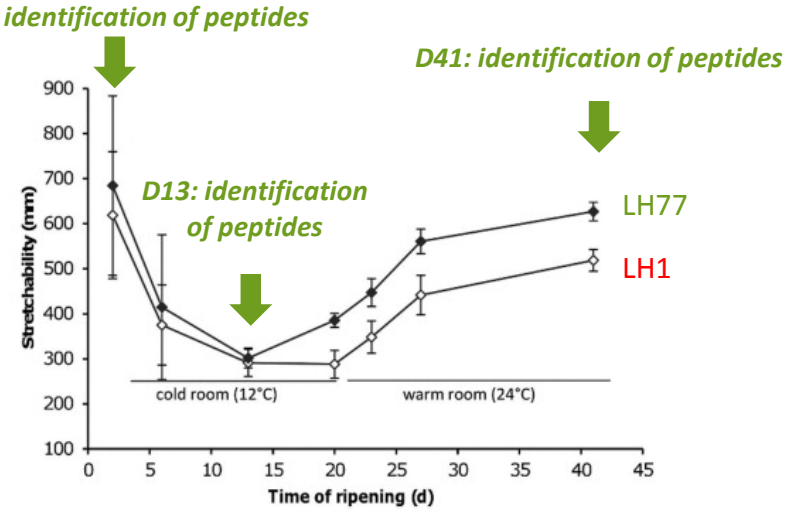
→ From the identification of peptides in the aqueous extract of cheese:

- 1/ Calculation of their size, charges, hydropathy, aliphatic index, pHi, secondary structure
- 2/ Establish the relationship between these characteristics and the stretchability of cheese

# *In silico* approach

Swiss-type cheeses

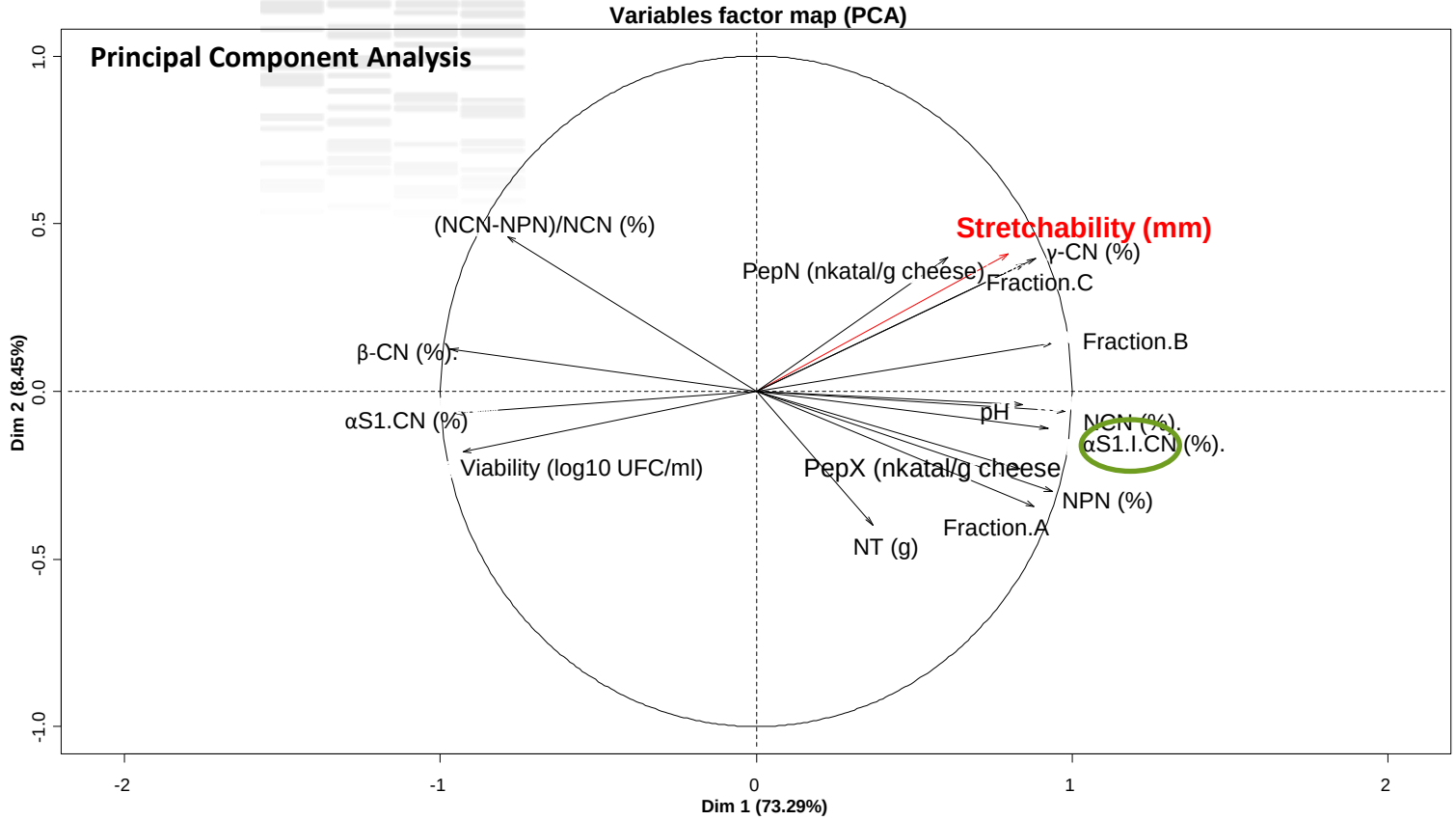
LH1 or LH77




(Sadat-Mekmene et al., 2013)

Proteolytic activities:
LH1 > LH77

| 6 cheeses | |
|---|---|
| **LH1-D1** | **LH77-D1** |
| **LH1-D13** | **LH77-D13** |
| **LH1-D41** | **LH77-D41** |




# Cheese characteristics

(microbiological, biochemical and technofunctional)

The stretchability is correlated with the proteolysis of caseins.

Casein αs1-(f24-199) has softening properties (Borsting et al. 2012, Brickley et al. 2007, Creamer et Olson 1982).

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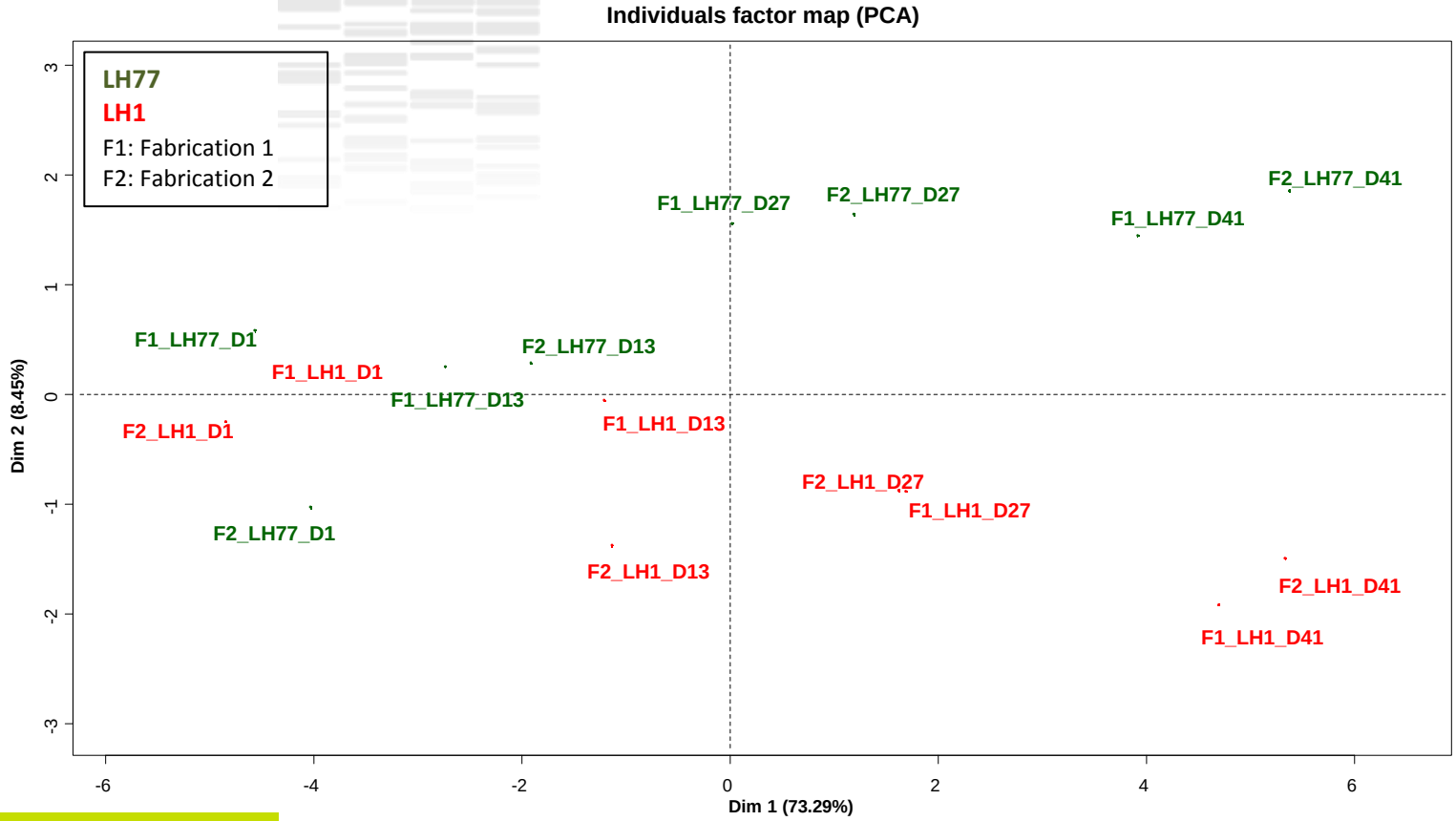
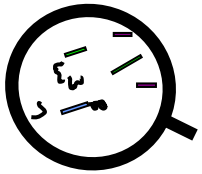
(Sadat-Mekmene et al., 2013)




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

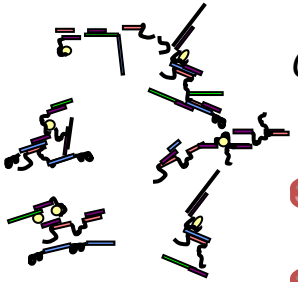
LH77-D41 generates the best stretchability.



*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.

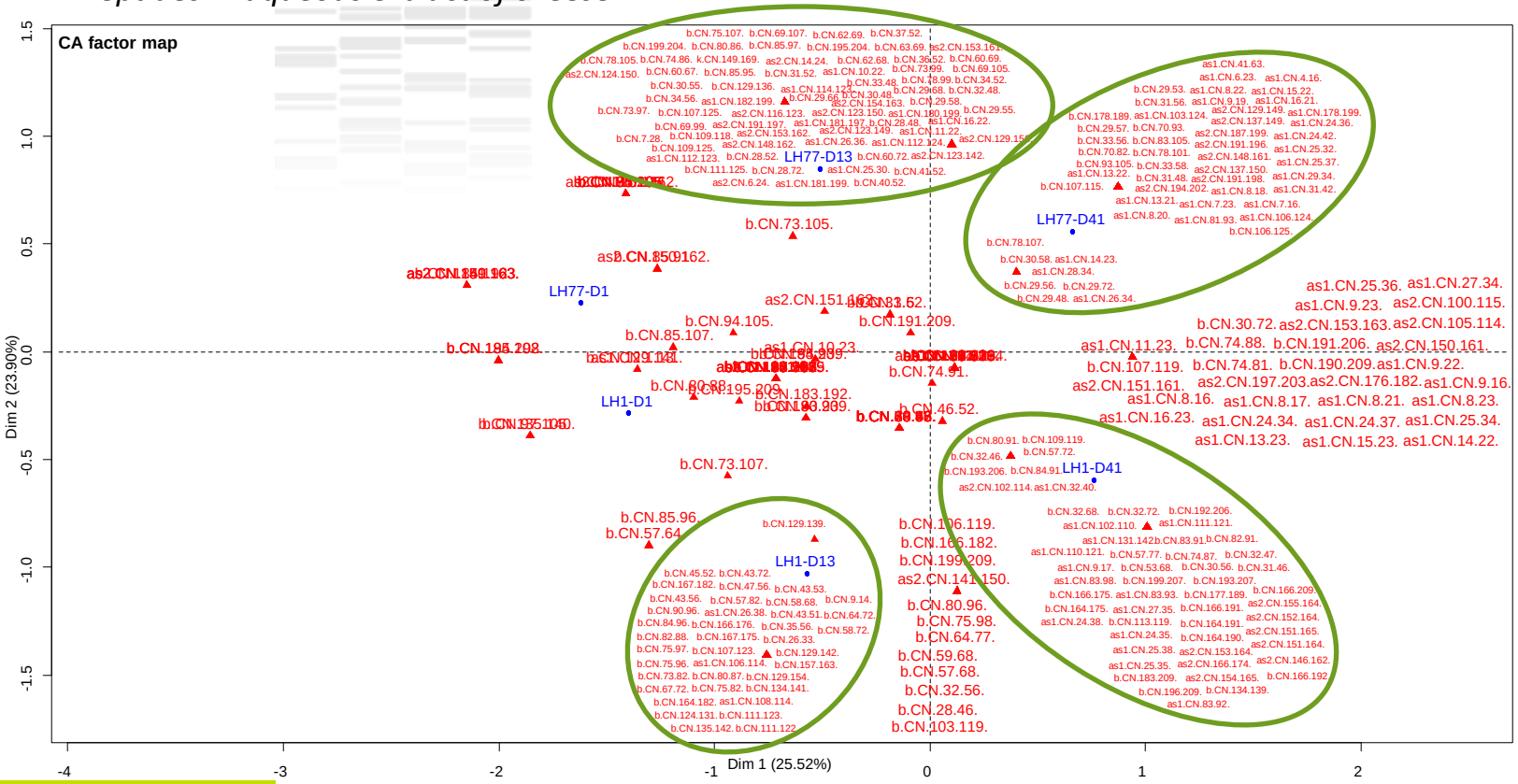


*Solid extract =*
*Cheese matrix after extraction of aqueous extract*

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*

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

| D1 | D13 | D41 | D41 |
|---|---|---|---|
| b.CN.84.93.=0 | b.CN.80.90.=1 | b.CN.74.88.=1 | as1.CN.9.23.=1 |
| b.CN.74.82.=0 | b.CN.47.52.=1 | b.CN.74.81.=1 | as1.CN.9.22.=1 |
| b.CN.53.72.=0 | b.CN.32.58.=1 | b.CN.30.72.=1 | as1.CN.9.16.=1 |
| b.CN.35.52.=0 | b.CN.195.207.=1 | b.CN.191.206.=1 | as1.CN.8.23.=1 |
| b.CN.32.52.=0 | b.CN.195.202.=1 | b.CN.190.209.=1 | as1.CN.8.21.=1 |
| b.CN.30.52.=0 | b.CN.194.207.=1 | b.CN.129.141.=0 | as1.CN.8.17.=1 |
| b.CN.29.52.=0 | b.CN.194.206.=1 | b.CN.107.119.=1 | as1.CN.8.16.=1 |
| b.CN.195.206.=0 | b.CN.167.176.=1 | as2.CN.197.203.=1 | as1.CN.27.34.=1 |
| b.CN.194.208.=1 | b.CN.135.141.=1 | as2.CN.176.182.=1 | as1.CN.25.36.=1 |
| b.CN.185.192.=1 | b.CN.126.133.=1 | as2.CN.153.163.=1 | as1.CN.25.34.=1 |
| b.CN.111.119.=0 | as2.CN.101.115.=1 | as2.CN.151.161.=1 | as1.CN.24.37.=1 |
| b.CN.103.113.=0 | as1.CN.181.189.=1 | as2.CN.150.161.=1 | as1.CN.24.34.=1 |
| as2.CN.101.114.=0 | as1.CN.10.23.=0 | as2.CN.105.114.=1 | as1.CN.16.23.=1 |
| as1.CN.24.30.=0 | | as2.CN.100.115.=1 | as1.CN.15.23.=1 |
| as1.CN.17.23.=0 | | | as1.CN.14.22.=1 |
| | | | as1.CN.13.23.=1 |
| | | | as1.CN.1.13.=0 |
| | | | as1.CN.11.23.=1 |

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

Peptides are significatively different at D1, D13 and D41.

Proteolysis is the main factor which modulate the stretchability.

# To verify our strategy…

Cheese at J13

↓

Water + crushing

↓

Centrifugation → Water extract

↓

Pellet

↓

EDTA 150mM + crushing

↓

Centrifugation → EDTA extract

↓

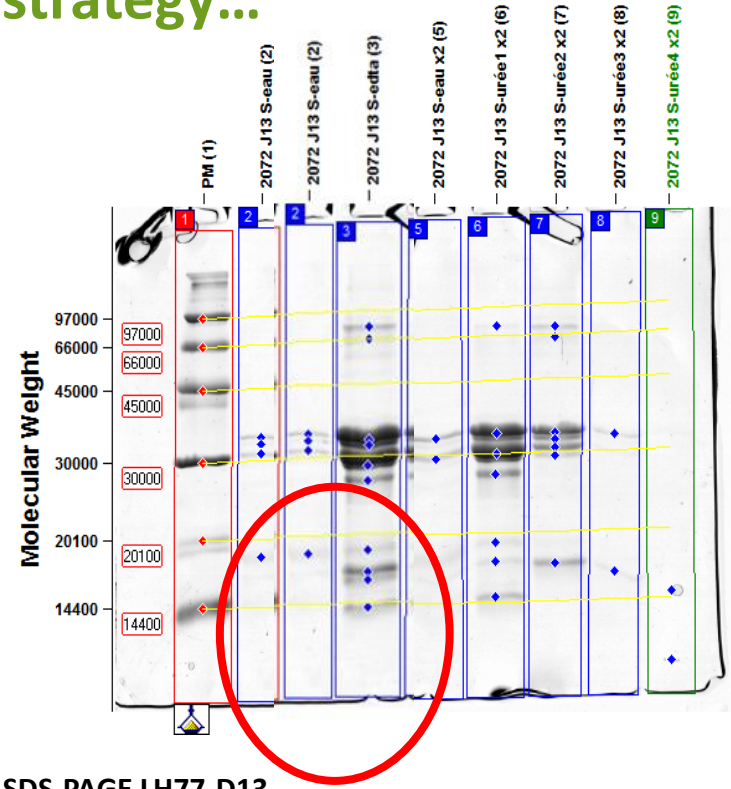
Pellet

↓

Urea 6M + crushing

↓

Centrifugation → Urea extract

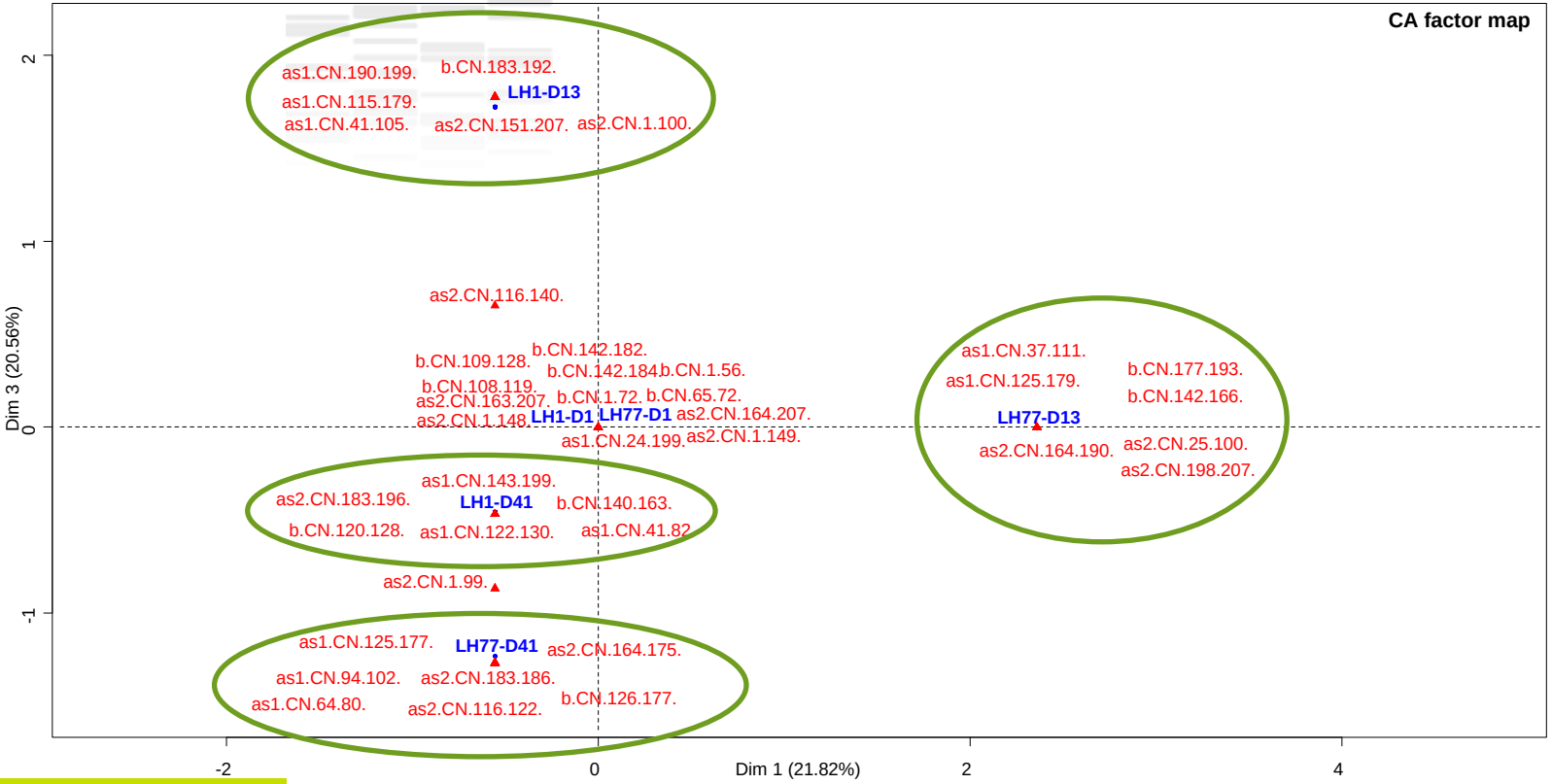



**SDS-PAGE LH77-D13**

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

Casein αs1-(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*



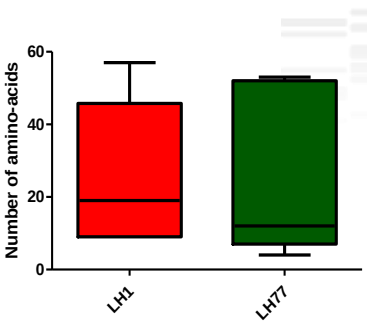

Each cheese possesses a different peptide profile.

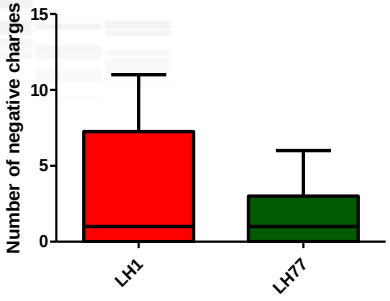
At D1, the peptide profiles are similar.

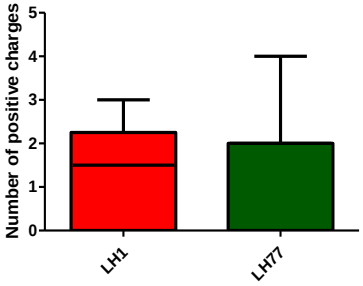
At D41, the majority of peptides is derived from αs1-casein and αs2-casein.

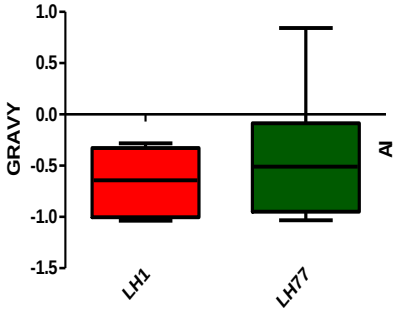
LH1 LH77

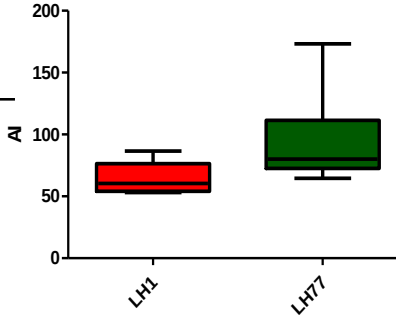
# Relationship between cheese stretchability and peptide characteristics (D41)

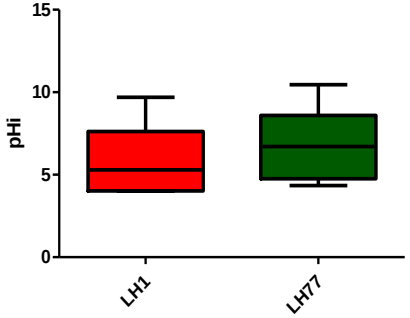


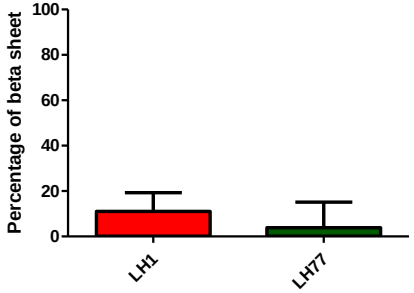



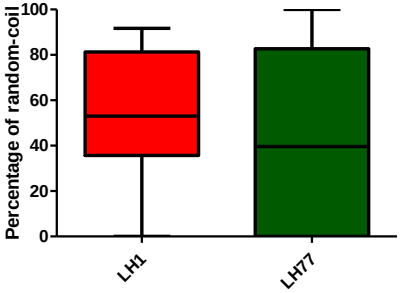



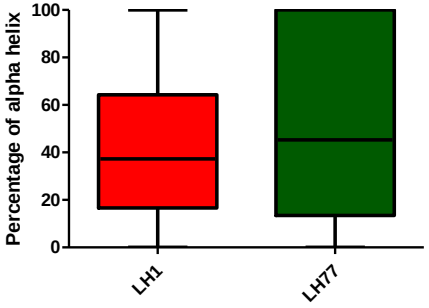



# Advantages / Disadvantages

- ✓ 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.

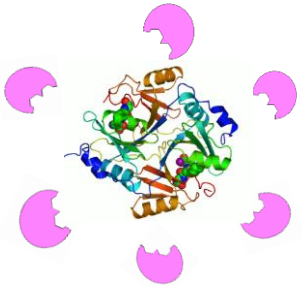
# Conclusion & Perspectives

## To recap:

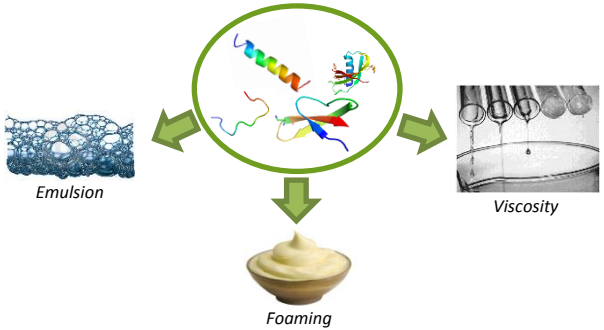
**Identification of peptides** in aqueous extract of cheese ⇨ Identification of **cleavage sites** ⇨ Deduction of **peptides in cheese matrix** ⇨ Multivariated analysis ⇩ **pools of peptides related to stretchability** ⇨ **Calculate the peptide characteristics** in each pool to connect these characteristics 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**



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# THANK YOU FOR YOUR ATTENTION

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