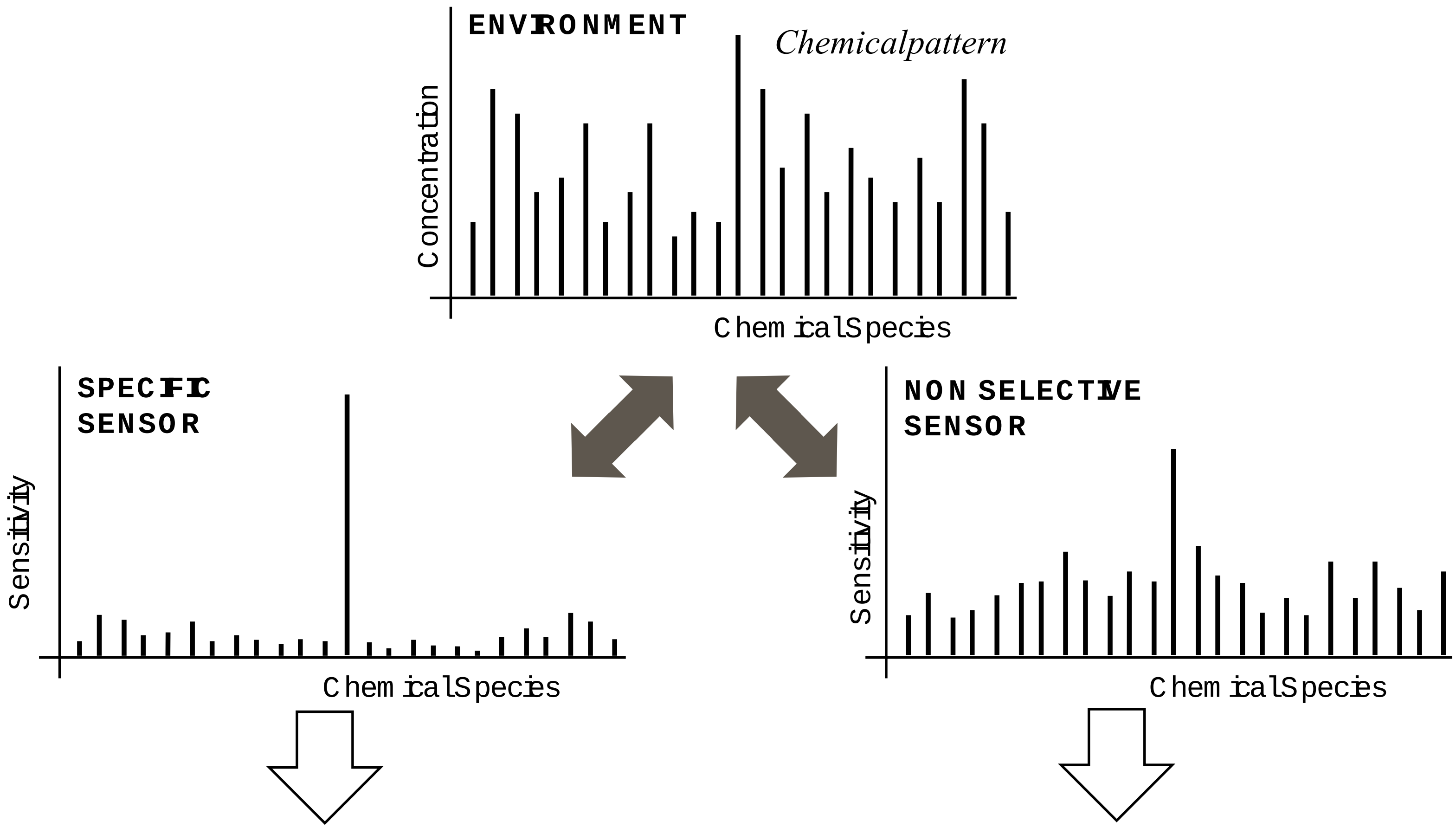
The Mistery of Olfaction

- Human senses can be separated in two main groups:
    - Physical Senses:
        - tactile, sight, hear
    - Chemical Senses:
        - smell, and taste
- Chemical Senses operate at incoscious level: perceptions are not fully expressed.

- 15 years ago the possibility to mimick the human olfaction became real
- It is a big scientific challenge involving many scientific realms:
    - Physics, chemistry, mathematics, neuro-sciences, electronics,...

Jan Bruegel de Velours
The Smell; Madrid, Museo del Prado

The Selectivity

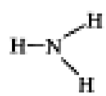


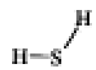
$$z \cong s_j \cdot C_j$$

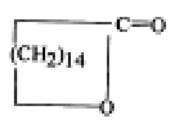
$$z = \sum_i s_i \cdot C_i$$

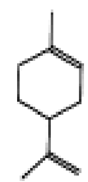
Odorous compounds

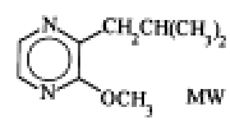
- Odorous compounds are very different at molecular level
- Molecular masses spans a range of 200 D
- The relation between molecular structure and odour perception is still rather obscure

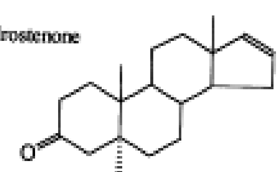
Ammonia  MW 17 Pungent

Hydrogen Sulphide  MW 34 Putrid

Cyclopentadecanone  MW 254 Musk

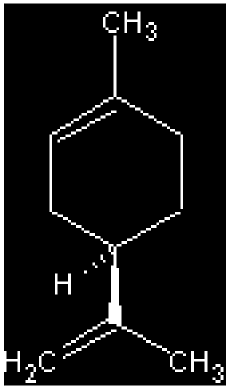
Limonene  MW 136 Lemons

2-methoxy-3-isobutyl pyrazine  MW 166 Bell peppers

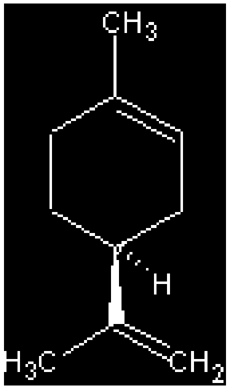
Androstenone  MW 272 , Urinous, Boar taint

Chirality and Odour

- Chiral compounds have an important role in biological interactions
- Odour perceptions and drug efficiency are strongly influenced by the spatial configuraton of the molecule
- Enantioselective sensors are then important in food scent and drug control applications.



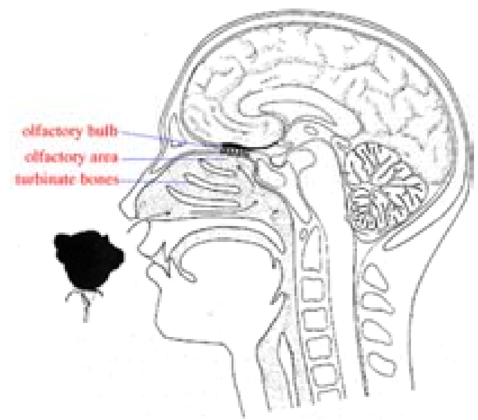
(R)-(+)-limonene
odour: fresh citrus, orange-like
olfaction resolution: 200 ppb



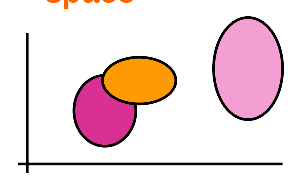
(S)-(-)-limonene
harsh, turpentine-like, lemon note
olfaction resolution: 500 ppb

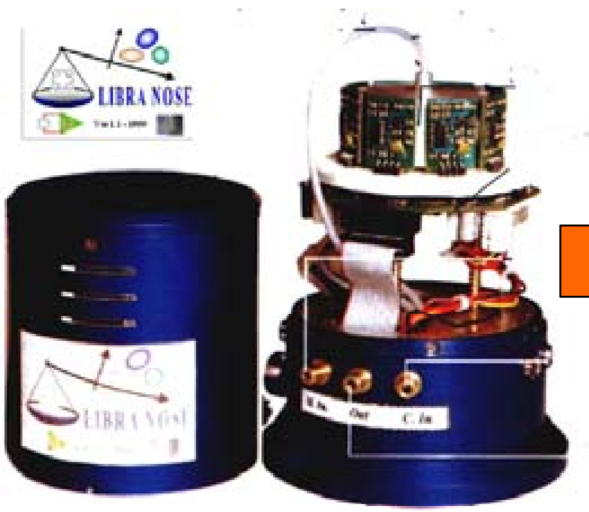
Natural and Artificial Olfaction

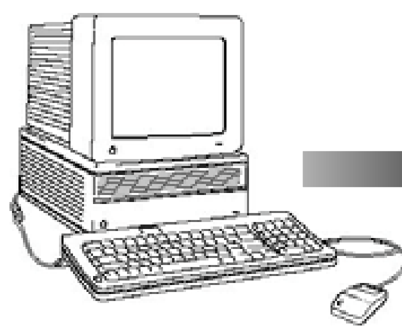
- *Olfaction components:*
    - *Sampling system*
    - *Measurement chamber*
    - *Sensors*
    - *Signal processing*
    - *Pattern recognition*



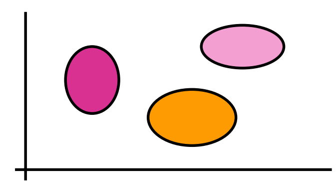
Classification space



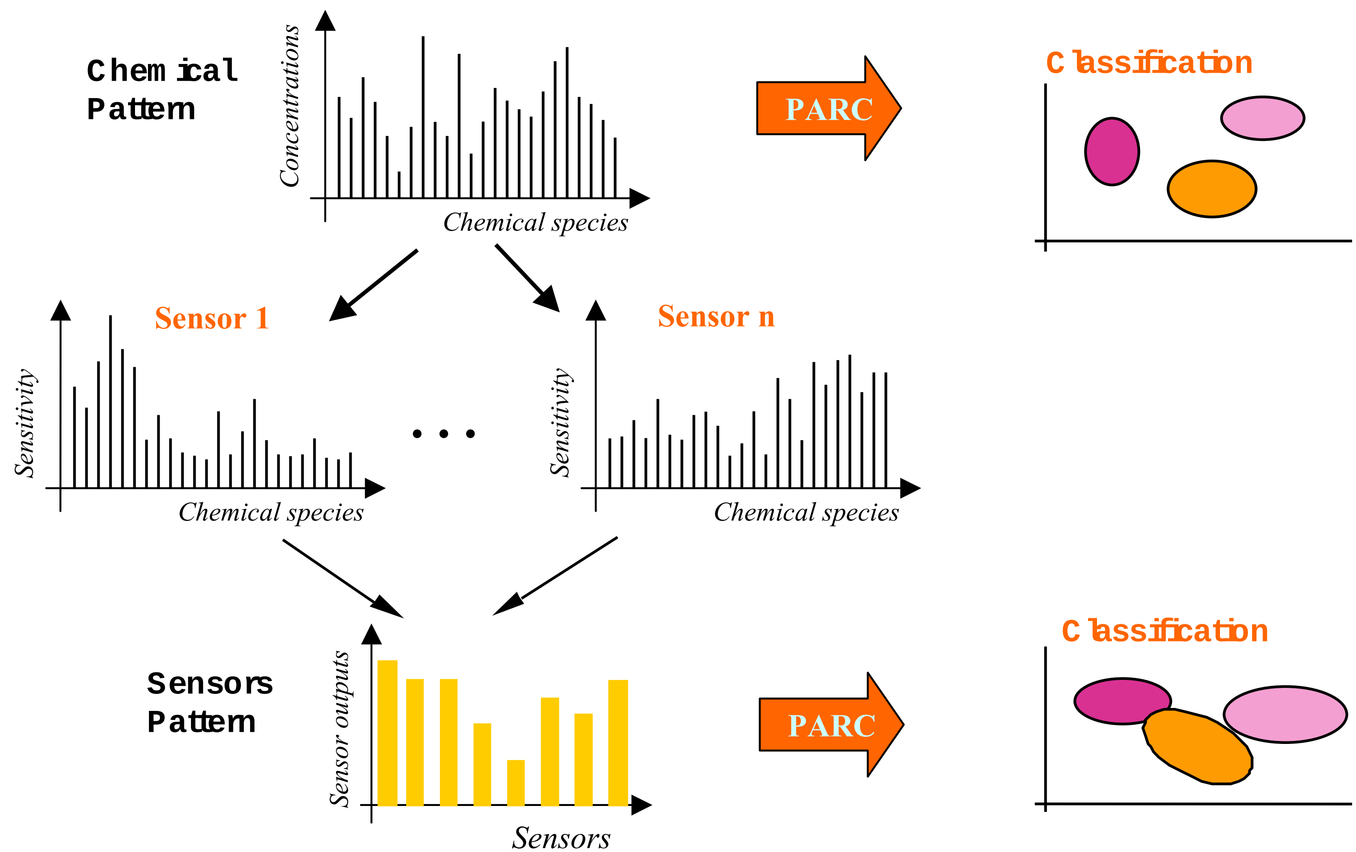




Classification space

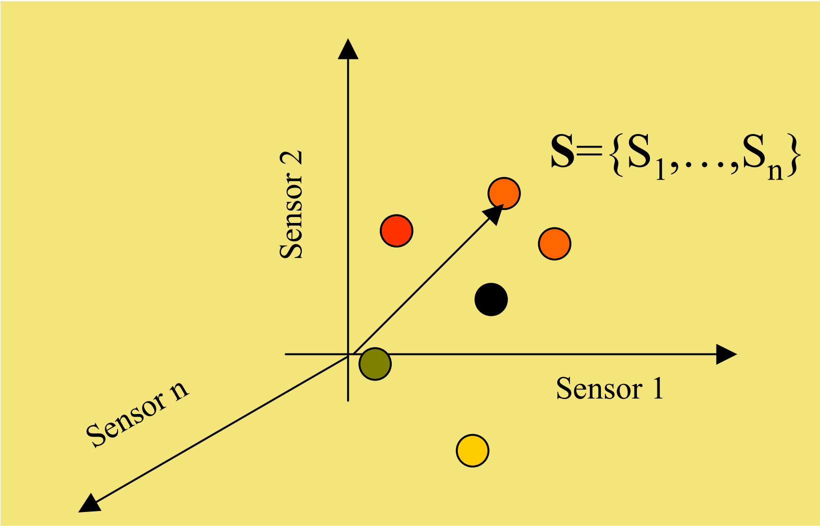


The Strategy for Qualitative Analysis with an artificial sense system



Electronic Nose Data Space

- As any other multisensor system, the data of an electronic nose are found in a multidimensional space: ***the sensor space***
- A single measure is an entity in this space, namely a measure is an n-dimensional vector.
- Suitable data analysis techniques allow visualise the space as a 2D plot.
- In the sensor space odours are mapped according to their similarities and differences.



The senses as instruments: the sensory analysis

- Sensory analysis is the science of extracting human perceptions elaborating them to characterise samples.
- It is typically applied in food analysis to evaluate features like quality and freshness of products.
- Human evaluations are always qualitative.
- Generally, all the senses are integrated and cooperate to the overall evaluation.

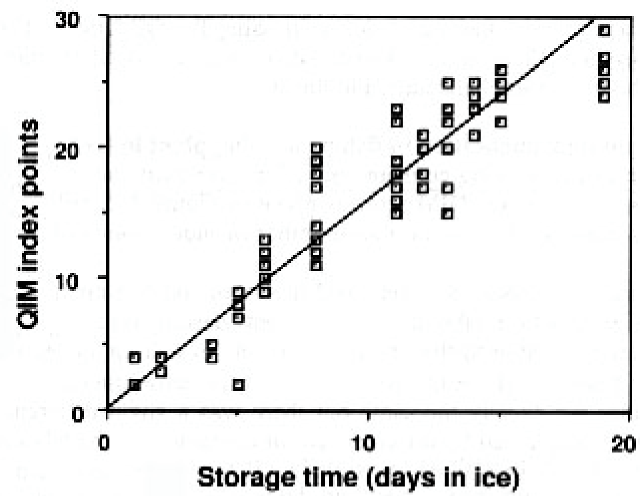
panel evaluation of fish freshness

Sensory analysis:
example: Quality Index Method for fish

Table III: QIM scheme for cod

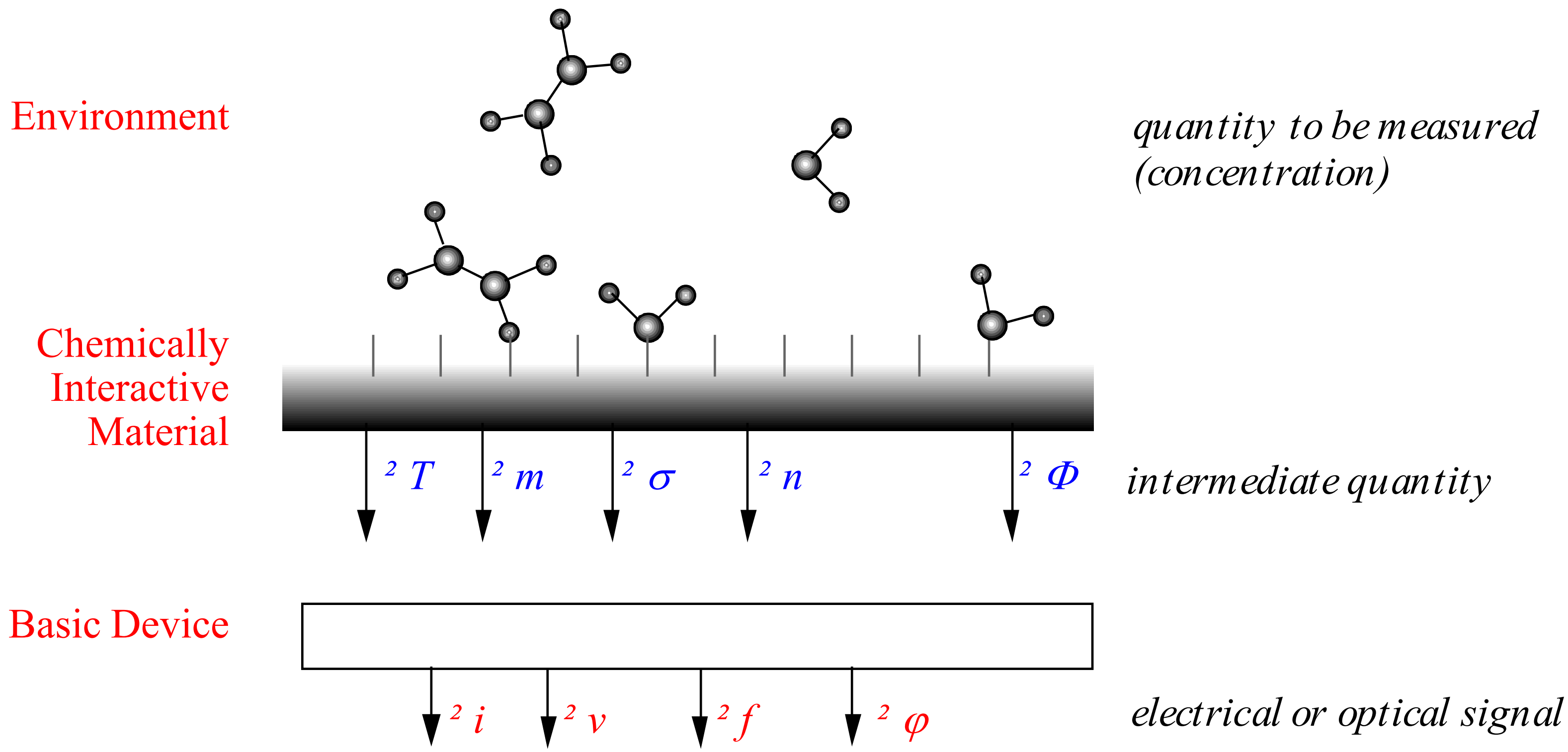
Quality parameter		Description	Score
Appearance	Skin	Bright, iridescent pigmentation	0
		Rather dull, becoming discoloured	1
		Dull	2
	Stiffness	In rigor	0
		Firm, elastic	1
		Soft,	2
		Very soft	3
Eyes	Cornea	Clear	0
		Opalescent	1
		Milky	2
	Form	Convex	0
		Flat, slightly sunken	1
		Sunken, concave	2
	Colour of pupil	Black	0
		Opaque	1
		Grey	2
Gills	Colour	Bright	0
		Less coloured, becoming discoloured	1
		Discoloured, brown spots	2
		Brown, discoloured	3
	Smell	Fresh. seaweedy, metallic	0
		Neutral, grassy, musty	1
		Yeast, bread, beer, sour milk	2
		Acetic acid, sulphuric, very sour	3
	Mucus	Clear	0
		Milky	1
		Milky, dark, opaque	2
Fillets	Colour	Translucent, bluish	0
		Waxy, milky	1
		Opaque, yellow, brown spots	2
Blood	Colour	Red	0
		Dark red	1
		Brown	2

- QIM involves the evaluation of various parameters in order to have a linear relationship versus the days in ice of fish.
- The method is calibrated for each species.

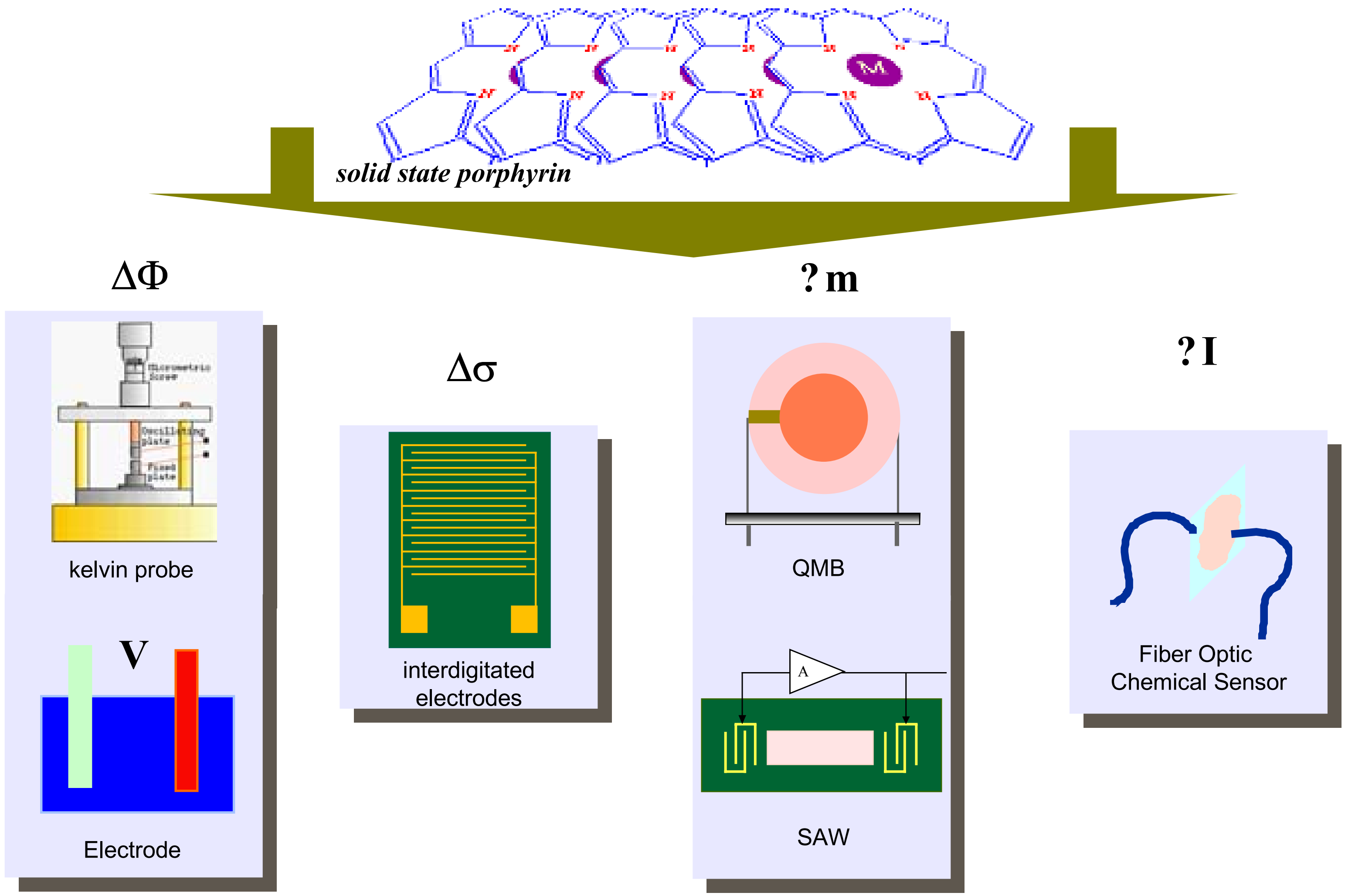


J. Luten, E. Martinsdottir in Evaluation of Fish Freshness, 1997

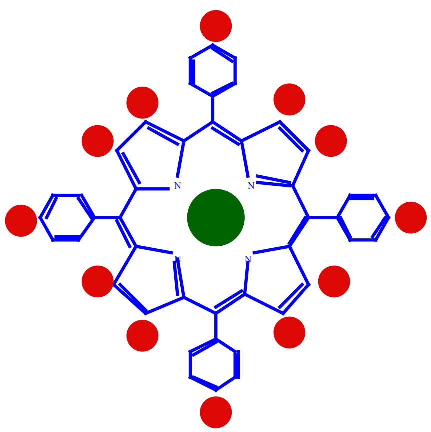
Structure of a generic solid-state chemical sensor

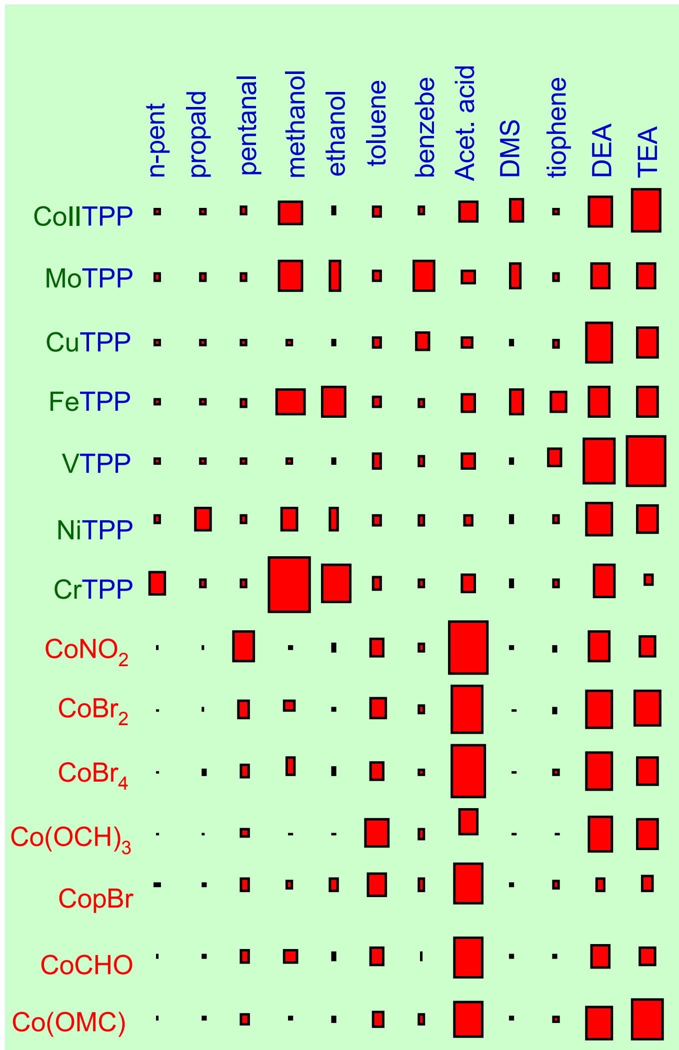


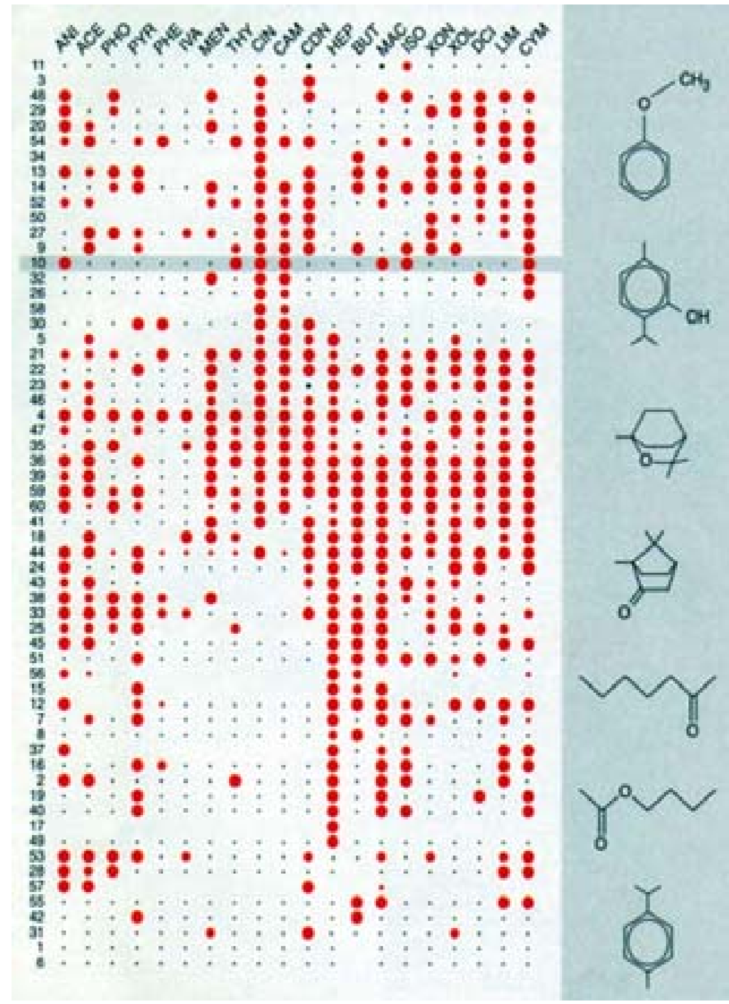
Chemical Sensors



The Electronic Nose paradigm: sensitivity of natural and artificial receptors

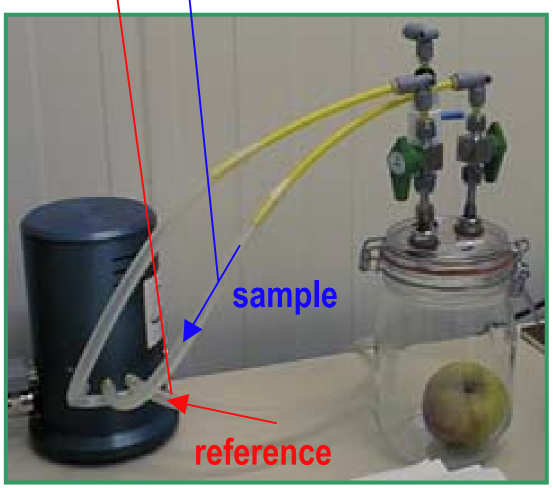


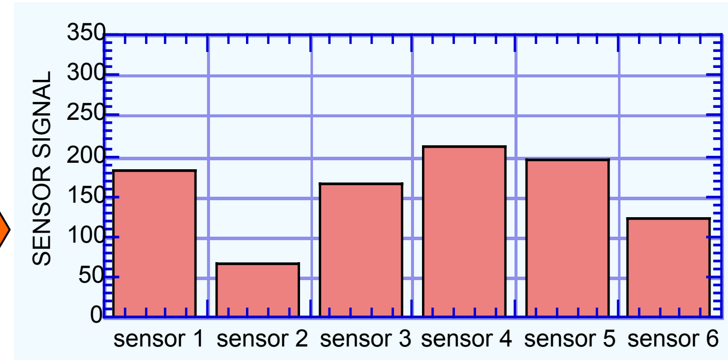




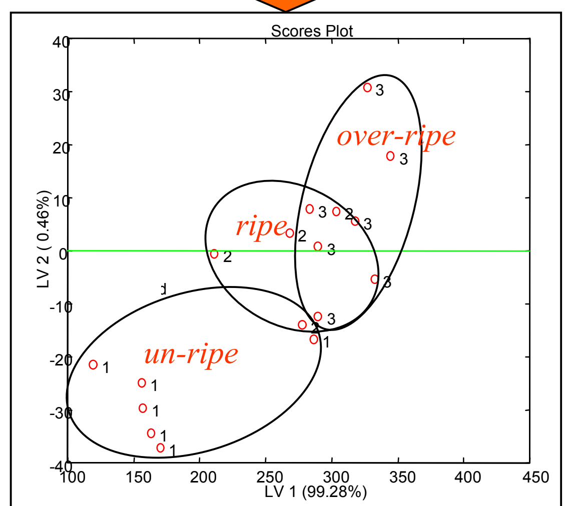
Sicard and Holley; Brain Res 1984; 292:283-96

Sensor signals





Pattern Recognition



Representation Space

Natural and Artificial Olfaction

Natural Olfaction

- Receptors
  - Non selective
  - Ultra High Redundancy (10^8)
  - Biochemical transduction
  - Signal: pattern of spikes
- Sample Delivery
  - Actuation of sniffing
  - Two sources of odor (outside and mouth)
- Signal processing
  - Data synthesis
- Data analysis
  - Ultra Wide Database
  - Drift compensation
  - High integration with other senses

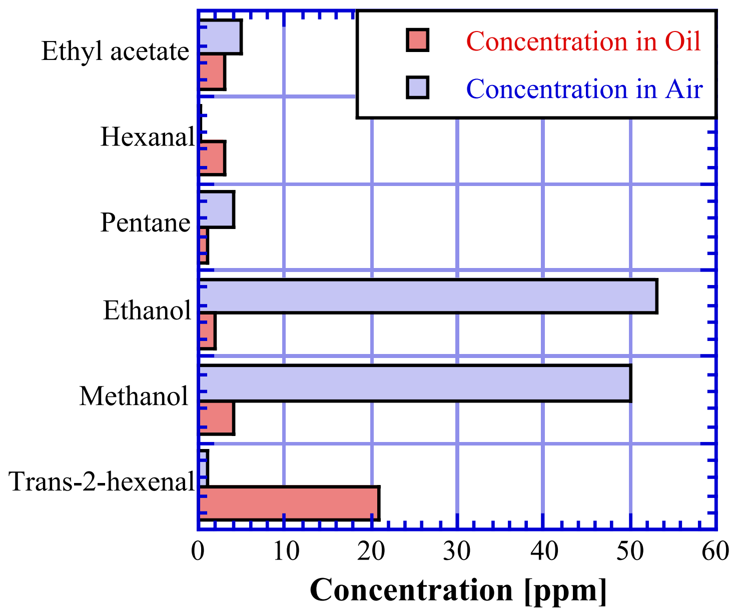
Artificial Olfaction

- Sensors
  - Non selective
  - Low Redundancy (10)
  - Chemical transduction
  - Signal: steady signal
- Sample Delivery
  - Continuous sniffing
  - One source of odour (outside)
- Signal processing
  - One sensor - one signal
- Data analysis
  - Limited Database
  - Poor Drift compensation
  - Integrability with other instruments

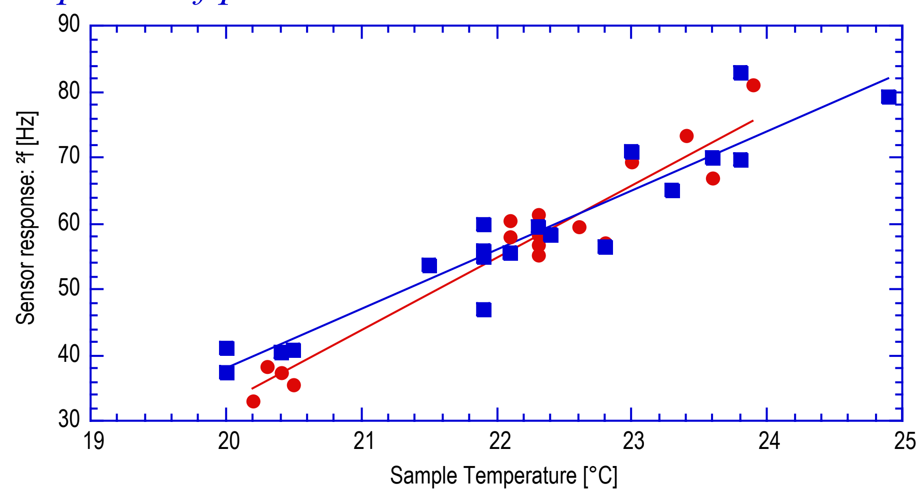
Odour generation

- There are two main problems connected with the physico-chemical processes of odour generation:
  - 1. The differences between headspace and real sample compositions
  - 2. The dependence of the headspace measure from the sample temperature

1. Concentrations in headspace and in the samples of some compounds in olive oils



2. Influence of T_{sample} in the measurement of two species of peaches



Odour sampling

- Given a certain sample (generally a liquid or a solid), the electronic nose measures its headspace.
- Odor sampling has to be reproducible and all the sample conditions have to be controlled.
- Examples of sample odour extraction