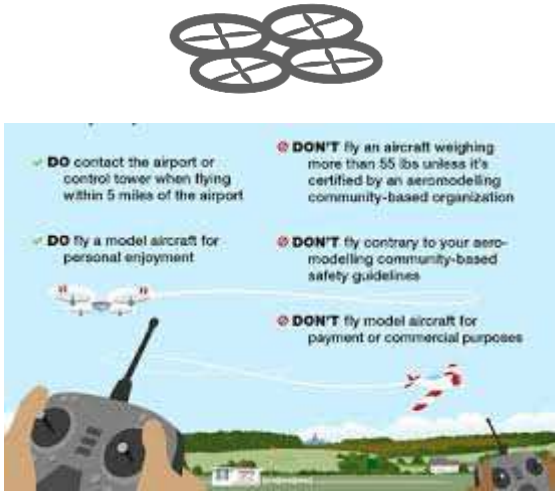
Vegetable oil speciation in processed foods

how legislation drives innovation

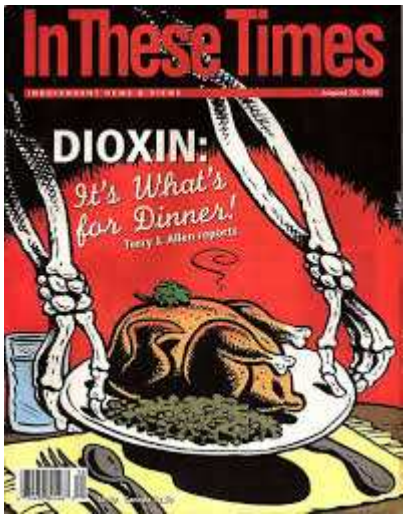
Dr Tassos Koidis

Lecturer in Food Science and Nutrition

legislation *vs* innovation



Food safety legislation is very strict



efsa
European Food Safety Authority

FOOD STANDARDS AGENCY

Supermarket apologises after food watchdog's findings

HORSE MEAT IN TESCO BURGERS

Food labelling*: the exemption*

The labels are complex and yet informative

INGREDIENTS
Water, Carrots, Onions, Red Lentils (4.5%) Potatoes, Cauliflower, Leeks, Peas, Cornflower, **Wheat**flour, Cream (**milk**), Yeast Extract, Concentrated Tomato Paste, Garlic, Sugar, **Celery** Seed, Sunflower Oil, Herb and Spice, White Pepper, Parsley
ALLERGY ADVICE
For allergens, see ingredients in **bold**

The EU has the stricter legislation in the world

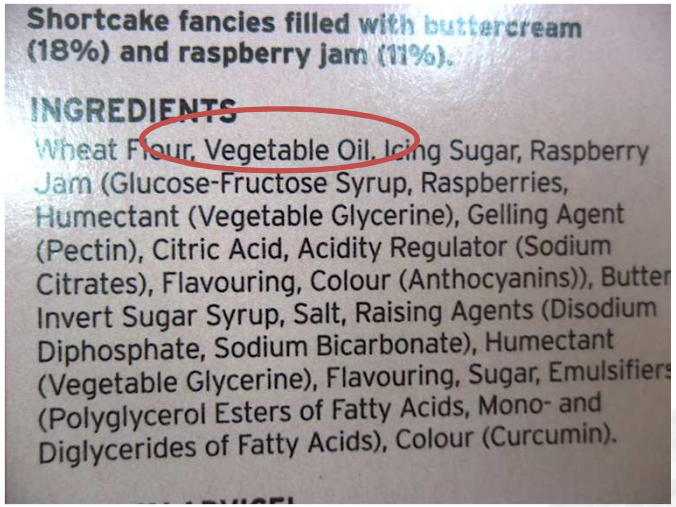
IN THERE THE REGULATOR PUTS SOME STRICT RULES THAT COMPANIES MUST ADHERE BUT NOT ALWAYS THE RESEARCH EXIST TO POLICE THE LEGISLATION PROPERLY…

New Regulation in place

for vegetable oils sold as ingredients in processed foods

- EC Regulation 1169/2011, food businesses required to declare the composition of the oil mixture in the food product label. [Dec 2014: live]
- vegetable oils of interest: **palm, sunflower, rapeseed; coconut oil**
- Monitoring the compliance of the regulation is challenging for national bodies and other enforcers.


Mr
KIPLING
Exceedingly good...
6 VIENNESE WHIRLS
WITH A RASPBERRY JAM AND BUTTERCREAM FILLING

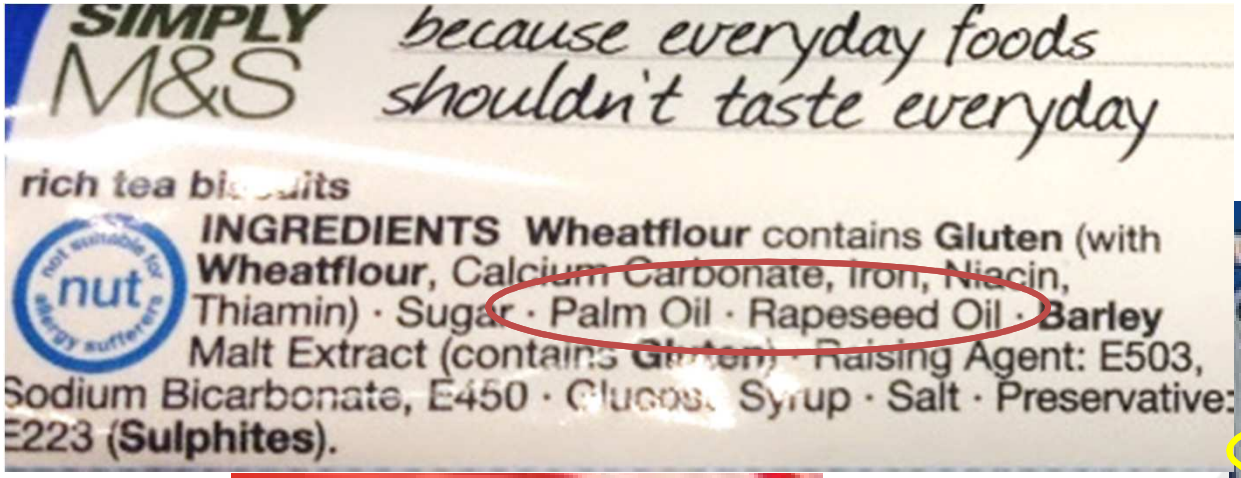

Shortcake fancies filled with buttercream (18%) and raspberry jam (11%).
INGREDIENTS
Wheat Flour, Vegetable Oil, Icing Sugar, Raspberry Jam (Glucose-Fructose Syrup, Raspberries, Humectant (Vegetable Glycerine), Gelling Agent (Pectin), Citric Acid, Acidity Regulator (Sodium Citrates), Flavouring, Colour (Anthocyanins)), Butter
Invert Sugar Syrup, Salt, Raising Agents (Disodium Diphosphate, Sodium Bicarbonate), Humectant (Vegetable Glycerine), Flavouring, Sugar, Emulsifiers
(Polyglycerol Esters of Fatty Acids, Mono- and Diglycerides of Fatty Acids), Colour (Curcumin).

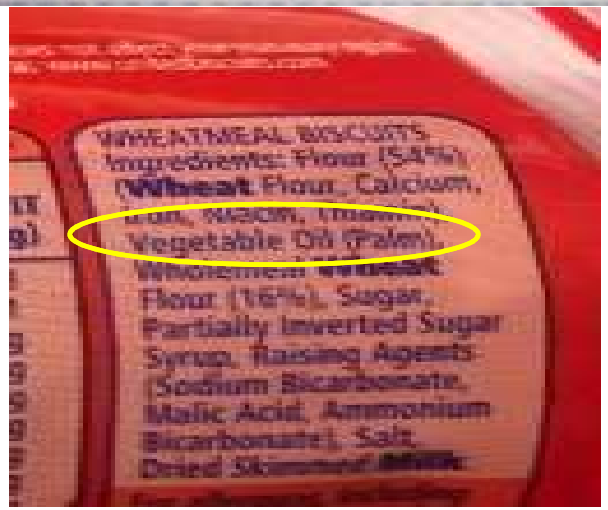

OLD EL PASO
8 Tortillas
MINI
SUPER SOFT
FLOUR
THE SAME GREAT TASTE
NOW WITH 40%


TESCO
SCONE
MIX
JUST ADD MILK
HOME BAKING


V Suitable for vegetarians
Ingredients
Wheat Flour, Sugar, Vegetable Oil, Raising Agents (Calcium Phosphate, Potassium Bicarbonate), Salt.
Our promise
We are happy to refund or replace any Tesco product which falls below the high standard you expect. Just ask any member of staff.


Ingredients: Wheat flour, water, stabiliser (glycerol), vegetable oil, raising agents (sodium bicarbonate, sodium acid pyrophosphate), emulsifier (mono and diglycerides of fatty acids), dextrose, salt, preservative (potassium sorbate). Packaged in a protective atmosphere.
CONTAINS WHEAT INGREDIENTS.


SIMPLY M&S
because everyday foods shouldn't taste everyday
rich tea bi uits
nut
INGREDIENTS Wheatflour contains Gluten (with Wheatflour, Calcium Carbonate, Iron, Niacin, Thiamin) · Sugar · Palm Oil · Rapeseed Oil · Barley Malt Extract (contains Gluten) · Raising Agent: E503, Sodium Bicarbonate, E450 · Glucose Syrup · Salt · Preservative: E223 (Sulphites).


Vegetable Oil (Palm),
Flour (16%), Sugar,
Partially Inverted Sugar
Syrup, Raising Agents
(Sodium Bicarbonate,
Malic Acid, Ammonium
Bicarbonate), Salt,


No hydrogenated
CRISP BISCUITS
Ingredients: Wheat Flour
(with Calcium, Iron,
Vegetable Oil (Sunflower),
Barley Malt Extract,
Raising Agents (Sodium
Bicarbonate, Ammonium
Bicarbonate), Salt.
For allergens, including
cereals containing gluten,
see ingredients in Bold.
May also contain Soya.

Can you find out what type of

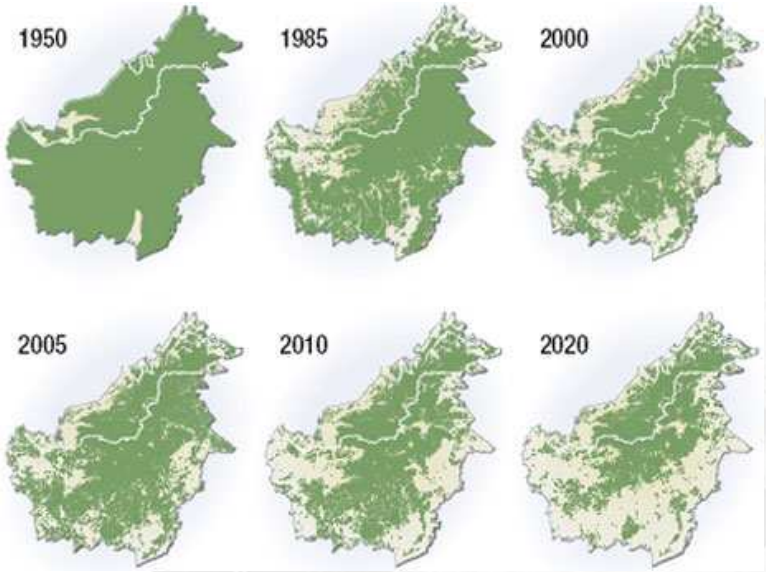
vegetable oil

is present in processed foods?

analytical method capable to identify oil species in the vegetable oil blends?

What is the issue with palm oil?

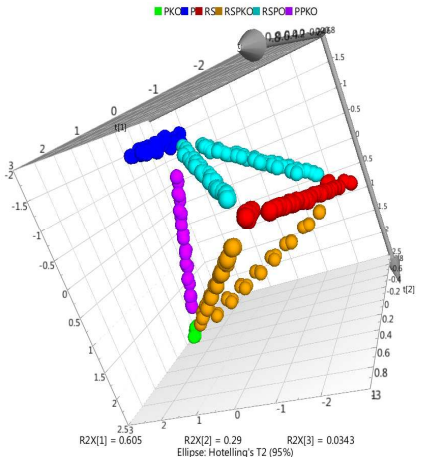
- sustainable production?
  production raised 500% during the last 20 years
- Fair trade / fair wages?
- Deforestation



In supermarkets, 50% of all baked goods, confectionery, spreads, cosmetics, cleaning agents, air fresheners etc.

the average first-world citizen consumes at least 10kg of palm oil each year!

Fusion of spectroscopy and chromatography



Fingerprinting

Staged procedure

Is to extract information about the whole of the sample product by analysing a wealth of variables that defines it which on their own they might not mean much but in systematically viewing them all together do supply a overview of the unique "character" (fingerprint) of the sample.

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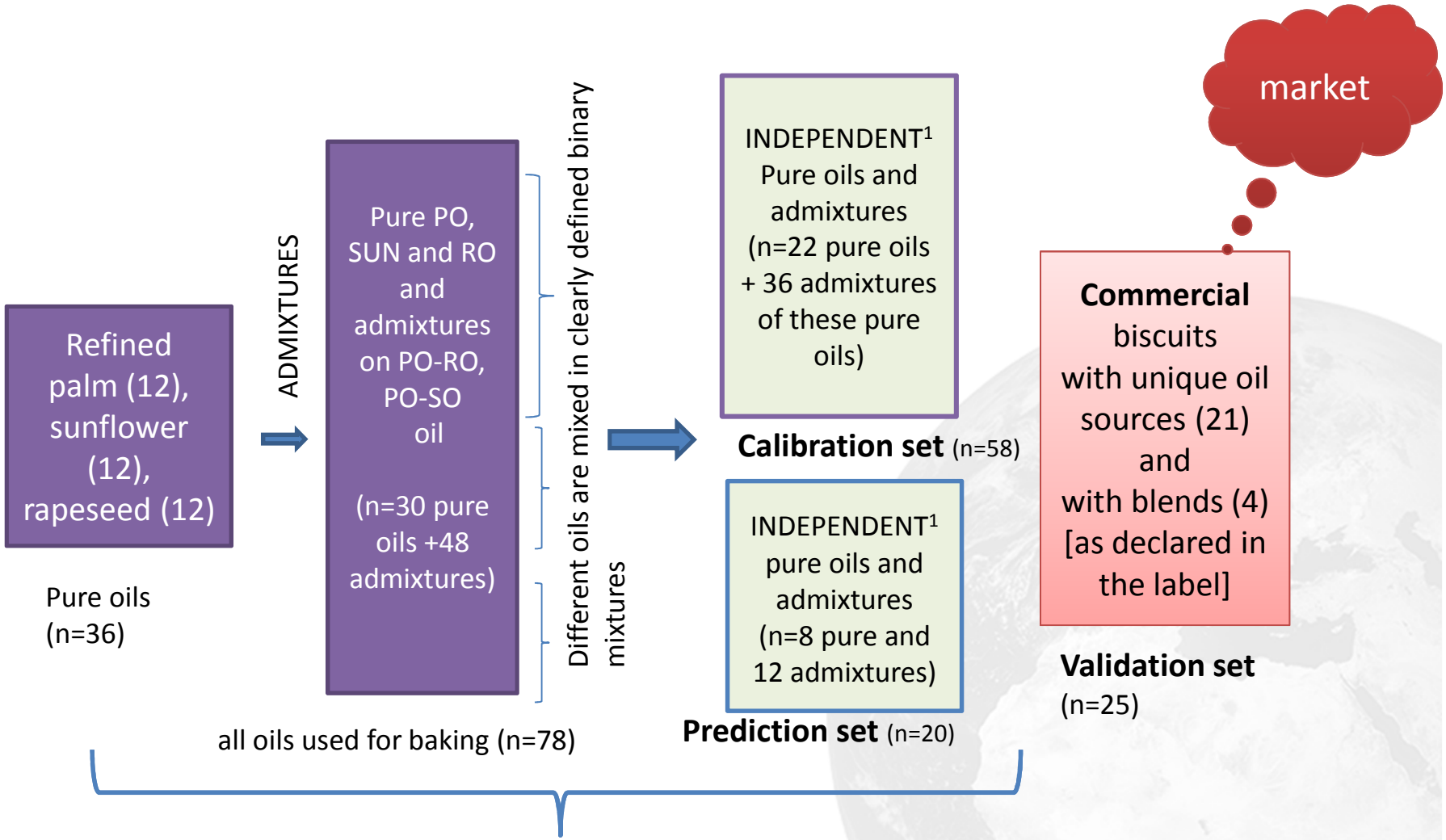

Osorio, M.T., Haughey, S., Elliott, C., **Koidis, A.** (2015).. *Food Chemistry,* 189, 67-73

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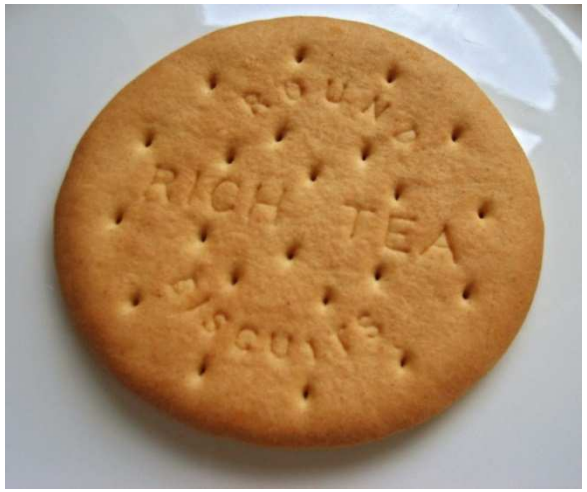
IDENTIFICATION OF VEGETABLE OIL SPECIES IN BISCUITS



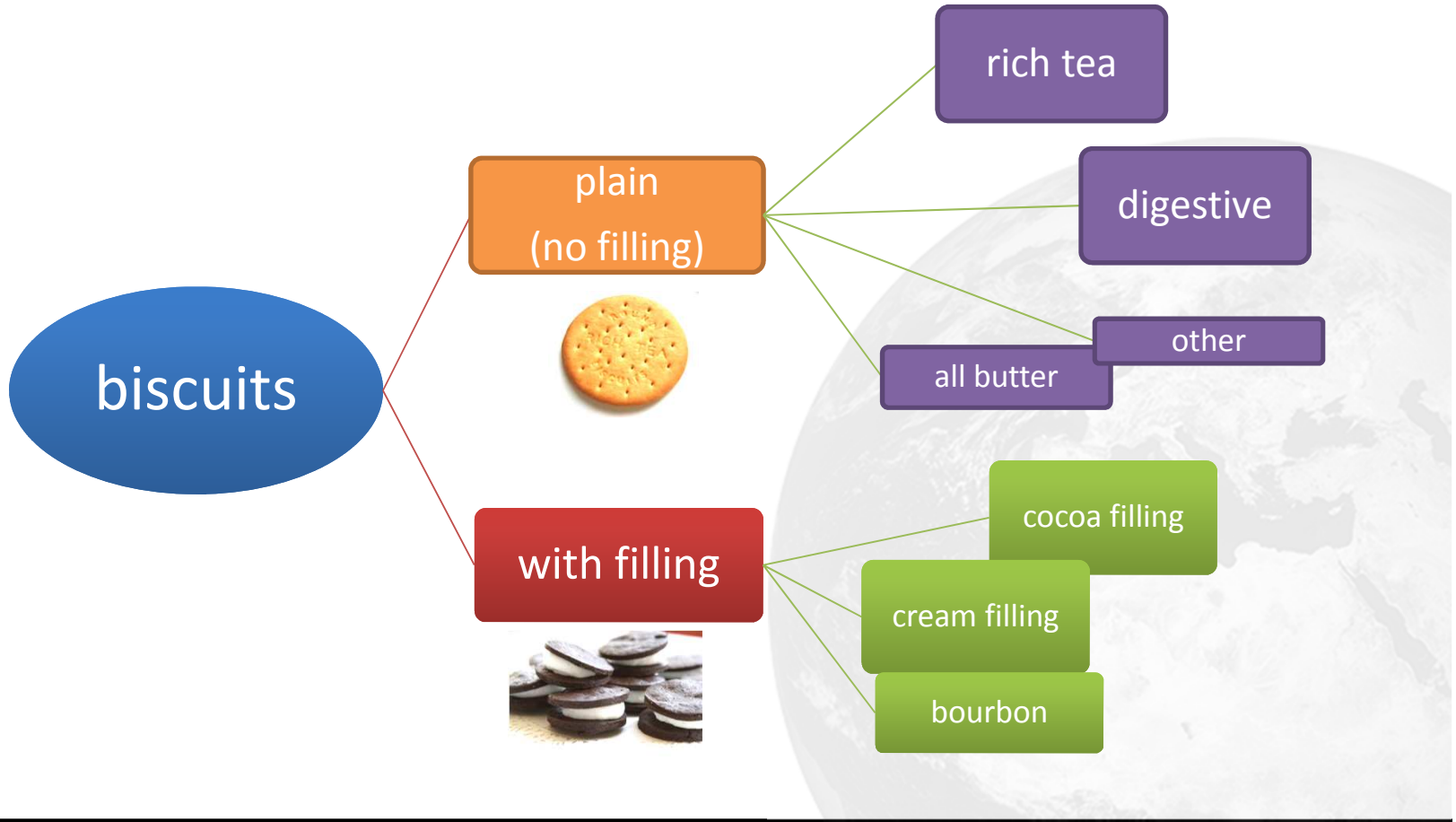
the use of vegetable oils in bakery products

A “crust” that has a “hard” oil like palm stearin
A “creamy” sauce that has a “soft” vegetable, fat, for example, palm olein, rapeseed oil or coconut oil

pastry Crust: Hard fraction → Palm Stearin

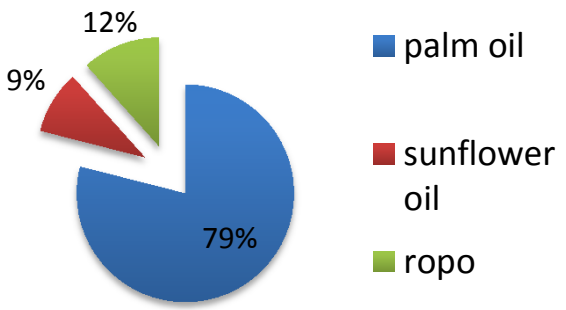
filling: Soft fraction→ Palm Olein

Bakery/pastry products



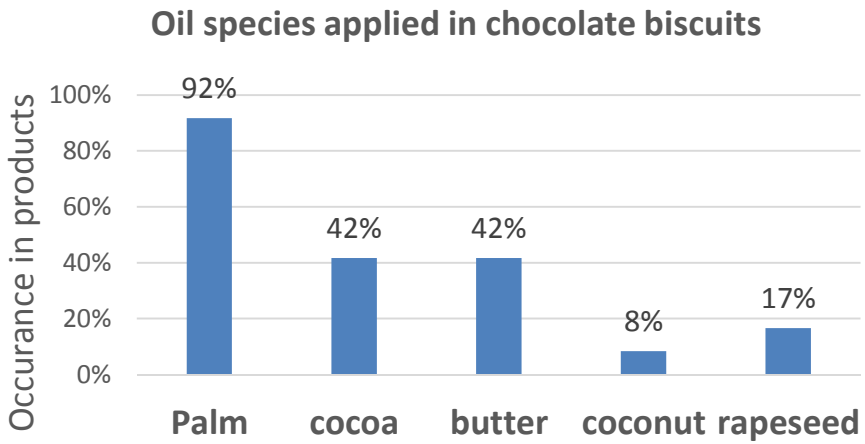
Market study / Industry intelligence

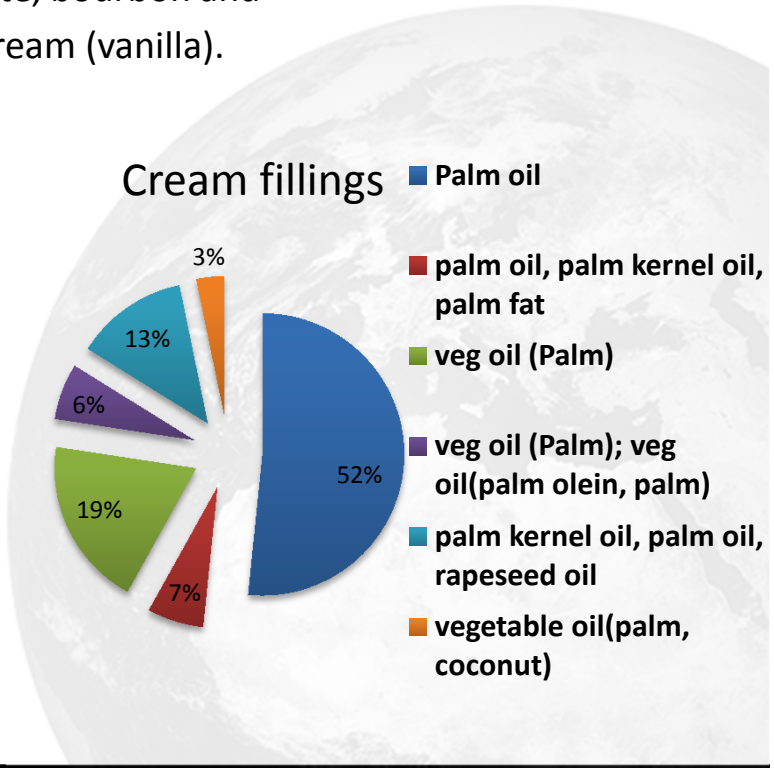
In biscuits without fillings



In biscuits with fillings..

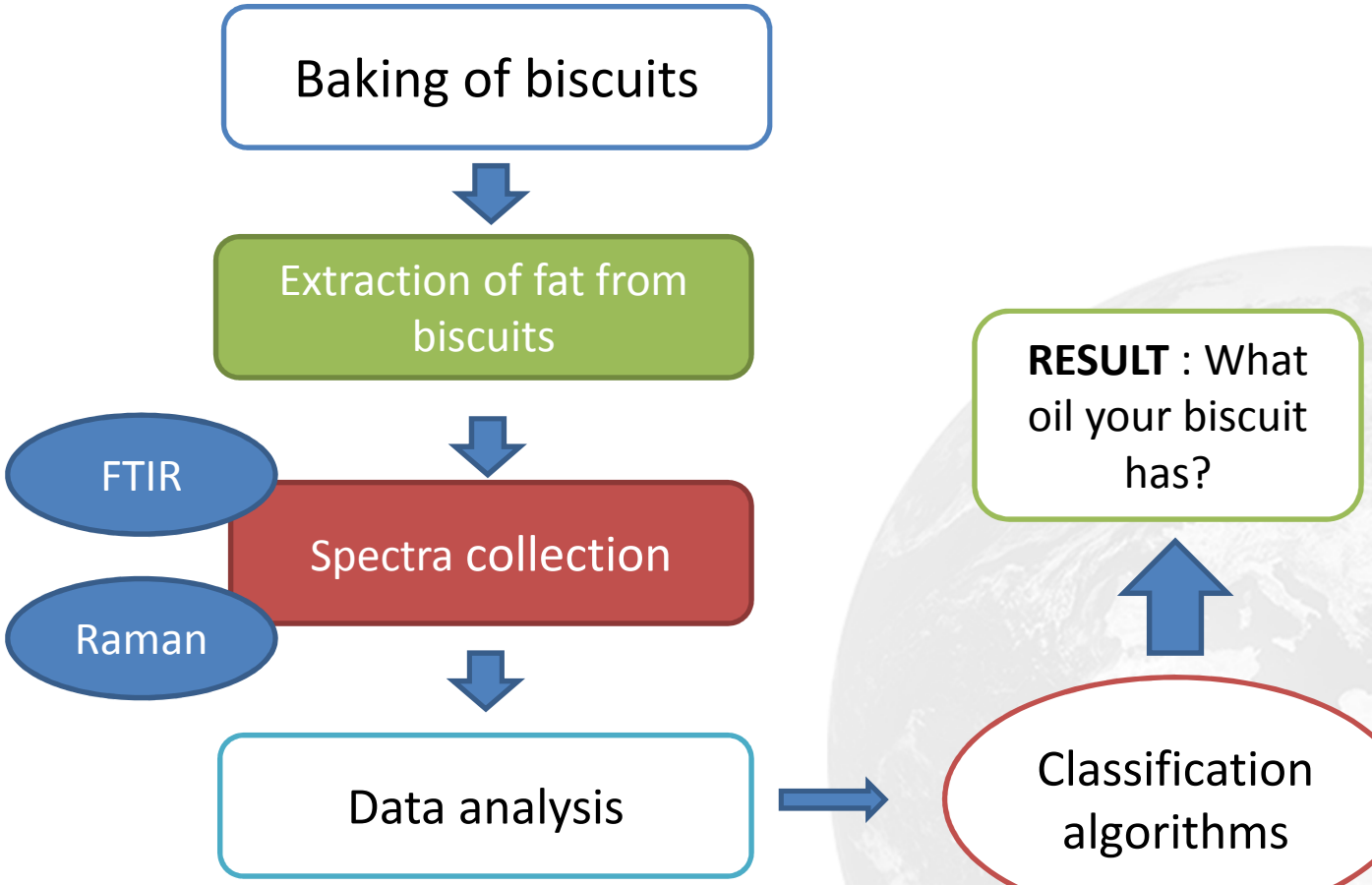
Common fillings include chocolate, bourbon and white cream (vanilla).



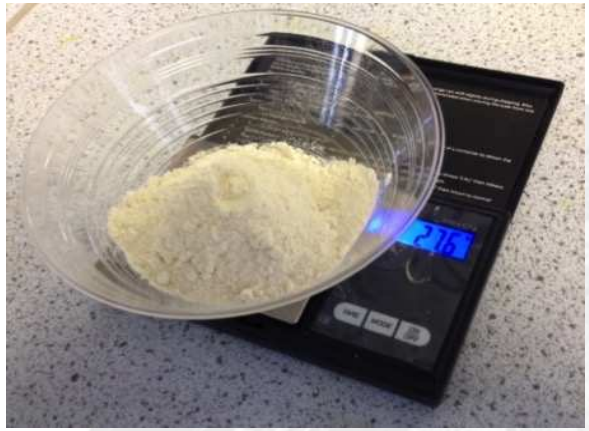


Key features of the study

- 36 authentic vegetable oil samples
  - 12 palm, 12 sunflower, 12 rapeseed oils
  - trusted sources from the industry
  - in house chemical analysis with official methods
- 48 admixtures of oils
  - (ROPO, SOPO)
- 5 oil classes (PO, SO, ROPO, SOPO, RO) trained with supervised discriminative algorithms
- 3+ layers of validation


Baking of biscuits
Extraction of fat from biscuits
FTIR
Raman
Spectra collection
Data analysis
Classification algorithms
RESULT : What oil your biscuit has?

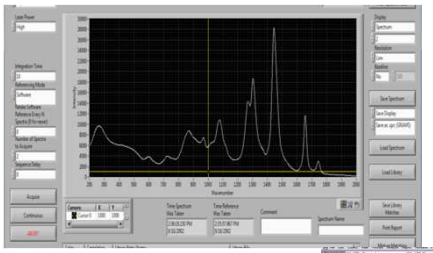
In-house baking

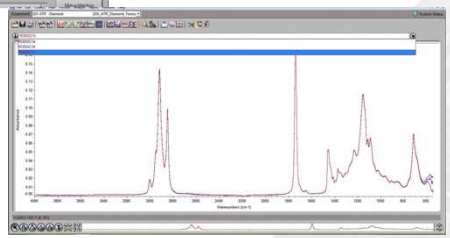


solvent extraction

spectra acquisitions

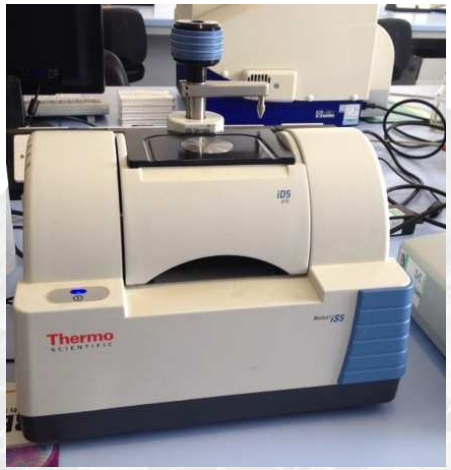
raman





- 1064 nm laser frequency
- 200 - 2000 cm^{-1} range
- 10 cm^{-1} resolution

ftir



- 400 - 4000 cm^{-1} range
  - DTGS detector on d-ATR
- number of scans: 32
- resolution: 4.0

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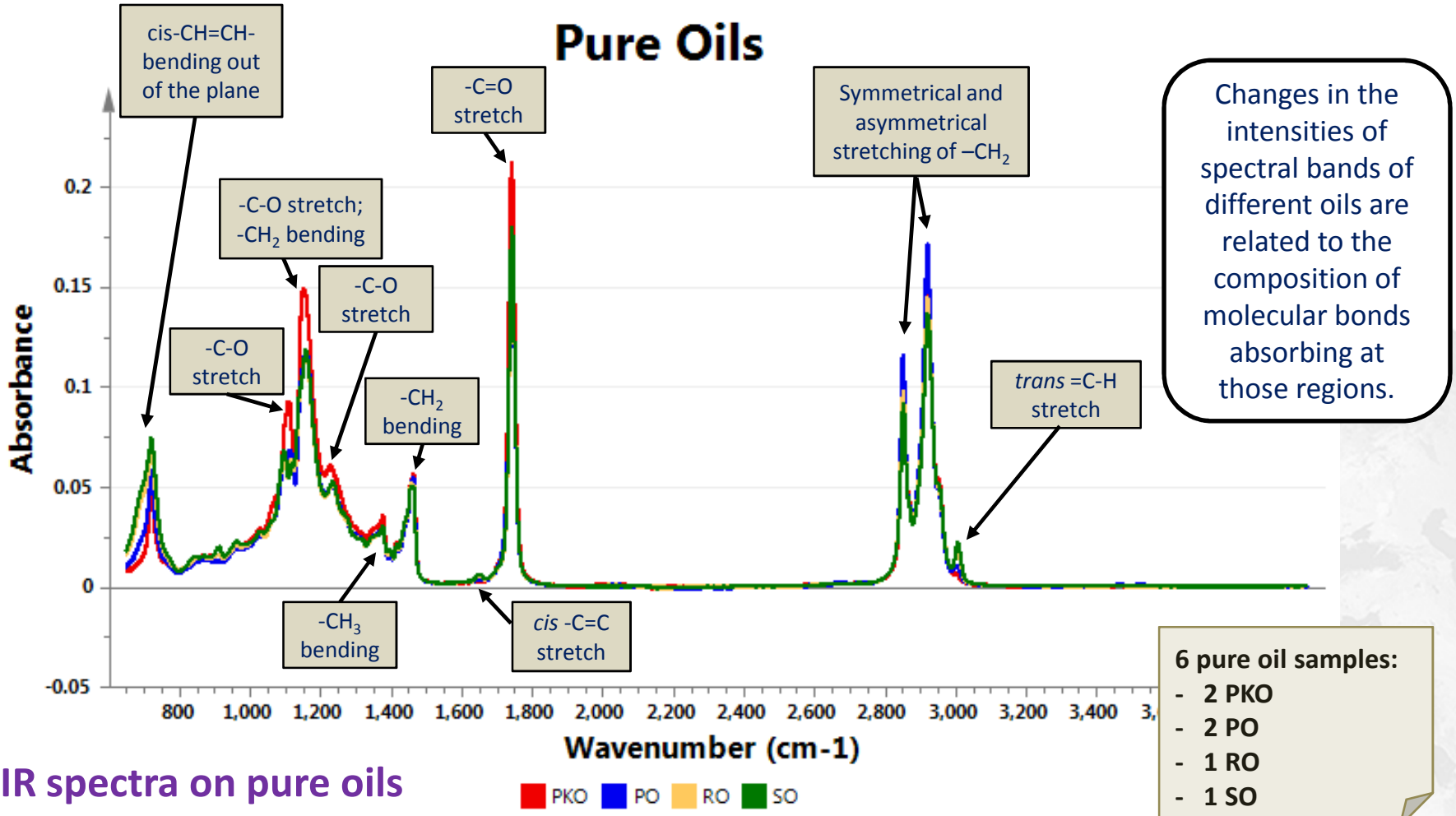


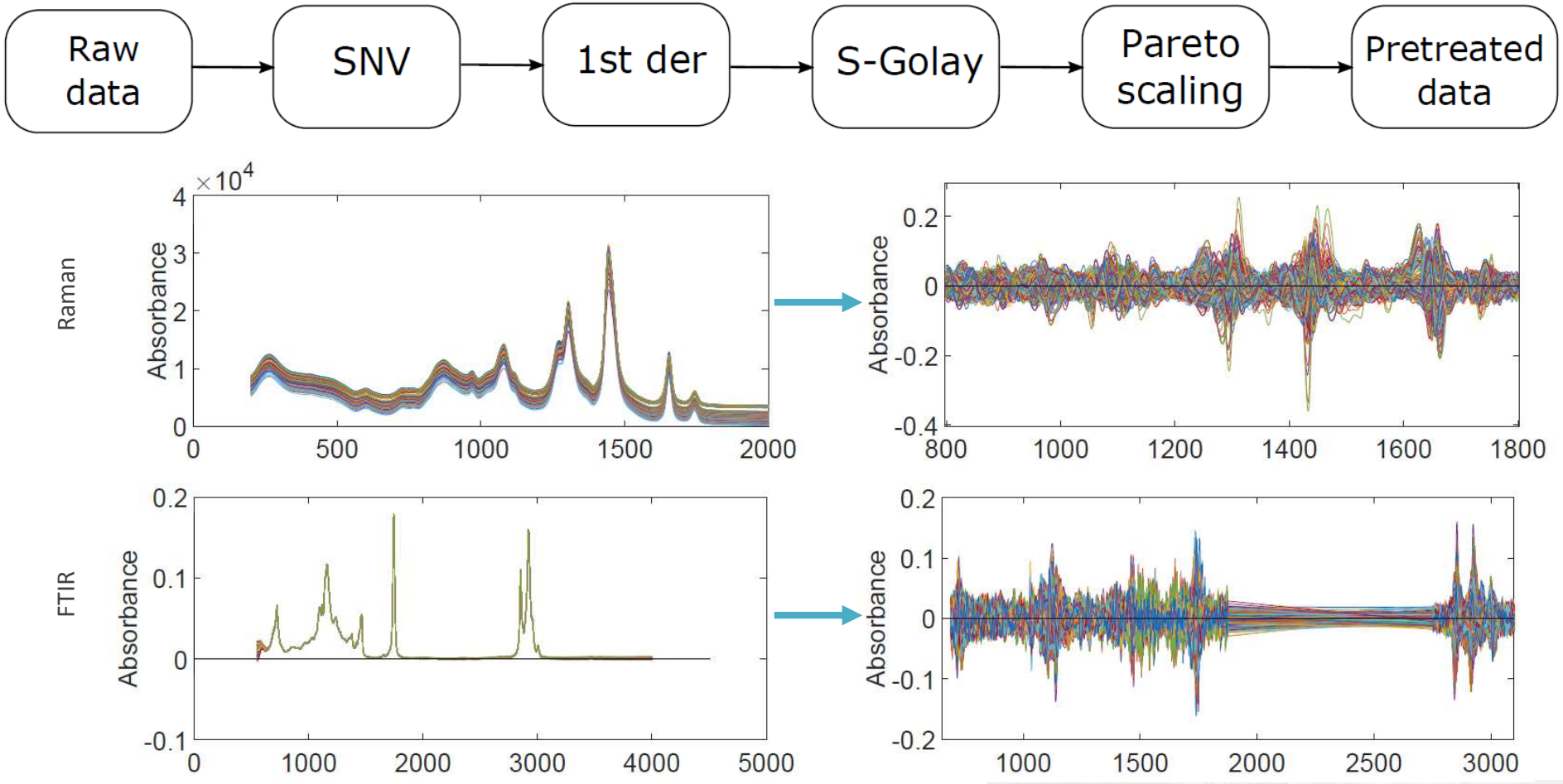
Changes in the intensities of spectral bands of different oils are related to the composition of molecular bonds absorbing at those regions.

6 pure oil samples:
- **2 PKO**
- **2 PO**
- **1 RO**
- **1 SO**

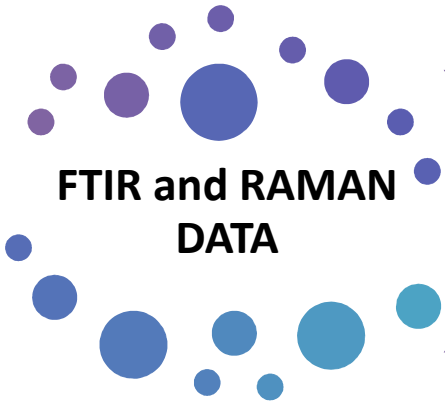
FTIR spectra on pure oils

PKO: Palm Kernel Oil; PO: Palm oil; RO: Rapeseed oil; SO: Sunflower oil

Pre-processing steps



Model and class development and validation

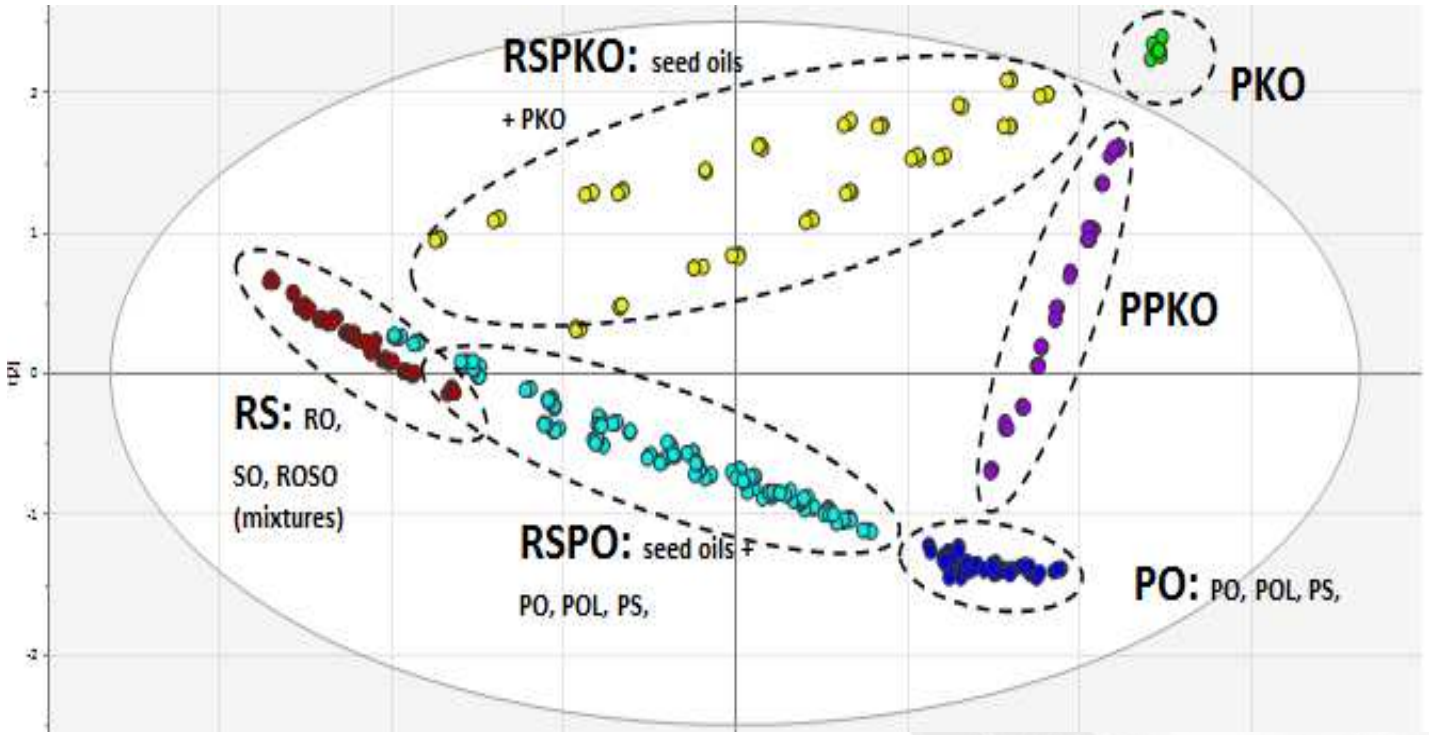


TRAINING of the MODEL using calibration set

VALIDATION

SIMCA	PLS-DA
• Soft Class Model of Class Analogy • Creates a PCA space for each class and determines DtModel	•Patrial Least Square – discriminant analysis •supervised classification

PCA scores plot of FTIR data of different vegetable oils



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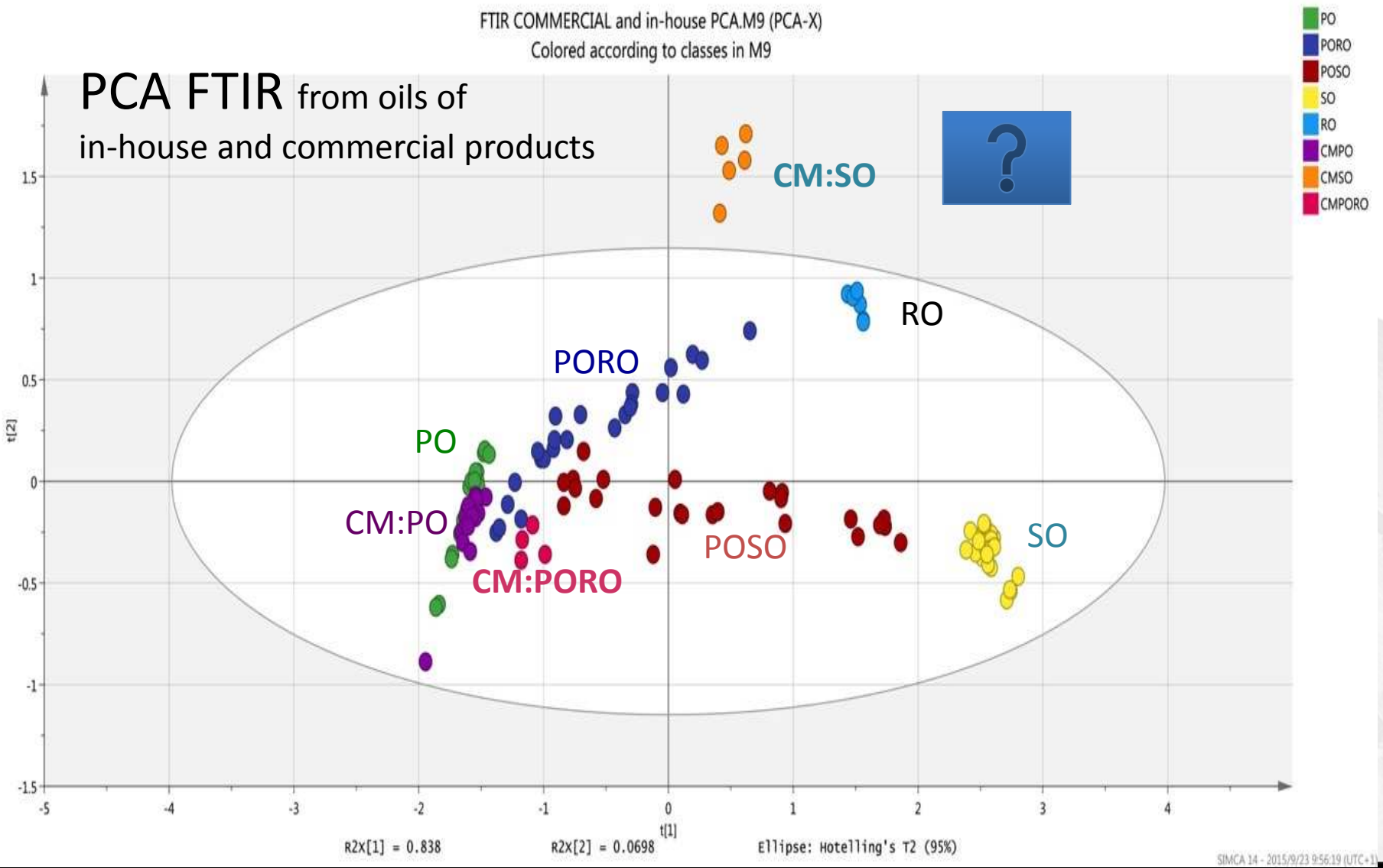
PCA FTIR from oils of in-house and commercial products



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Classification results: for in-house samples

SIMCA and PLS-DA model performance on prediction dataset using Raman and FTIR (26 samples from in-house-baking biscuits for Raman and FTIR in separate)							
	TARGET GROUP	SENSITIVITY (%)		SPECIFICITY (%)		OVERALL CLASSIFIC RATE (%)	
		RAMAN	FTIR	RAMAN	FTIR	RAMAN	FTIR
SIMCA	PO	66.7	83.3	100	100	83.0	92.0
	PORO	66.7	83.3	100	100	83.0	92.0
	POSO	83.3	66.7	100	100	92.0	83.0
	SO	83.3	83.3	100	100	92.0	92.0
	RO	50.0	100.0	100	100	75.0	100
	TOTAL (%)	19/26 70.0	21/26 83.3	100	100	85.0	92.0
PLS-DA	PO	100	100	100	90.0	100	95.0
	PORO	100	100	100	90.0	100	95.0
	POSO	100	(a)33.3	100	100	100	66.7
	SO	100	100	100	90.0	100	95.0
	RO	100	100	100	91.7	100	95.8
	TOTAL (%)	26/26 100%	21/26 86.7%	100	92.3	100	90.0

for SIMCA we accept samples with Pconf>0.05 and for PLD-DA with Pconf >0.5; if no limits are applied. correct classification is at 100% at all cases

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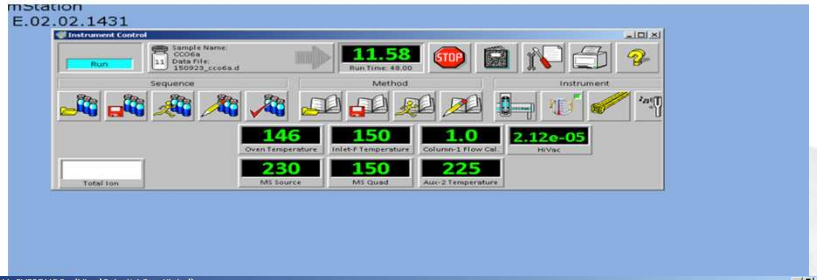
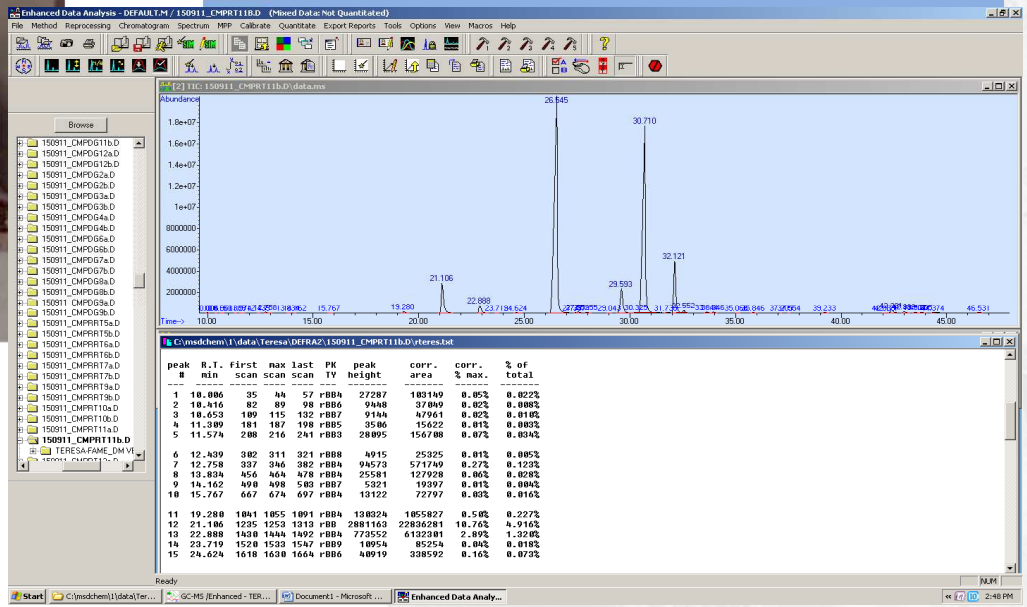
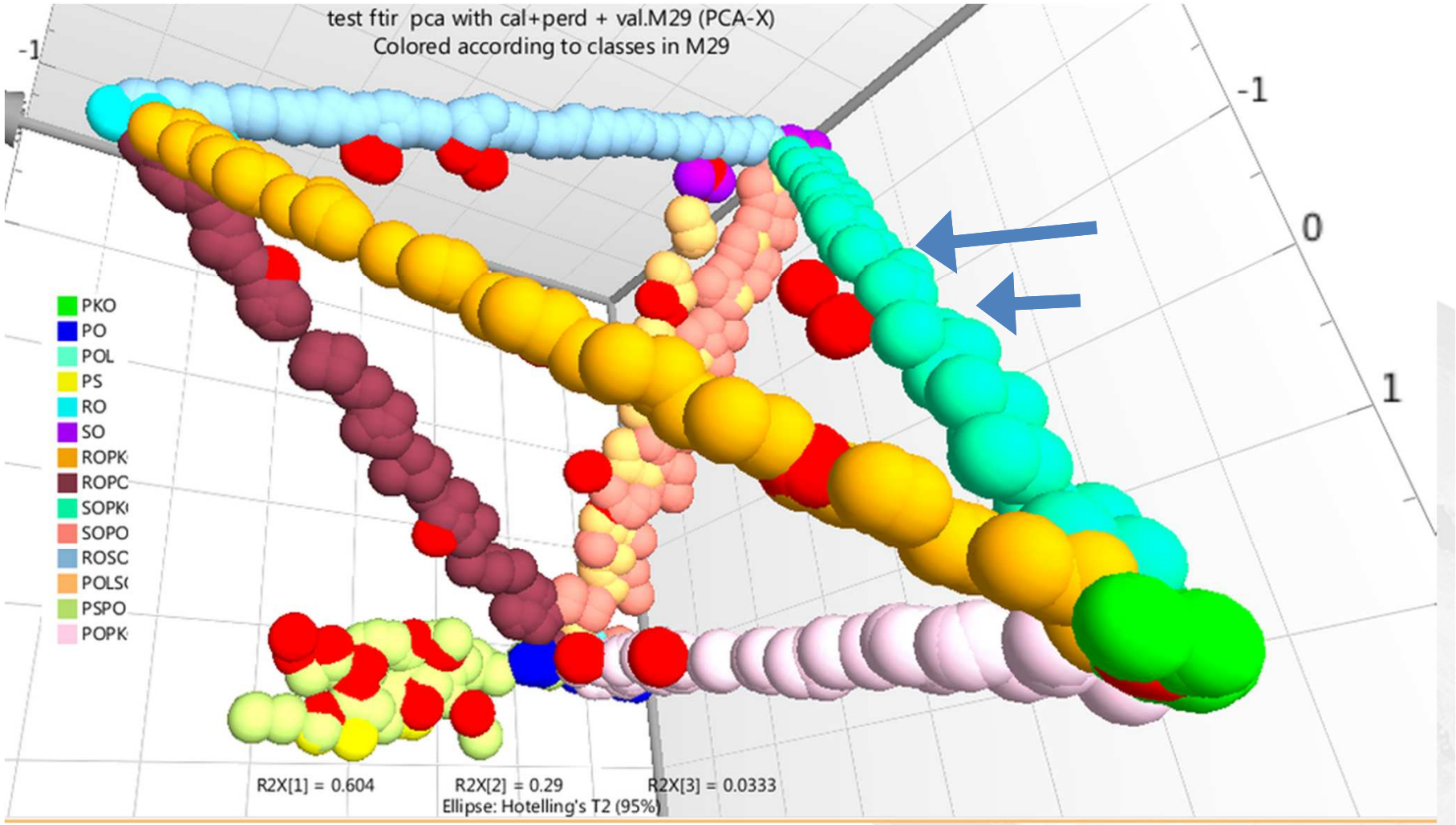
Gas Chromatography/Mass Spectroscopy






test ftir pca with cal+perd + val.M29 (PCA-X)
Colored according to classes in M29
-1
-1
0
1
PKO
PO
POL
PS
RO
SO
ROPK
ROPC
SOPK
SOPO
ROSC
POLS
PSPO
POPK
R2X[1] = 0.604
R2X[2] = 0.29
R2X[3] = 0.0333
Ellipse: Hotelling's T2 (95%)

Fatty acids profiles

Oil species	OIL SOURCES	C14:0	C16:0	C18:0	C18:1c	C18:2c	C20:0	C22:0
PO	In-house biscuits	1.3 ± 0.1	44.9 ± 0.5	4.2 ± 0.1	36.9 ± 0.6	11.1 ± 0.4	0.3 ± 0.0	0.1 ± 0.0
	Commercial bisc.	1.3 ± 0.1	45.3 ± 2.0	4.1 ± 0.2	36.2 ± 1.5	11.0 ± 1.6	0.3 ± 0.0	0.1 ± 0.0
	Untreated oils	1.1 ± 0.1	43.4 ± 0.9	4.8 ± 0.2	34.8 ± 0.9	8.2 ± 0.4	0.4 ± 0.1	0.0 ± 0.0
SO	In-house bisc.	0.1 ± 0.0	7.1 ± 0.2	3.3 ± 0.2	28.6 ± 2.2	59.1 ± 2.2	0.1 ± 0.0	0.7 ± 0.0
	Commercial bisc.	0.1 ± 0.0	5.5 ± 1.3	2.9 ± 0.2	78.0 ± 2.5	11.2 ± 1.4	0.2 ± 0.0	0.8 ± 0.1
	Untreated oils	0.1 ± 0.0	6.1 ± 0.2	3.6 ± 0.2	26.8 ± 1.8	55.9 ± 1.9	0.1 ± 0.0	0.7 ± 0.0
RO	Untreated oils	0.0 ± 0.0	4.5 ± 0.2	1.7 ± 0.1	55.9 ± 2.3	17.5 ± 0.8	0.5 ± 0.0	0.3 ± 0.0
OO	Untreated oil (lit.)	0.0 ± 0.0	13.8 ± 6.2	2.7 ± 2.2	69.0 ± 14.0	12.2 ± 8.7	0.4 ± 0.4	0.1 ± 0.1

further challenge: to identify the type of oils used in confectionery products

Fat extraction with solvent (hexane, ethyl acetate)

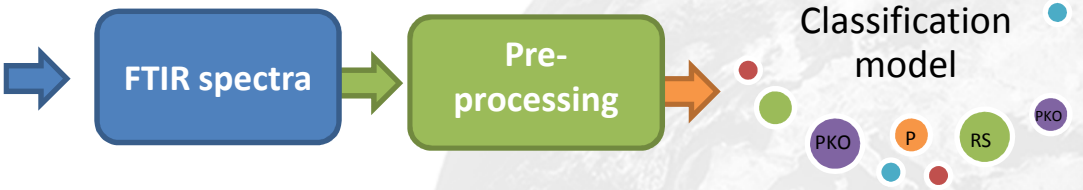
↓

Analysis (screening, confirmation)

Palm components:
-Confectionary fats
-Cocoa butter replacers (CBR)
-Cocoa butter equivalents (CBE)

An interlaboratory trial with 14 participants having different brands of Fourier-transform infrared spectrometers for the identification of oil species in mixtures of oils

VALIDATION
9 oil samples
(Pure oils and admixtures)



an instrument agnostic FTIR method

a different approach to model transfer

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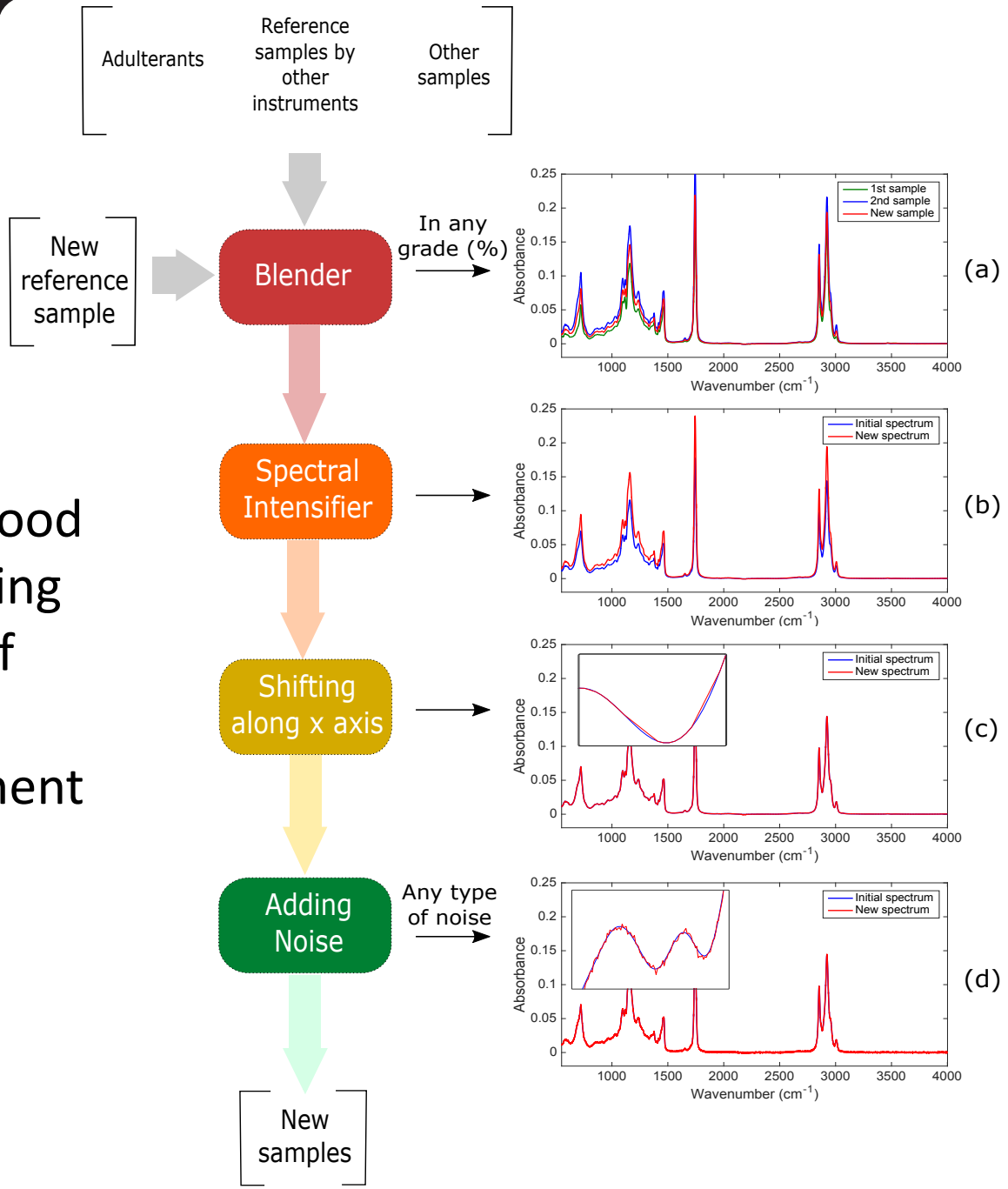
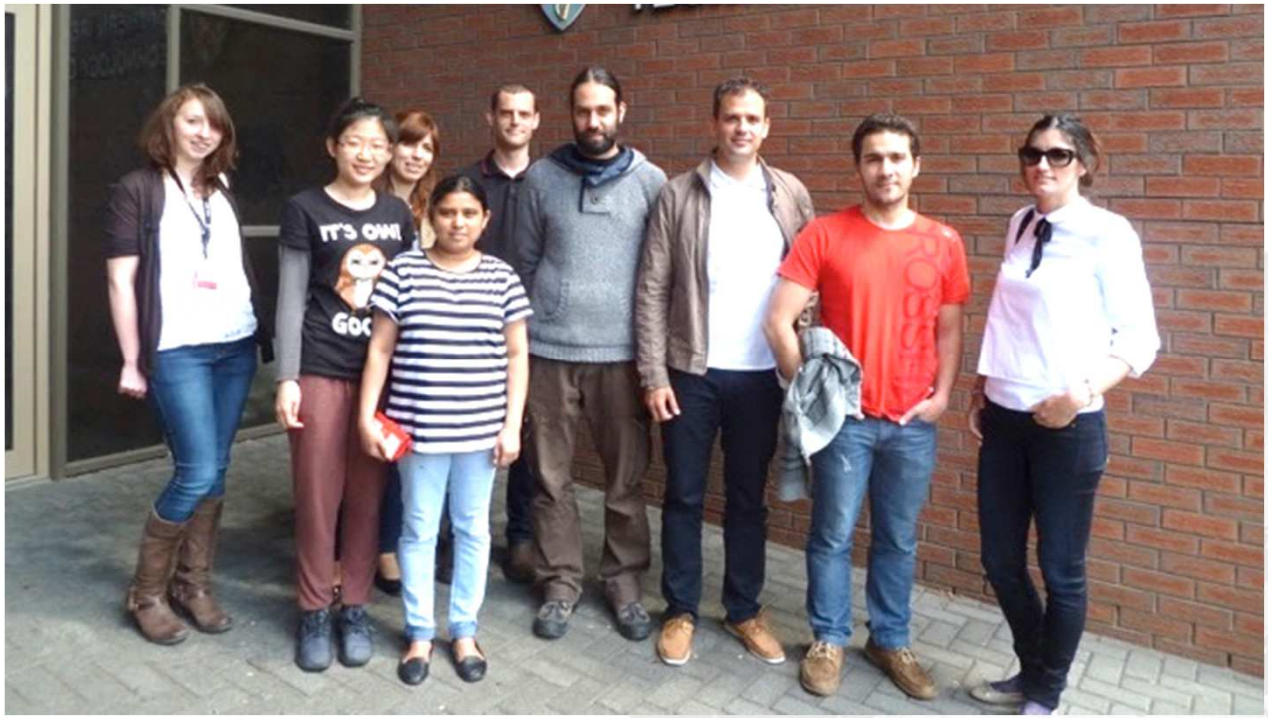
Data augmentation in food authenticity: synthesizing spectroscopic data of vegetable oils for performance enhancement



the team



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