Does aroma composition allow to discriminate groups of dark chocolates categorized on the basis of their organoleptic properties? Inputs of direct-injection mass spectrometry (PTR-ToF-MS) and GC-Olfactometry

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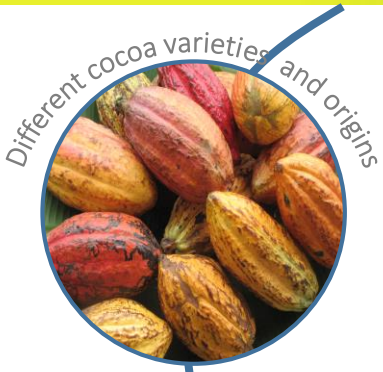


Same process of fabrication

Sensory evaluation

Final Objective:
Find key aroma compounds typical for each sensory poles in chocolate

1st hypothesis:
The sensory classification of the chocolates is mainly based on their composition in volatile organic compounds (VOCs)

1st objective:
Obtain the volatile compounds fingerprints of the 187 chocolates

Obtain the VOCs fingerprints

Samples preparation

+ 1mL of artificial saliva *

Stirring in a water bath at 36.2°C

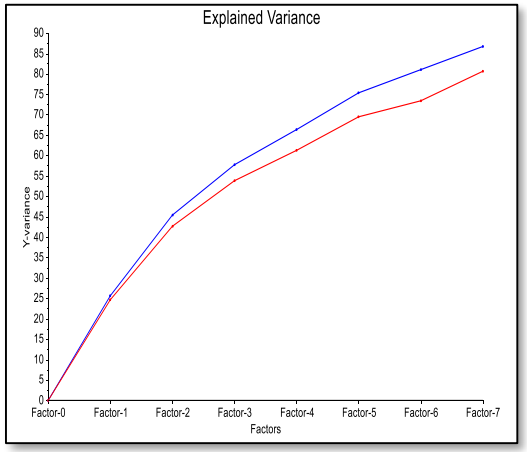
Equilibrating for 2h

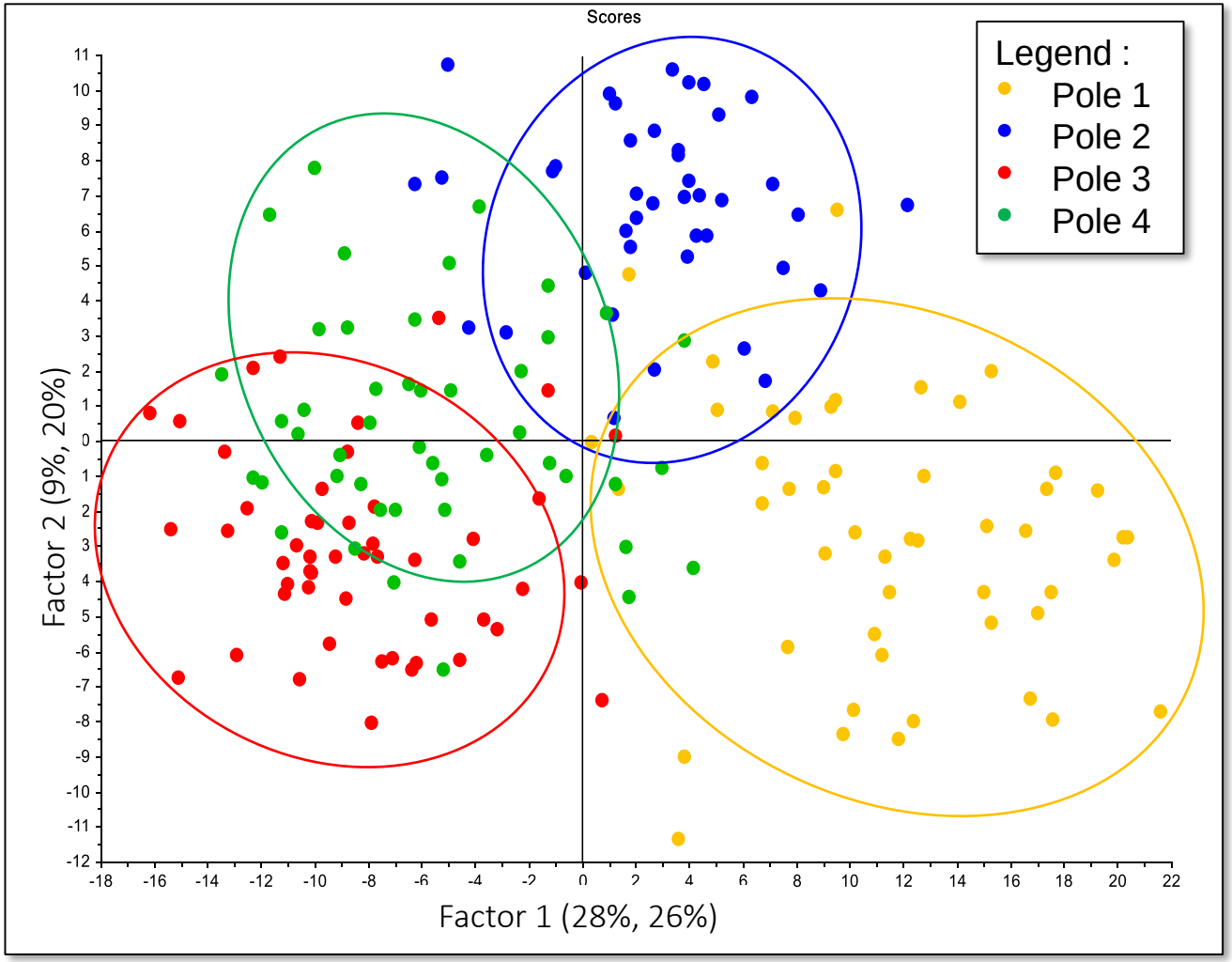
* water + salt + alpha amylase + mucins

Samples analysis: PTR-ToF-MS

Obtain the VOCs fingerprints

R-Square :
Calibration : 0.84
Validation: 0.80

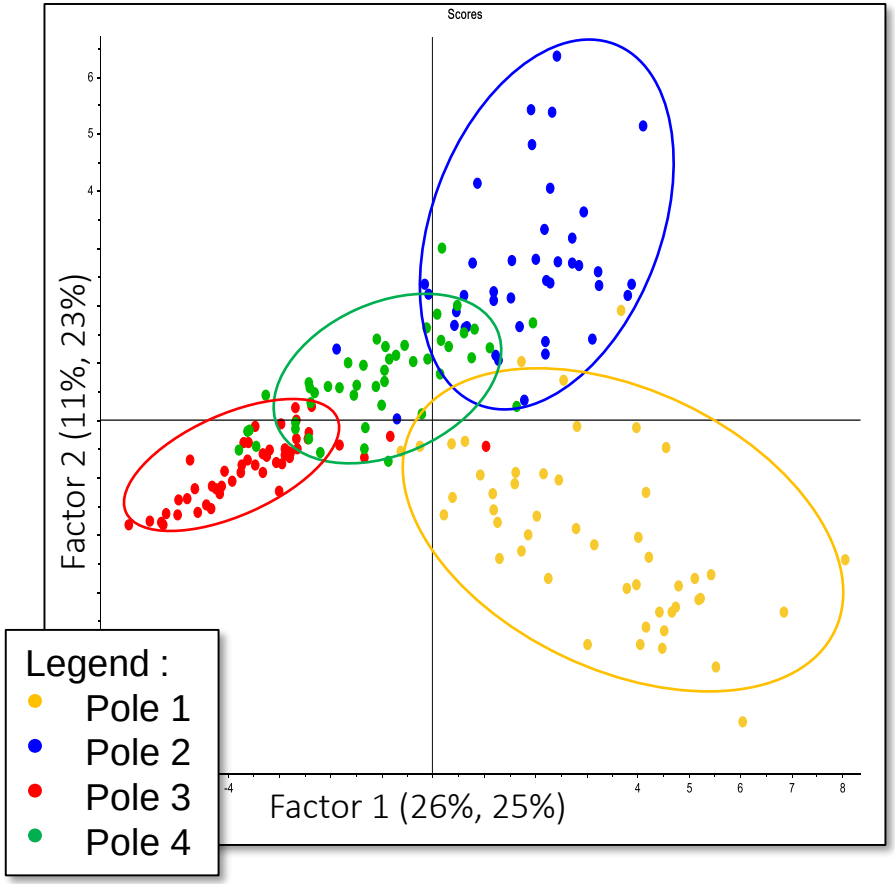




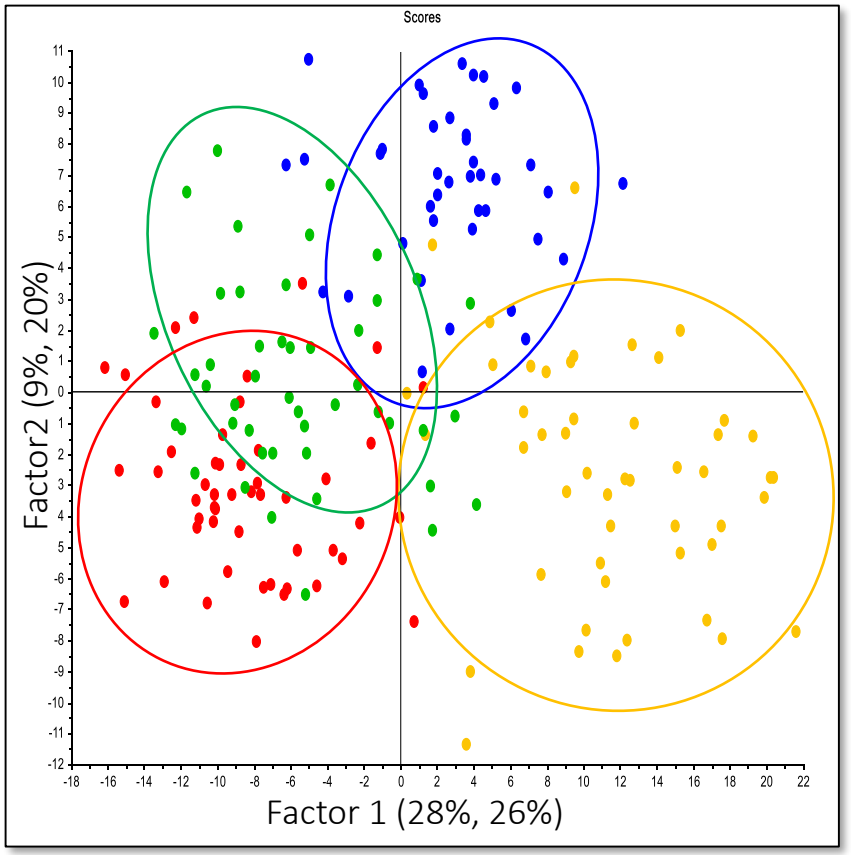
PLS-DA with chemical data (factors 1 and 2) 187 samples distributed in 4 sensory poles (Y variables) / 314 ions (X variables)

Obtain the VOCs fingerprints

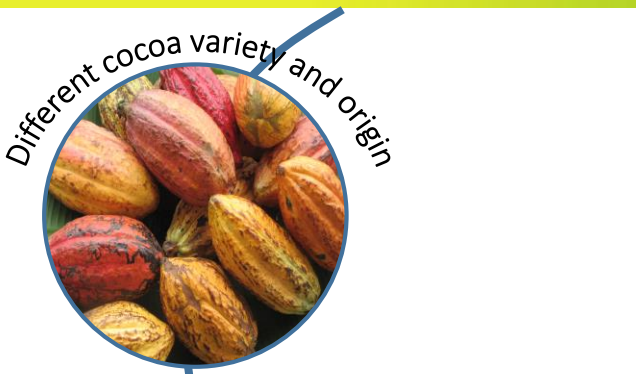
PLS-DA with **sensory data** (factors 1 and 2), 187 samples /36 sensory descriptors



PLS-DA with **chemical data** (factors 1 and 2), 187 samples/ 314 ions



The produced “chemical maps” showed that the headspace PTR-MS analyses of the chocolates allowed retrieving the classification of the 187 samples into the four sensory categories previously determined



Same process of fabrication

Sensory evaluation

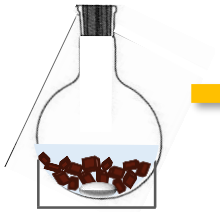
The 1st hypothesis is validated

2nd hypothesis:
There are volatile organic compounds typical for each pole

2nd objective:
Analyse compounds which have an olfactive impact, identify them and find key organic compounds for each pole

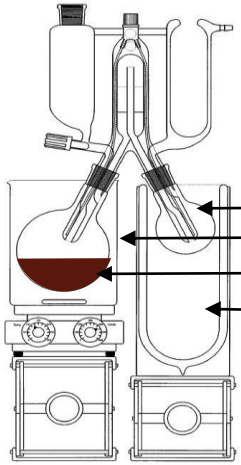
Identification of key aroma compounds

Flavour extraction

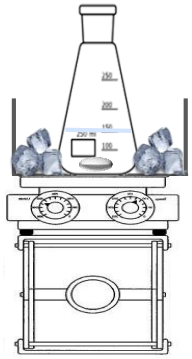


30 g of chocolate
+ 300 µL internal standard
+ 100 mL of MiliQ water

SAFE

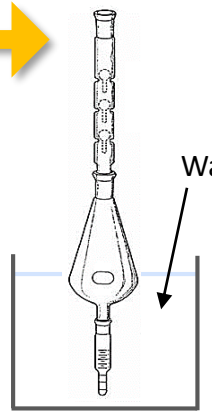


Liquid-liquid extraction

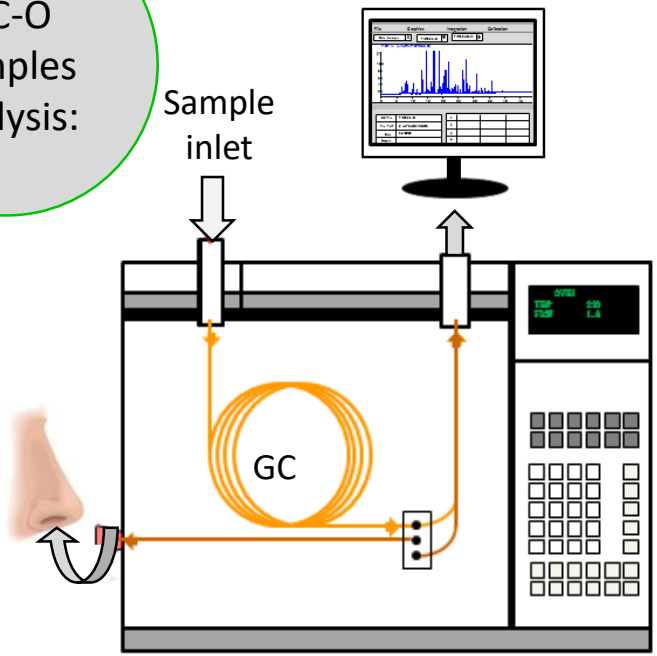


extraction with CH_2Cl_2
(3 x 15ml)

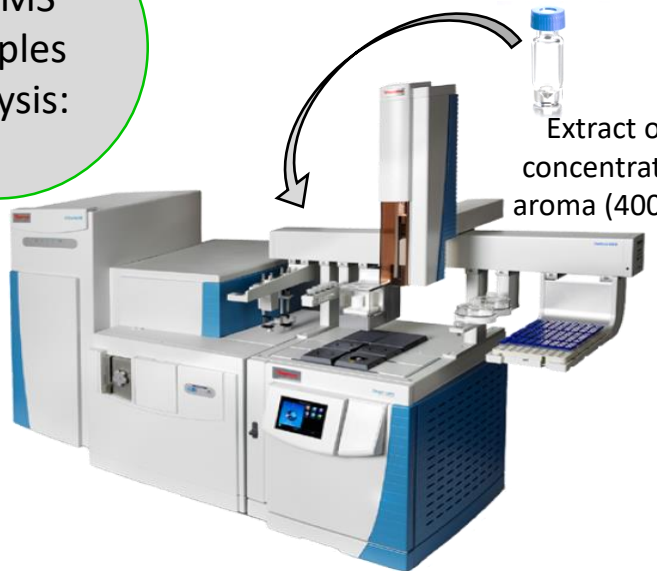
Concentration with Kuderna-Danish



GC-O samples analysis:



GC-MS samples analysis:



Identification of key aroma compounds

One average index = one odorant area
Number of repetition = detection frequency

Average index	Number of repetition	Common descriptors
1072	4	Fruity, floral
1109	3	Roasted
1173	6	Solvent, fruity
1195	5	Fruity
1248	3	Unpleasant
1293	7	Butter, fruity
1296	4	Fruity, floral
1308	11	Mushrooms
1326	4	Roasted, peanuts
1346	8	Cereal, roasted
1384	8	Metal

Samples

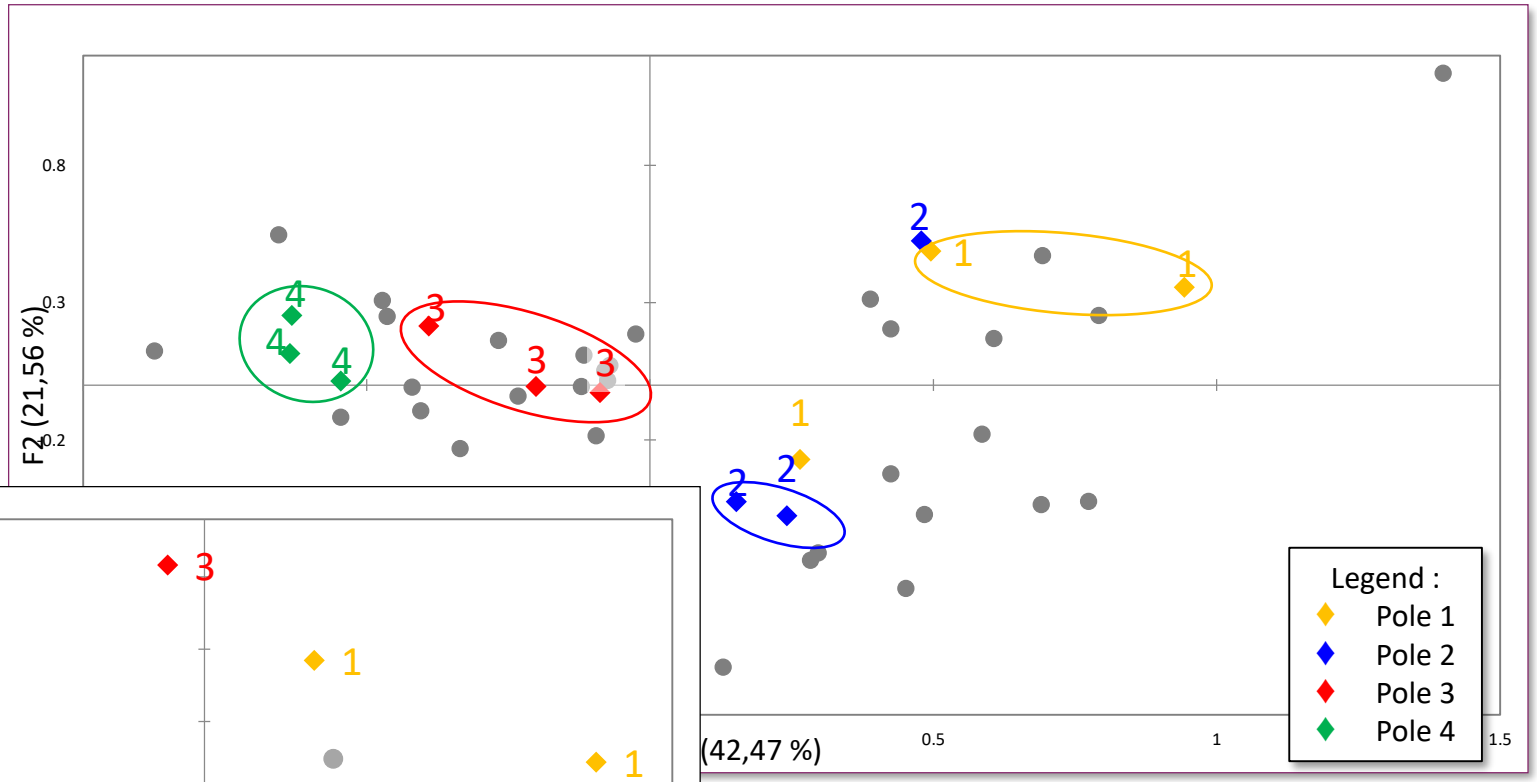
	1-51	1-52	1-53	2-45	2-47	2-48
994	12	10	10	11	12	12
1054	6	7	5	6	6	7
1065	4	3	2	5	4	2
1072	4	9	5	6	8	5
1109	3	3	1	2	5	9
1127	1	4	0	2	5	6
1140	0	0	0	0	1	3
1172	6	5	2	4	1	3
1183	0	4	2	1	6	7
1196	5	5	2	1	9	6
1201	2	4	0	0	3	5
1211	2	4	0	5	6	4
1250	3	2	4	2	4	4
1267	2	5	0	1	12	9
1293	7	9	10	6	9	6
1296	4	0	0	0	2	0
1309	11	10	12	12	12	12
1323	4	5	2	4	7	6
1332	0	0	2	0	6	4
1336	1	2	0	2	2	0
1346	8	8	6	9	11	9

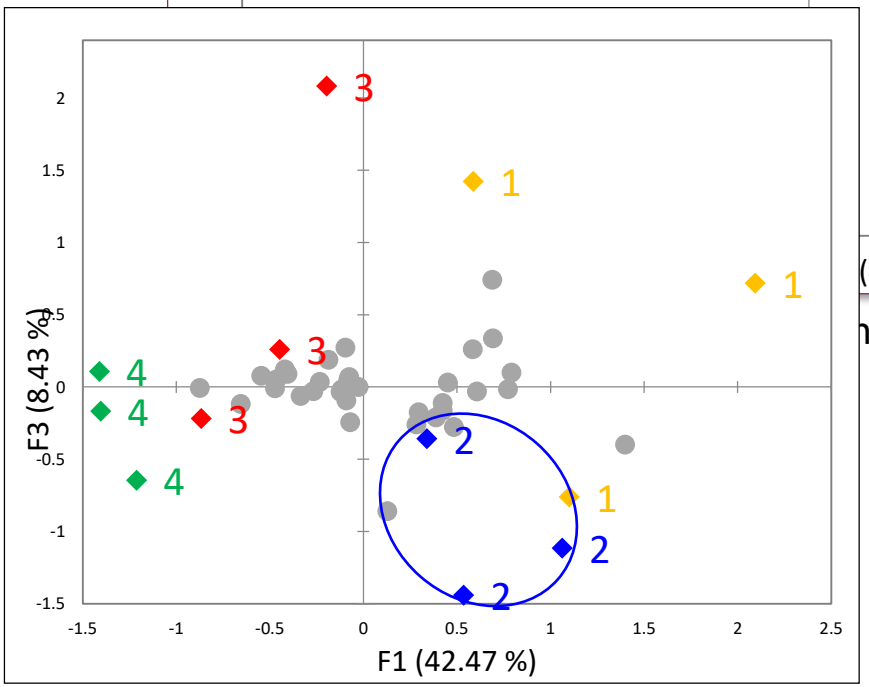
OAs

Extract of the table with detection frequencies of 124 odorant areas (OAs) in 12 samples

Selection of discriminant OAs showing differences between higher and lower detection frequencies values in samples > 30%

Identification of key aroma compounds





Correspondence analysis (factors 1 and 3)

nd 2): detection frequencies of 34 OAs (grey

OAs	Compounds	Odor attribute
1126	Pentan-2-ol	Fruity
1461	Acetic acid	Vinegar
1795	Ethyl phenylacetate	Floral
1824	2-phenylethyl acetate	Fruity, floral
2204	δ-Decalactone	Fruity, floral

Take home messages

- The analysis of VOCs allows retrieving the classification of the 187 samples into the four sensory categories previously determined
- Sensory classification of the chocolates could be explained chiefly by the profiles of flavour compounds released by the matrix but not in its entirety
- There are OAs for each pole which have been identified thanks to correspondence analysis. Unidentified OAs due to coelutions will be resolved using a GC-2D analysis.

Yes, aroma composition allows to discriminate groups of dark chocolates categorized on the basis of their organoleptic properties

Thanks

Jean Luc Le Quéré & Hélène Labouré & Renaud Boulanger

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The International Cocoa Organization

Thanks for your attention

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