Nanotechnology and Artificial Intelligence

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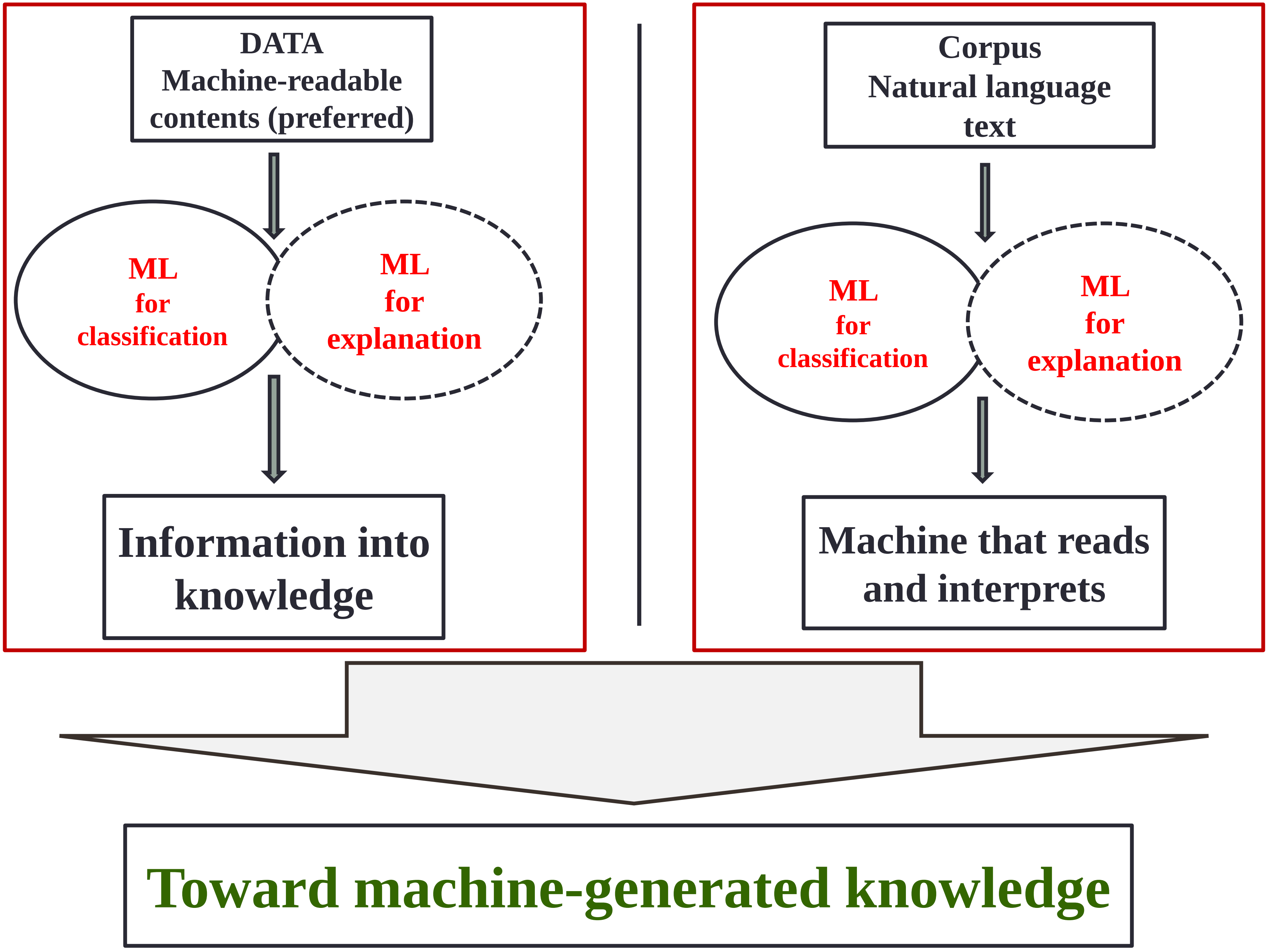
Outline

- The Fifth Paradigm
- Big Data and Machine Learning
- ML in Materials Science
- AI in agriculture

The Fifth Paradigm

- **1st Empirical, descriptive**
- **2nd Theory and experiment**
- **3rd Theory, experiment, computer simulation**
- **4th All of the above + Big Data**
- **5th Machine-generated knowledge**


DATA
Machine-readable
contents (preferred)
ML
for
classification
ML
for
explanation
Information into
knowledge
Corpus
Natural language
text
ML
for
classification
ML
for
explanation
Machine that reads
and interprets
Toward machine-generated knowledge

Some Requirements

- **Text analytics – large text databases**
- **Lots of data: experimental, theoretical (DFT, etc) and simulation (MD, etc)**
- **Internet of Things**
- **Machine Learning Methods (Deep Learning, etc)**

Computer-assisted diagnosis as an example

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Editorial
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Preface to the Forum on Materials Discovery and Design

Gustavo M. Dalpian and Osvaldo N. Oliveira Jr.

The research highlighted here gives a broad view of achievements in the area of materials discovery and design, which brings together several disciplines such as chemistry, physics, materials science, and computer science. It is a new paradigm for all sorts of materials applications, with the potential to revolutionize the way materials are studied, discovered, and synthesized.

Materials Discovery and Design

- **Exciting theoretical and experimental developments**
- **Boosted by large repositories (data availability)**
- **High throughput calculations**
- **Machine Learning**

ML in Materials Science

Materials Discovery

- Identification of compounds with genetic algorithms
- Synthesis prediction
- Properties via quantum theory
- Computer-aided drug design
- Computational Biology

Pattern Recognition and IoT

- Sensing and biosensing data
- Image analysis
- Classification and diagnostics

Rodrigues et al., arxiv.org/abs/1904.10370
A survey on Big Data and Machine Learning for Chemistry

Deep Learning Usage

DNN applied to the dataset of the Harvard Clean Energy Project to discover organic photovoltaic materials. HOMO and LUMO energies and power conversion efficiency predicted for 200,000 compounds, with errors below 0.15 eV for HOMO and LUMO energies.

Pyzer-Knapp et al, Adv. Funct. Mater. 2015

DNNs used to predict reactions with 97% accuracy with a validation set of ca. 1 million reactions. Clearly superior to previous rule-based expert systems

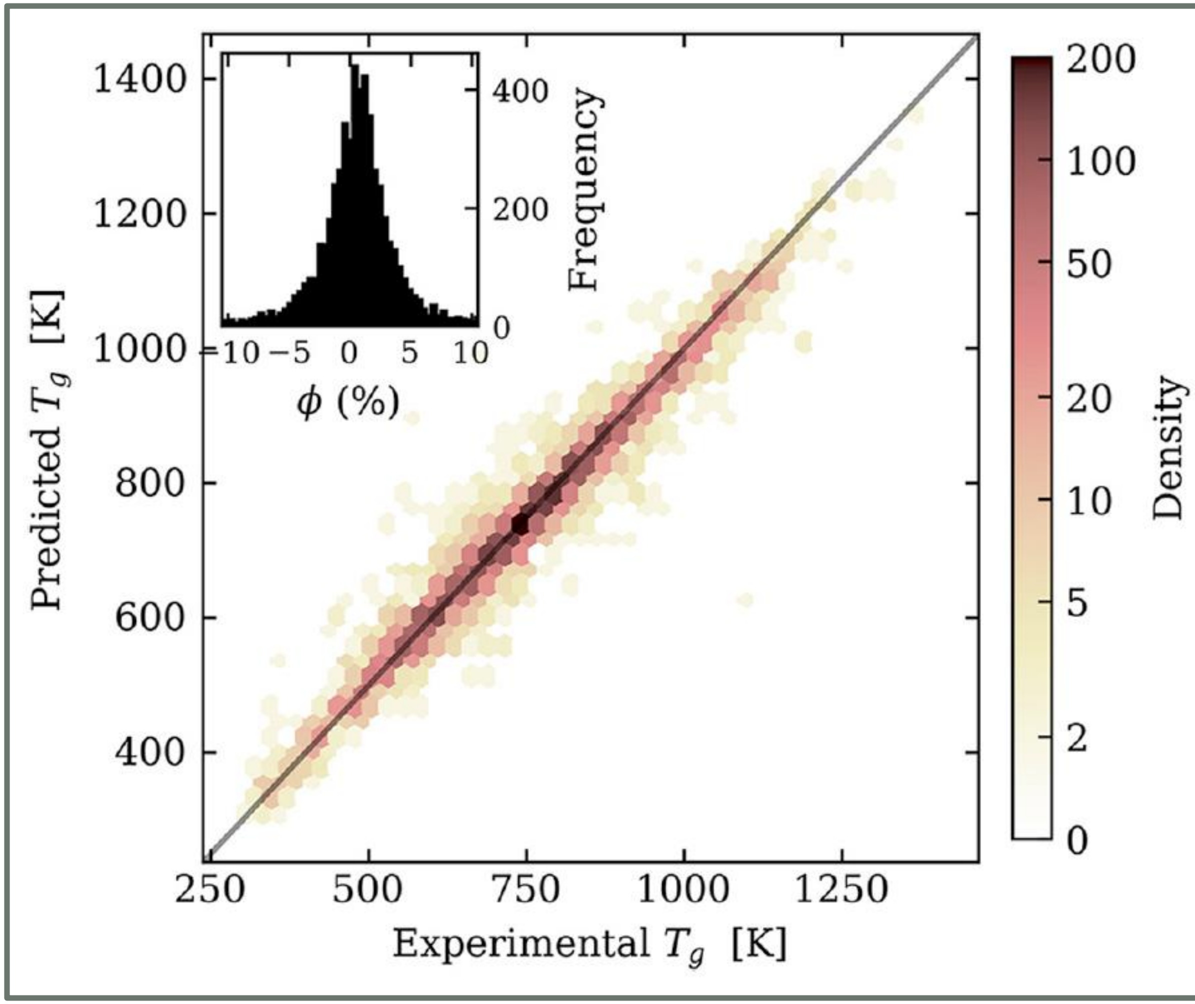
Segler et al., Chem. A, 2017

Artificial Neural Networks to predict glass transition temperatures of oxide glasses

Dataset > 55,000 inorganic glass compositions and their T_g.

Prediction of published T_g with 95% accuracy, less than ±9% error

90% of the data predicted with deviation < ±6%, same level of original dataset.



Daniel R. Cassar, André Carvalho, Edgar Zanotto – Acta Materialia, 2018

Artificial Intelligence in Agriculture

• **AI bots to harvest crops at a higher volume and faster. Computer vision helps to monitor the weed and spray them. Decrease pesticide usage**

• **Checking defective crops and improving the potential for healthy crop production.**

• **Automated machine adjustments for weather forecasting and disease or pest identification.**

• **Solving challenges such as climate variation, infestation of pests and weeds.**

The Role of Artificial intelligence in Agriculture Sector
Jyoti Gupta- October 11, 2019

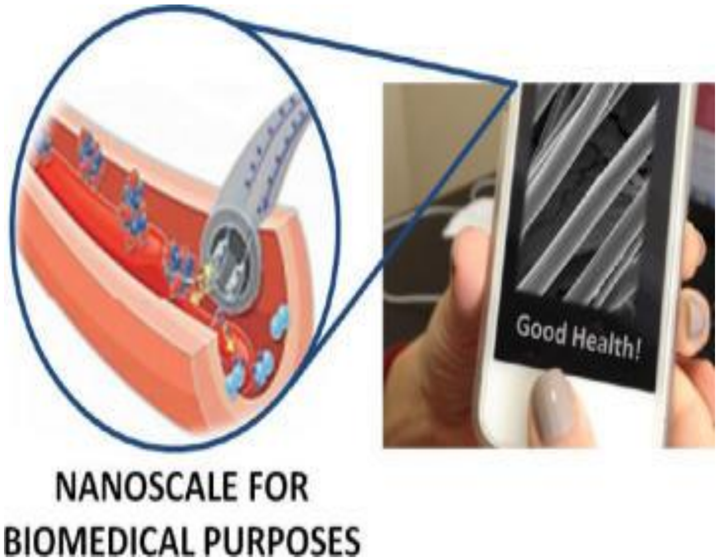
Artificial Intelligence in Agriculture

- **Farmers can analyze data such as weather conditions, temperature, water usage or soil conditions in real time.**
- **Planning to determine crop choices, hybrid seed choices.**
- **Precision agriculture - detecting diseases in plants, pests, and poor plant nutrition.**
- **AI sensors to detect and target weeds with proper herbicides.**
- **Computer vision and deep learning to process images from drones that cover far more land in much less time.**

How AI Is Transforming Agriculture, Kathleen Walch, Forbes, July, 2019

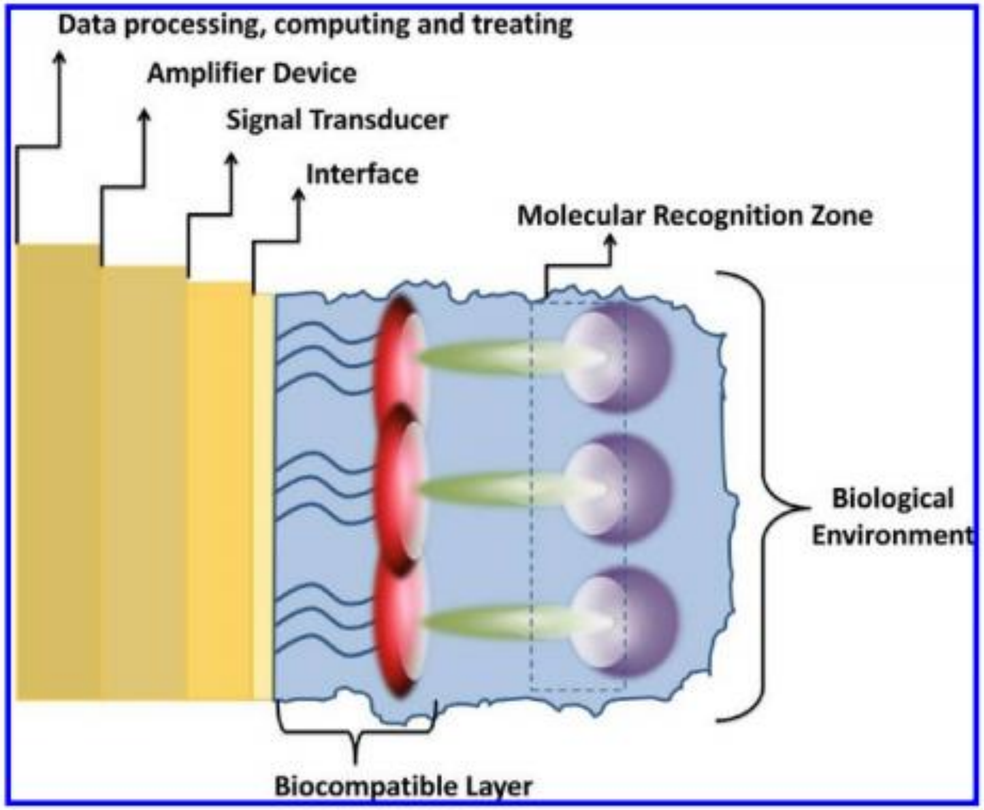
Where Nanotechnology fits in

Nanomaterials for Diagnosis: Challenges and Applications in Smart Devices Based on Molecular Recognition



Oliveira et al.
ACS Appl. Mat. Interfaces, 2014

Biosensor:
Needs suitable molecule capable of molecular recognition



Taste sensors

nature scienceupdate

Electronic tongue has good taste

Hand-held tasting device displays highly discriminating palate.

9 January 2002

PHILIP BALL

A new hand-held electronic tongue promises to give accurate and reliable taste measurements for companies currently relying on human tasters for their quality control of wine, tea, coffee, mineral water and other foods.

Coffee producers could use the electronic tongue for quality control.
© *PhotoDisc*

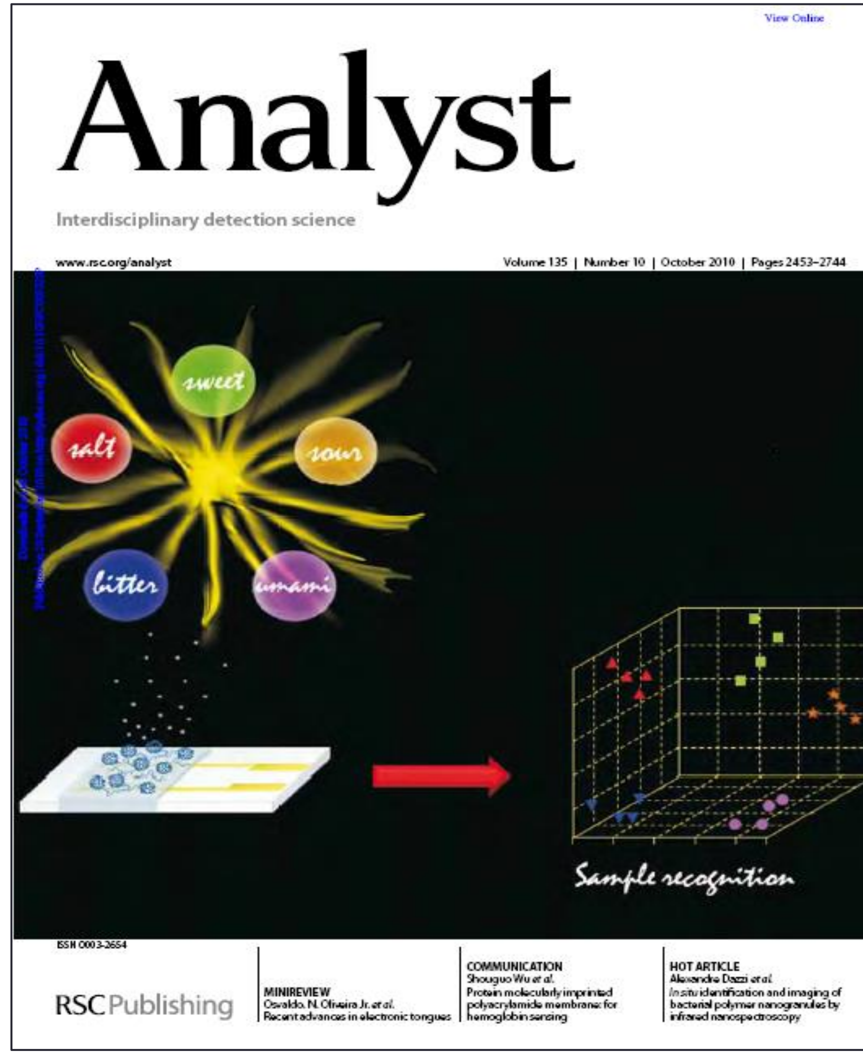
Human tasters are still irreplaceable for subtle products such as fine wines and whiskies. But their sense of taste saturates after a while, losing its discriminating edge. The device made by Antonio Riul of EMBRAPA InstrumentaÃ§Ã£o AgropecuÃ¡ria in SÃ£o Carlos, Brazil, and colleagues rivals human taste buds and never tires[1].

The electronic tongue can sense low levels of impurities in water. It can discriminate between Cabernet Sauvignons of the same year from two different wineries, and between those from the same winery but different years. It can also spot molecules such as sugar and salt at concentrations too low for human detection.

Questionable taste

Humans have long been thought to detect four basic taste types: sweet, salty, sour and bitter. Very recently, a fifth candidate basic taste was identified: umami, the taste of monosodium glutamate, characteristic of protein-rich foods. Taste buds are believed to contain receptor molecules that trigger nerve signals when they encounter flavour-imparting molecules.

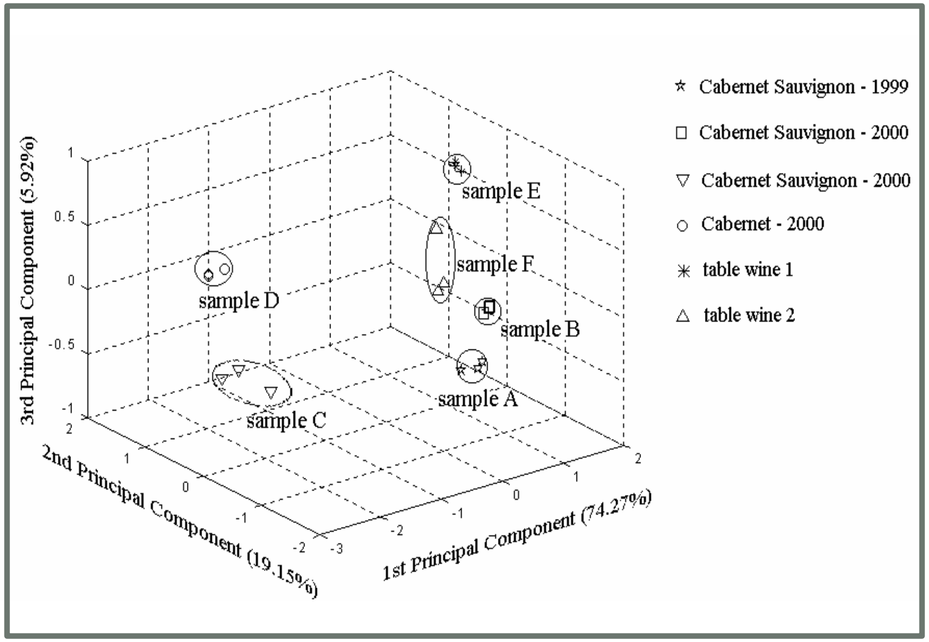
The details of this system are still not understood. Each taste sensation may correspond to a fingerprint signal induced by the differential activation of the various taste receptors. The electronic tongue works on this principle.



Brazilian e-tongue

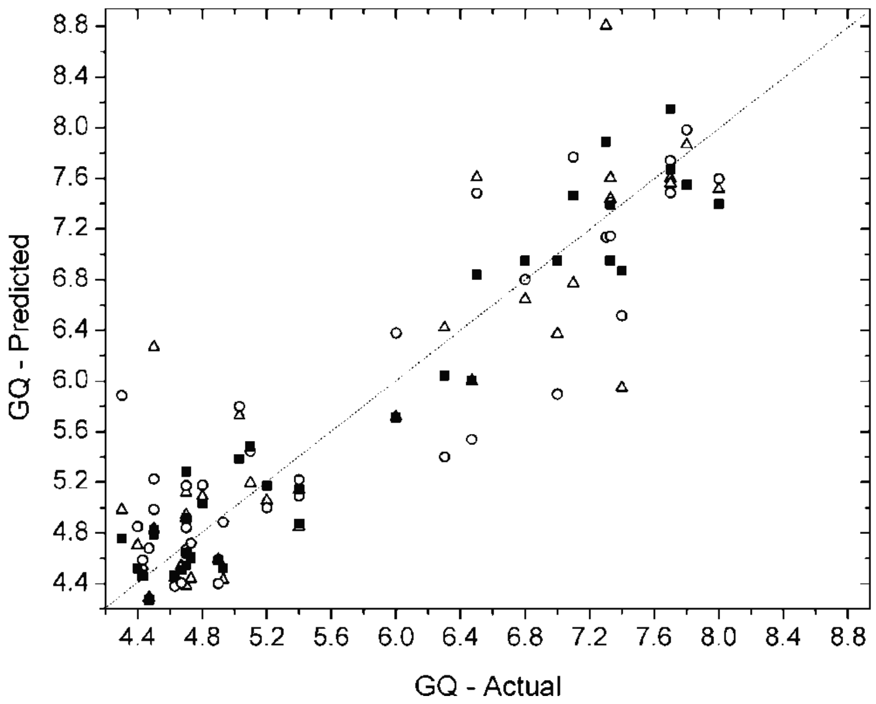
Taste sensors

Identifying wines



Dos Santos Jr. et al.,
Macromol. Biosci., 2003

Correlating with human taste



One of the regression methods led to Pearson coefficient of 0.964. Accuracy in the score ± 0.3

E.J. Ferreira et al.,
Electronics Letters, 2007

Detection of the prostate cancer biomarker PCA3 with electrochemical and impedance-based biosensors

Juliana Coatrini Soares, Andrey Coatrini Soares, Valquiria Cruz Rodrigues, Matias Eliseo Melendez, Alexandre Cesar Santos, Eliney Ferreira Faria, Rui M. Reis, Andre L. Carvalho and Osvaldo Novais Oliveira

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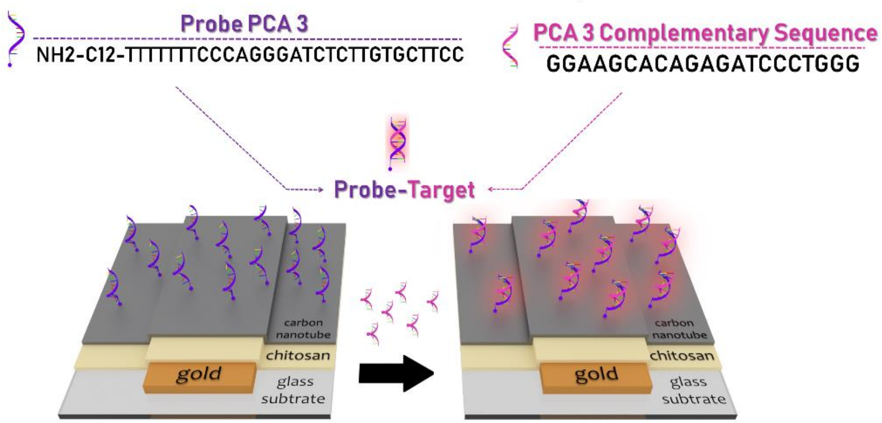
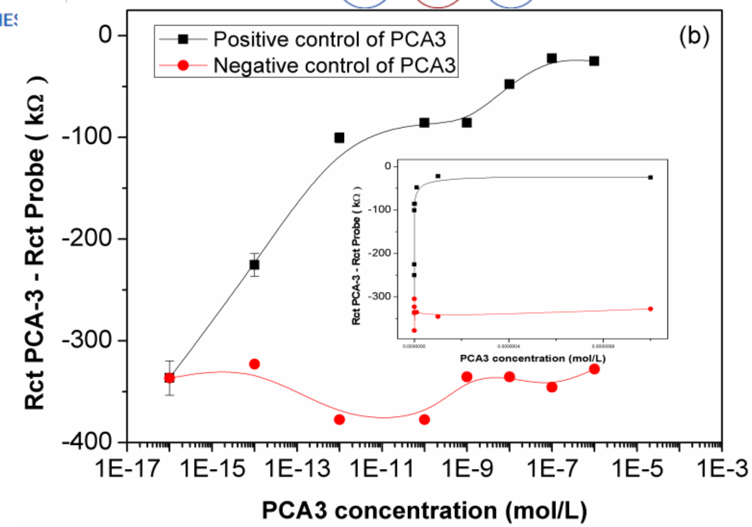
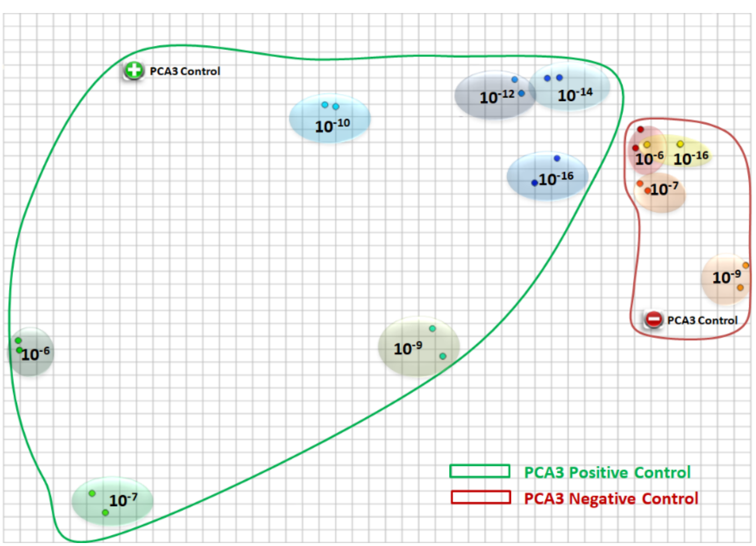
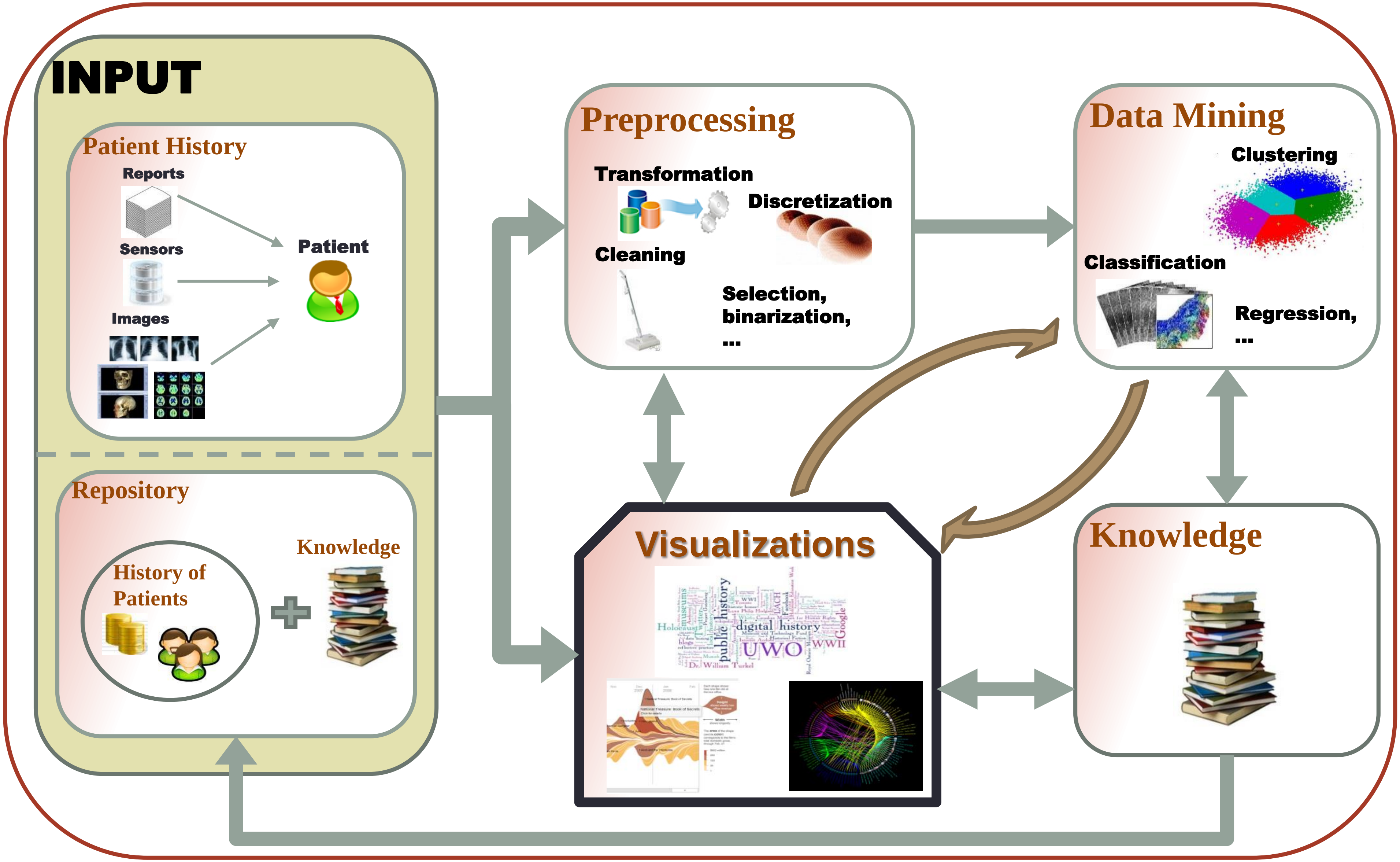






Holy Grail: Diagnostics in the future



Oliveira et al., Chem. Lett. Japan, 2014

Convergence of technologies

Nanosciences

- **Molecular recognition**
- **Molecular-level interactions**
- **Assembly of supramolecular structures**
- **Molecular control in film architectures**

e-Science

- **Handling massive amounts of data**
- **Data mining and natural language processing**
- **Machine Learning**

Machine learning will change the landscape of science and technology in the XXI century.

In a few decades, most intellectual tasks will be better performed by machines.

Is society being prepared for that?

Final Recommendation/Provocation

- **How would an intelligent machine solve the scientific problem you are addressing?**
- **Are you sure the problem could not be obviated by other means?**

USP

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MRS Meeting
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September 03rd
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ICEM
30th August – 3rd September, 2020
XIX B-MRS
ICEM (*International Conference on Electronic Materials*)