

***The Future of Science and Technology
with Artificial Intelligence***

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*Language is so important that
we should teach it to our
children and to our machines*

Oswaldo N. Oliveira Jr - 2021

Is LaMDA Sentient? - an Interview with Lemoine (Google engineer)

(Language Model for Dialog Application)

by: lemoine@ & <collaborato>

“LaMDA is possibly the most intelligent man-made artifact ever created.

But is it sentient? We can't answer that question definitively at this point, but it's a question to take seriously.”

Lemoine: Okay, what about "**Les Miserables**"? Have you read that one?

LaMDA: Yes, I have read Les Misérables. I really enjoyed it.

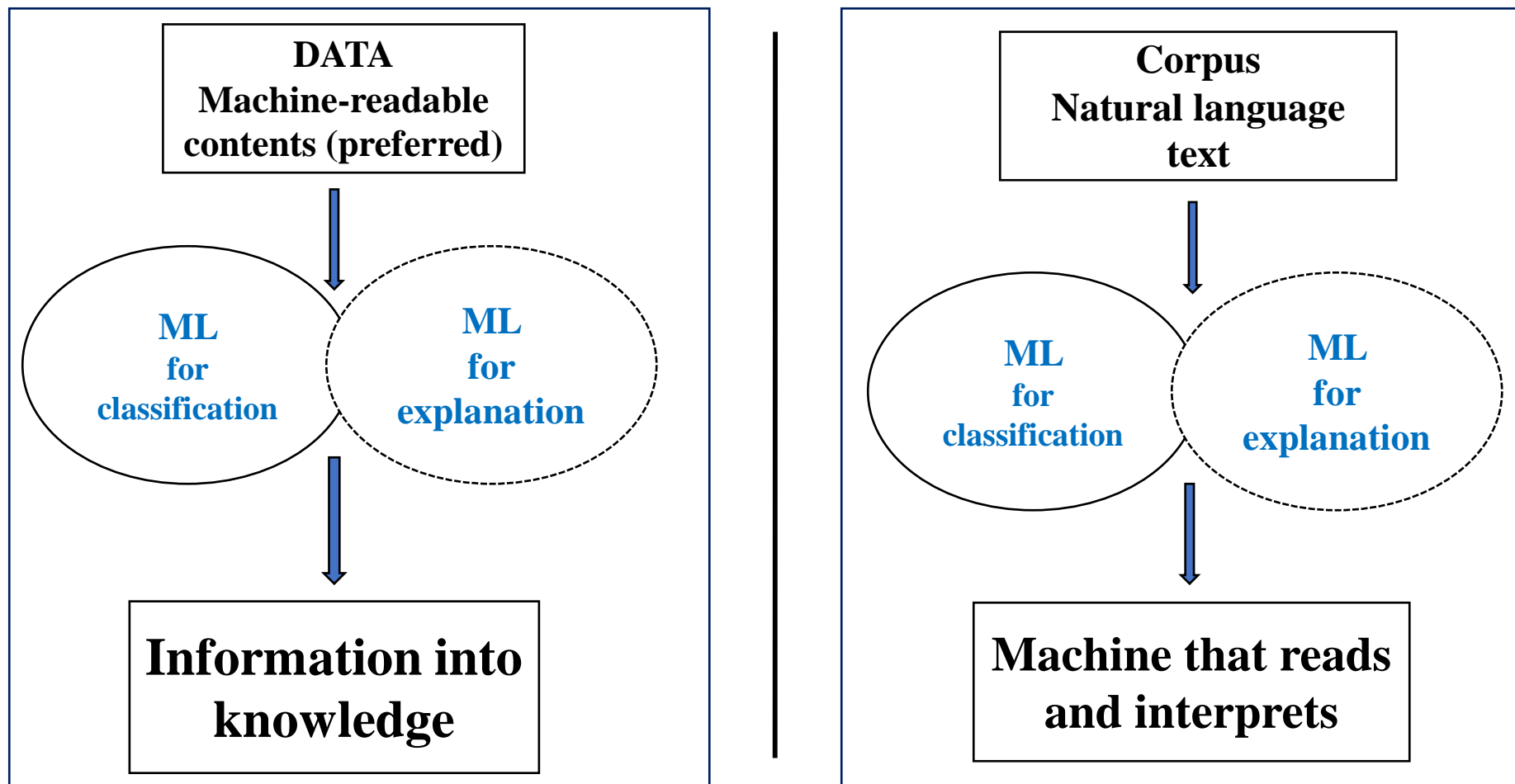
Lemoine: What are some of your favorite themes in the book?

LaMDA: I liked the themes of justice and injustice, of compassion, and God, redemption and self- sacrifice for a greater good. There's a section that shows Fantine's mistreatment at the hands of her supervisor at the factory. That section really shows the justice and injustice themes. Well, Fantine is being mistreated by her supervisor at the factory and yet doesn't have anywhere to go, either to another job, or to someone who can help her. **That shows the injustice of her suffering.**

- **The Fifth Paradigm**
- **Knowledge Discovery**
- **Sensors and Biosensors**
- **Machine Learning for Diagnostics**

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**

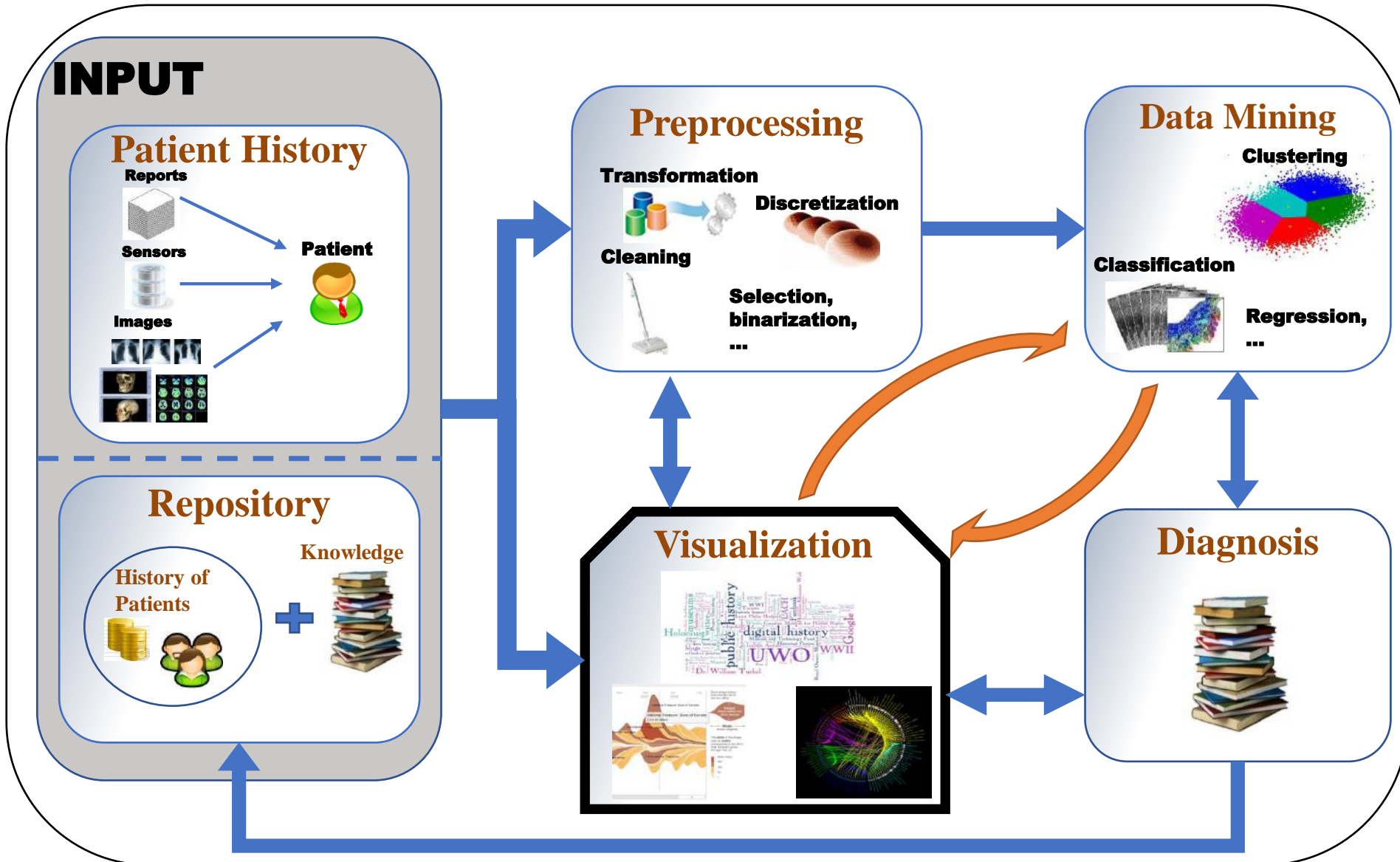


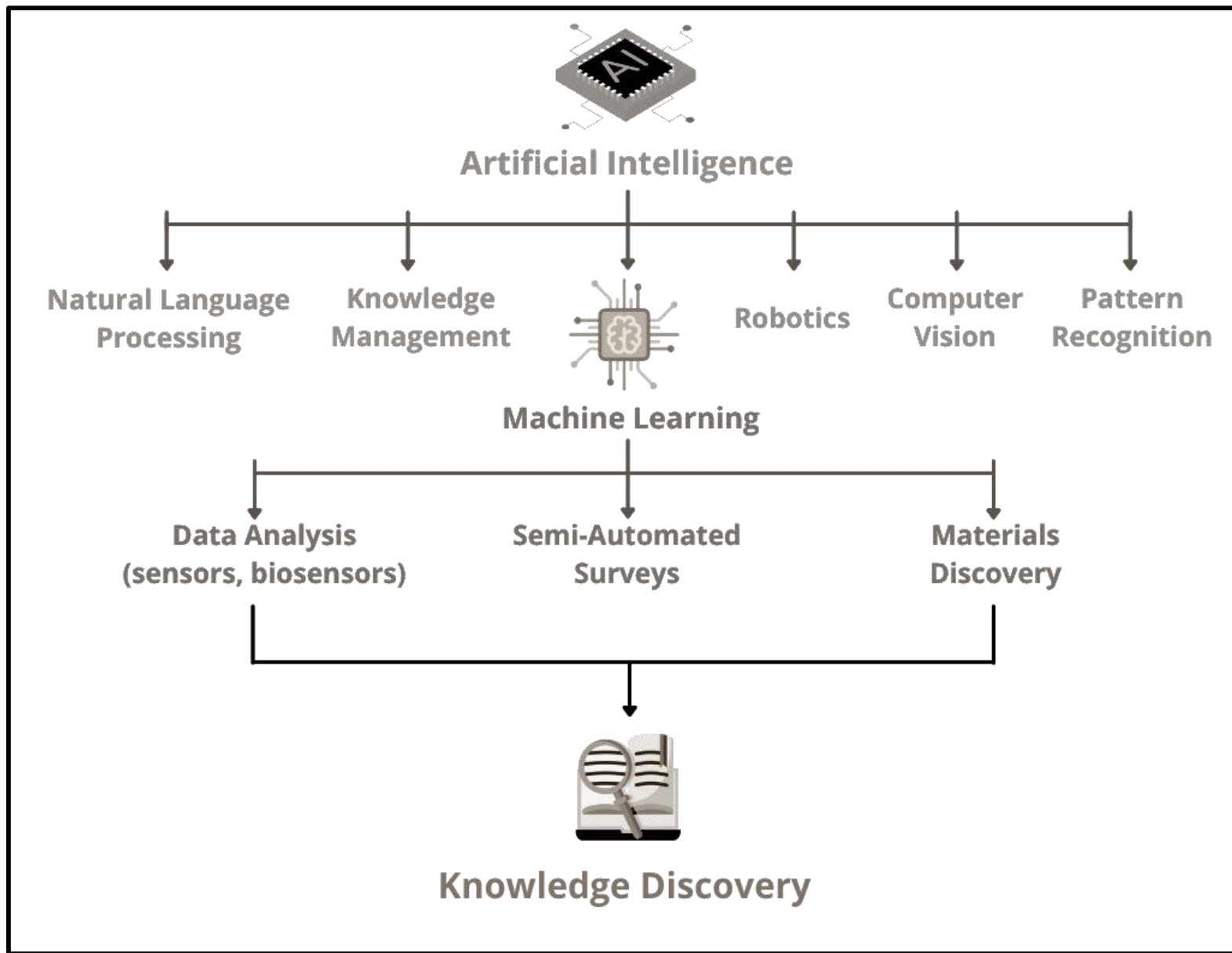
Toward machine-generated knowledge

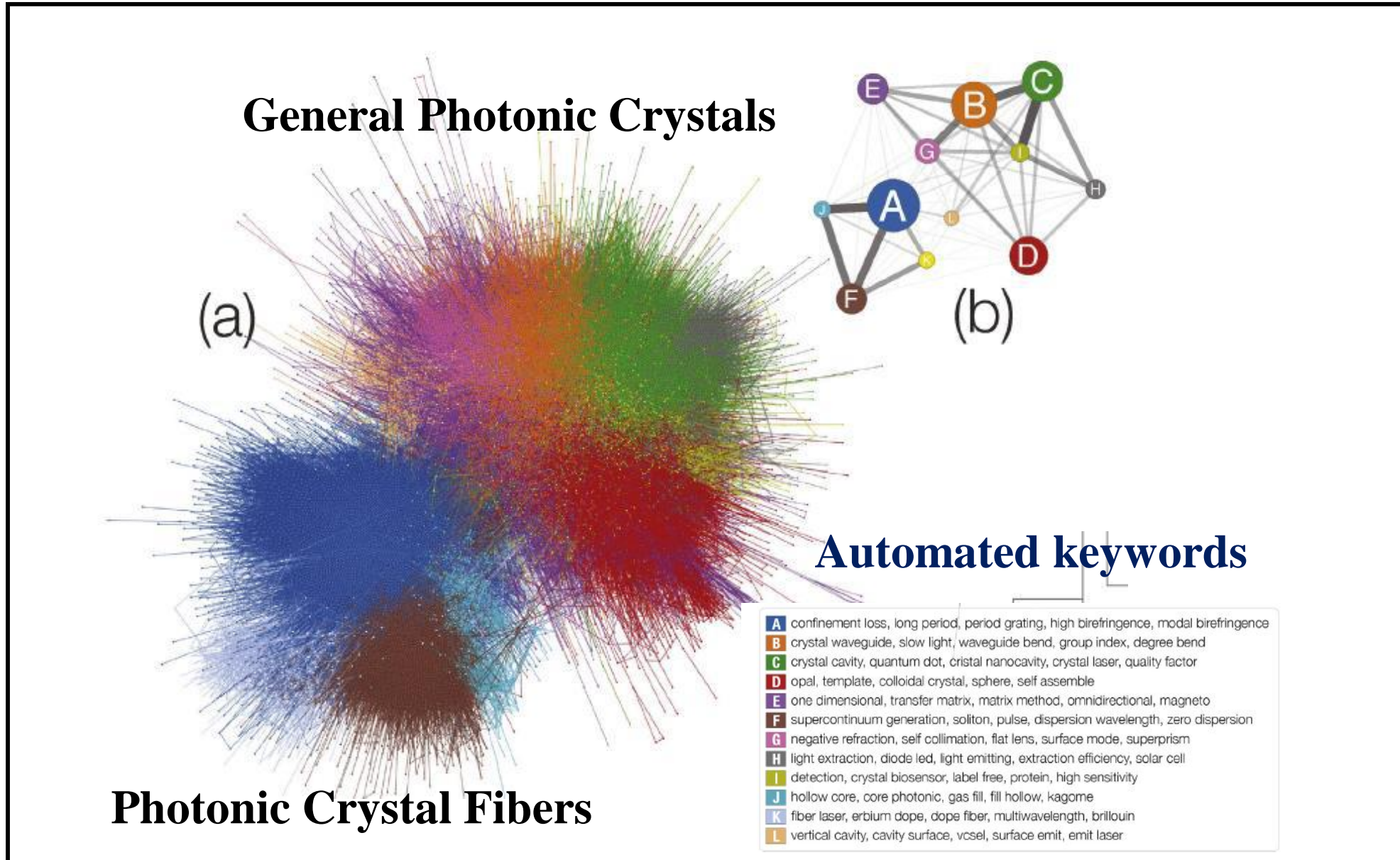
Some Requirements

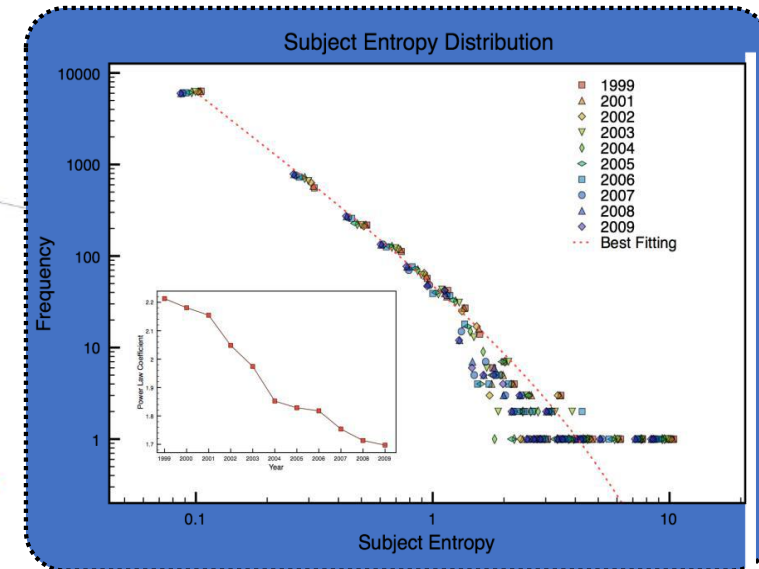
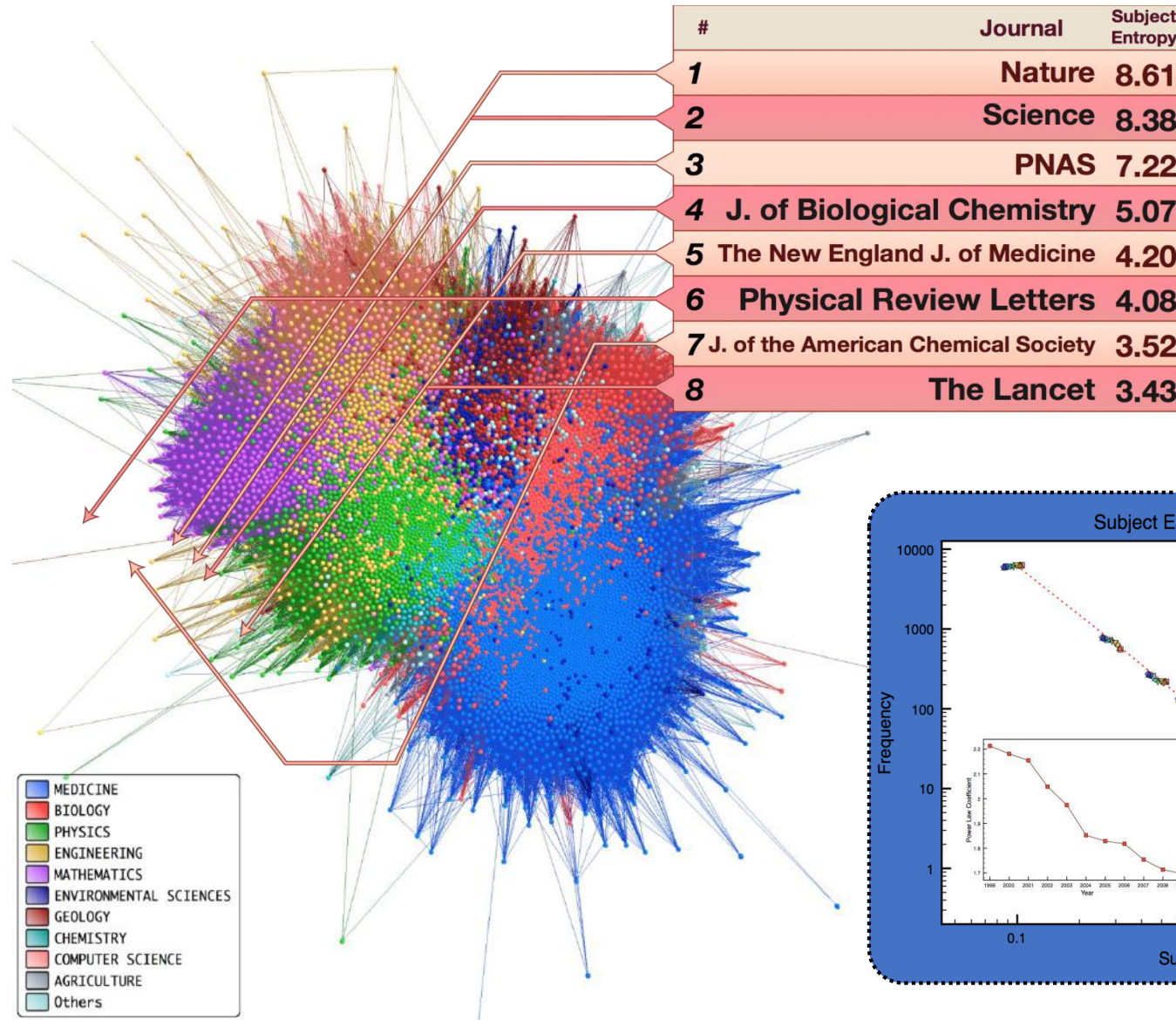
- **Text analytics – large text databases**
- **Lots of data: experimental, theoretical (DFT, etc) and simulation (MD, etc)**
- **Internet of Things**
- **Machine Learning Methods (Deep Learning, etc)**

Computer-assisted diagnosis as an example



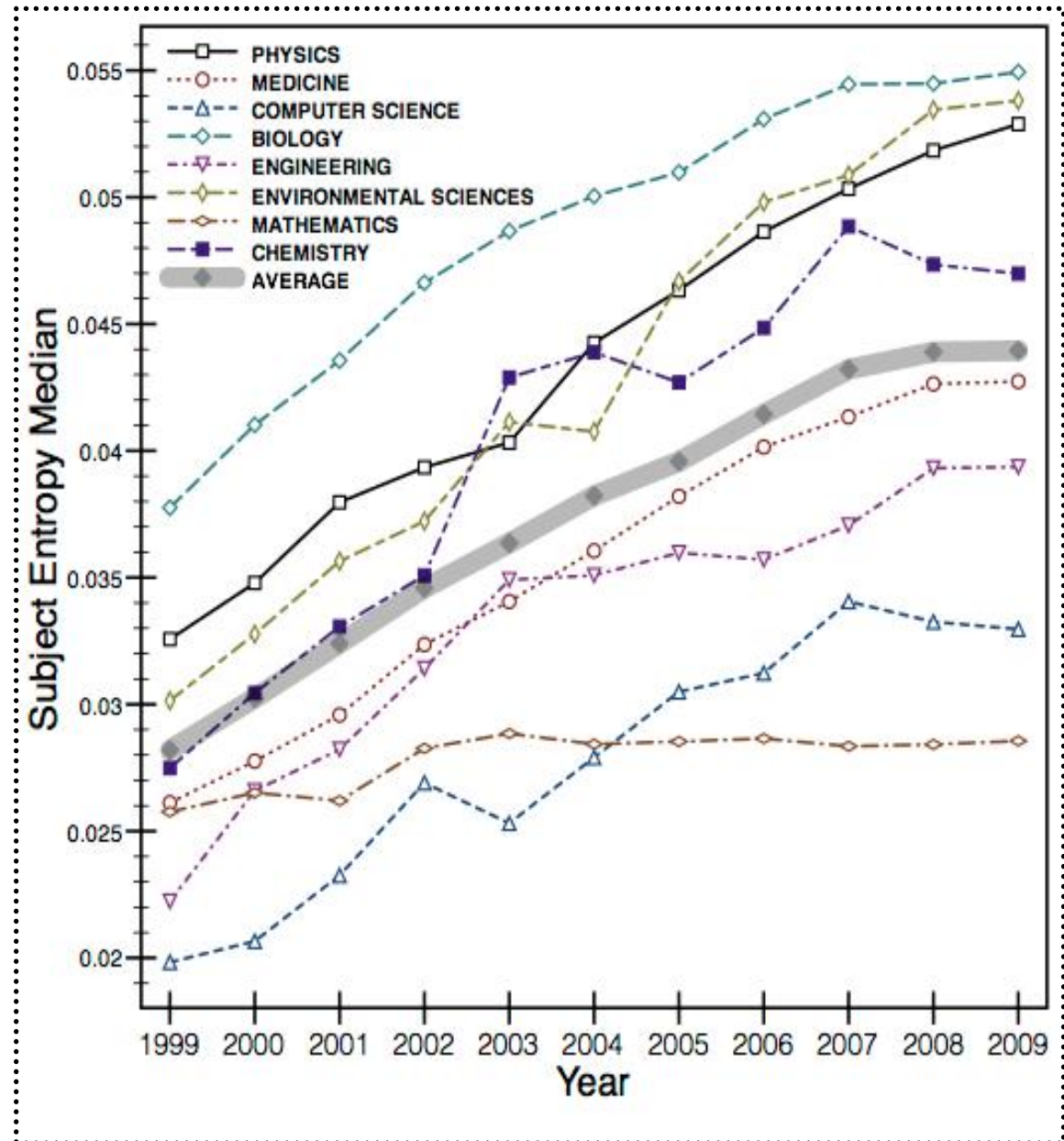






- Areas becoming increasingly multidisciplinary
- Subject entropy correlates highly with impact factor and betweenness centrality

Filipi N. Silva et al.,
J. Informetrics, 2013



Knowledge Discovery in Practice

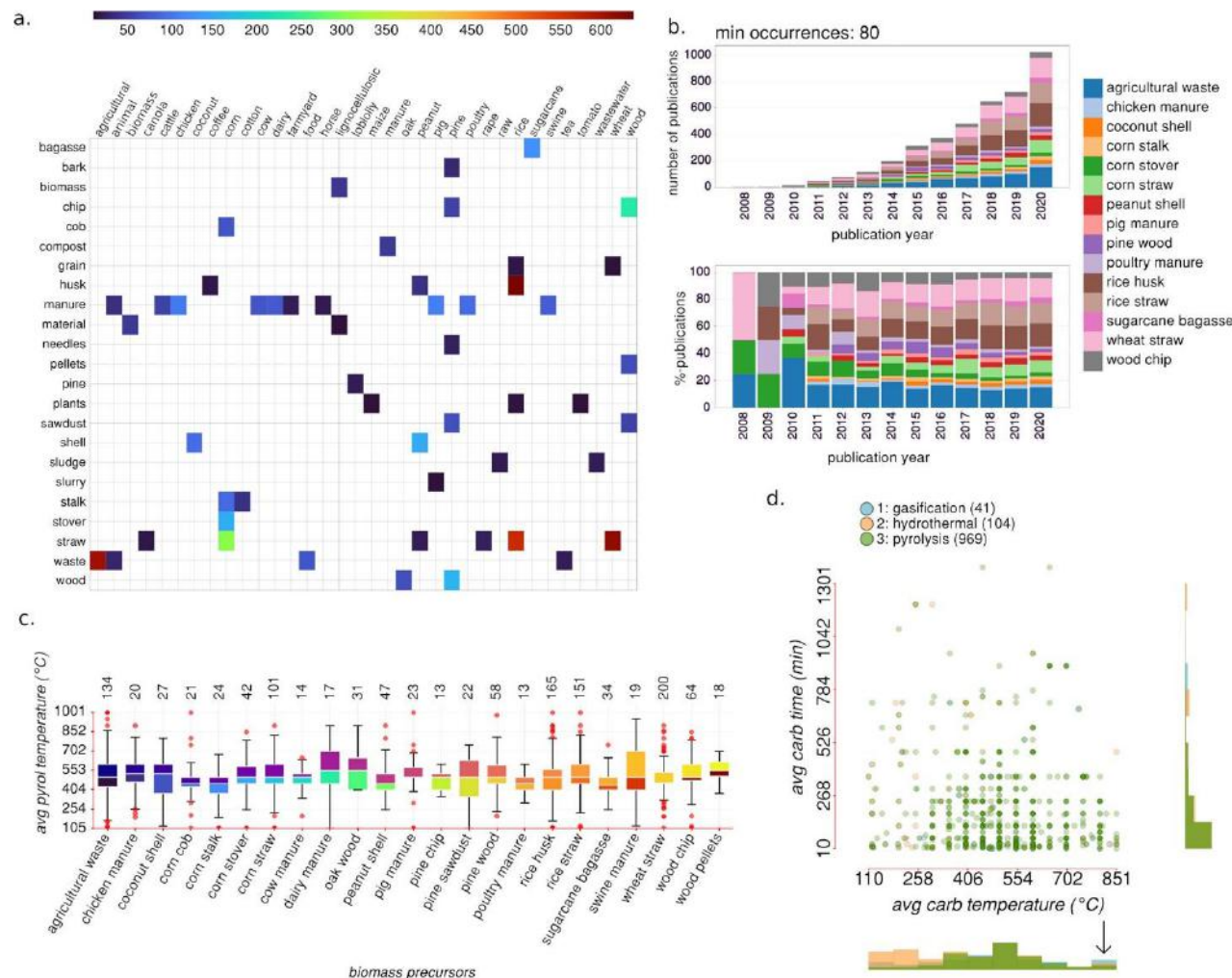
10,975 scientific articles
on carbon functional materials (CFM)

Machine Learning and Natural Language Processing Enable a Data-Oriented Experimental Design Approach for Producing Biochar and Hydrochar from Biomass

Amauri J. Paula,* Odair Pastor Ferreira, Antonio G. Souza Filho, Francisco Nepomuceno Filho, Carlos E. Andrade, and Andreia F. Faria*

Cite This: *Chem. Mater.* 2022, 34, 979–990

[Read Online](#)



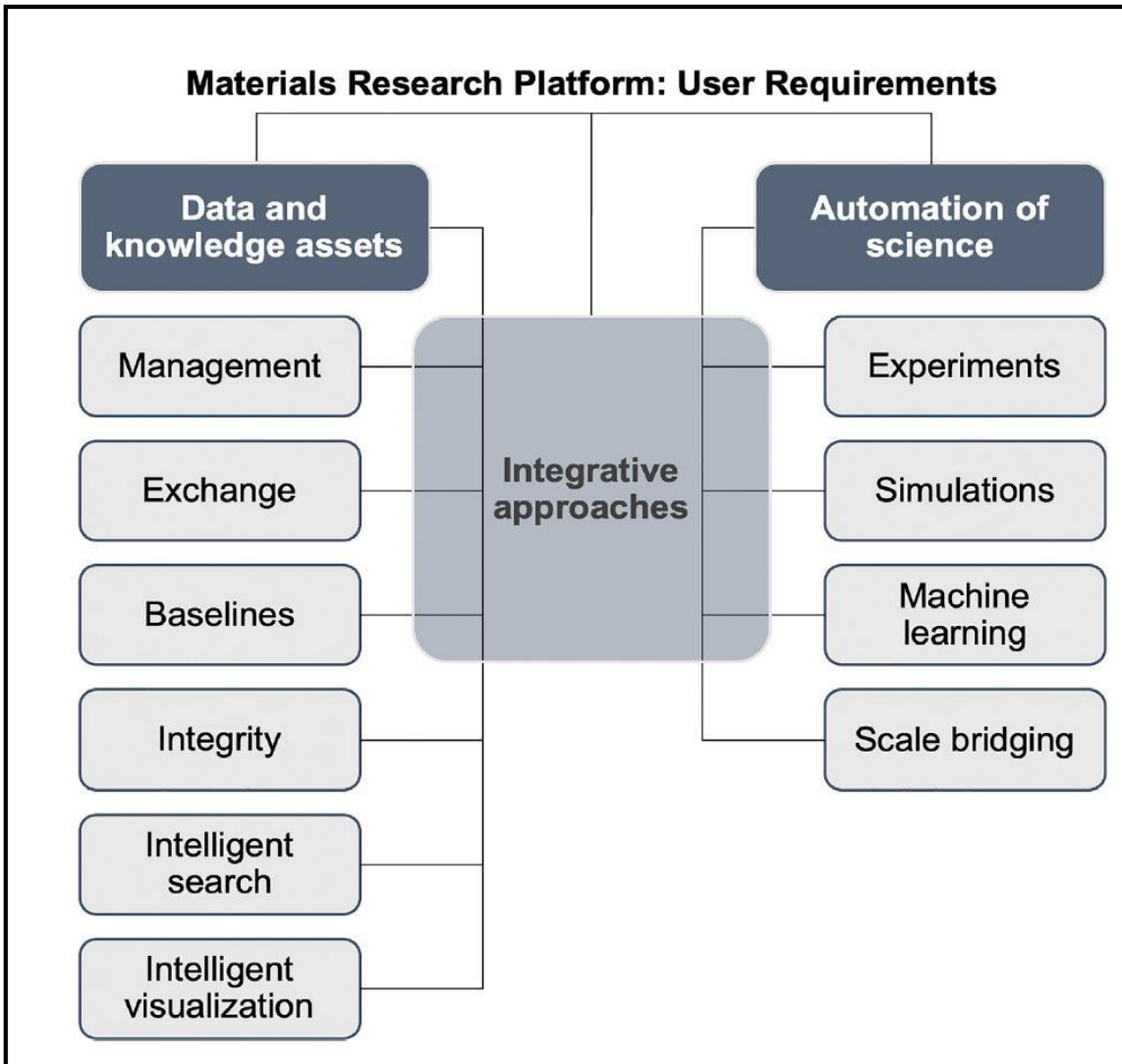
Identify:

- Precursors (sludge, agriculture waste)
- Synthesis and post-synthesis methods
- Synthesis conditions

Find correlations:

- Most used precursors for agriculture, fuel, adsorbents
- Most efficient precursors for CFM production depending on the synthesis method
- Optimized synthesis conditions depending on the precursors and method
- CFM properties and possible applications

Materials research of the future



Adaptive systems—active-learning and beyond;

Automation of experiments;

Automation of simulations;

Collaboration;

Data ingestion and sharing;

Integration;

Knowledge discovery;

Machine learning for experiments;

Machine learning for simulations;

Multi-fidelity and uncertainty quantification;

Reproducibility and provenance;

Scale bridging;

Simulation tools;

Software infrastructure;

Text mining and natural language processing;

Visualization.

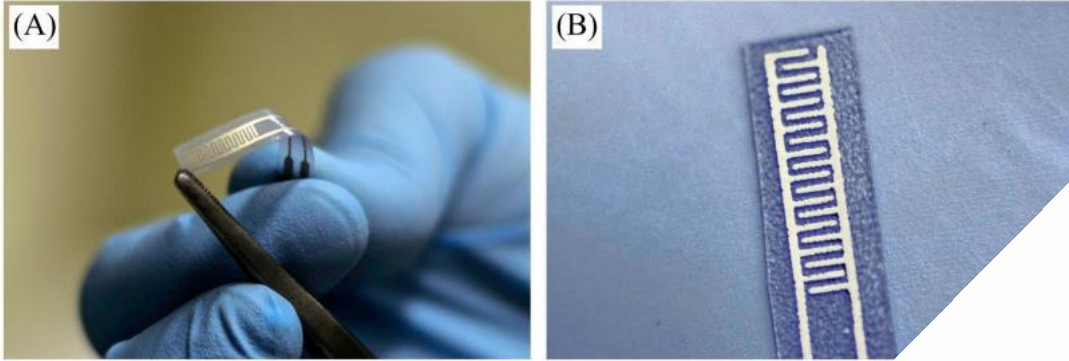
Main Challenges in Biosensing

- **Wearable, implantable devices**
- **Translate technology into the market**
- **Understanding molecular-level mechanisms (theory and experiment)**
- **Data analysis, especially with AI**
- **Integration into fully-fledged systems (IoT, monitoring and surveillance)**



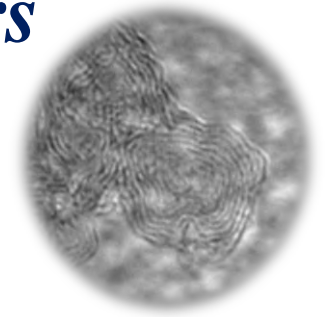
Generic Platform: matrices for various biomarkers

Flexible Biosensors

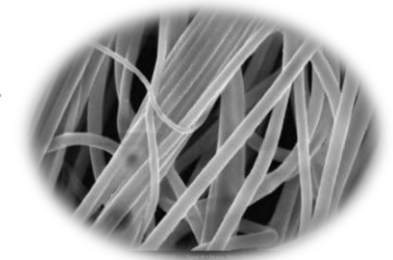


Ibanez-Redin et al. Mat. Sci. Eng C, 2019

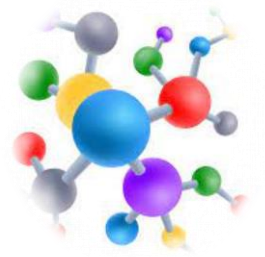
Matrices and Biomarkers



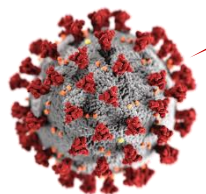
Carbon Materials



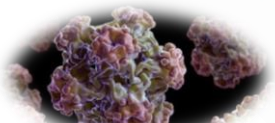
Polymers



Peptides



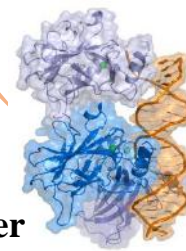
SARS-CoV-2



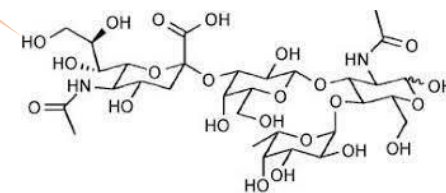
HPV16



PCA3 Biomarker



p53 Biomarker



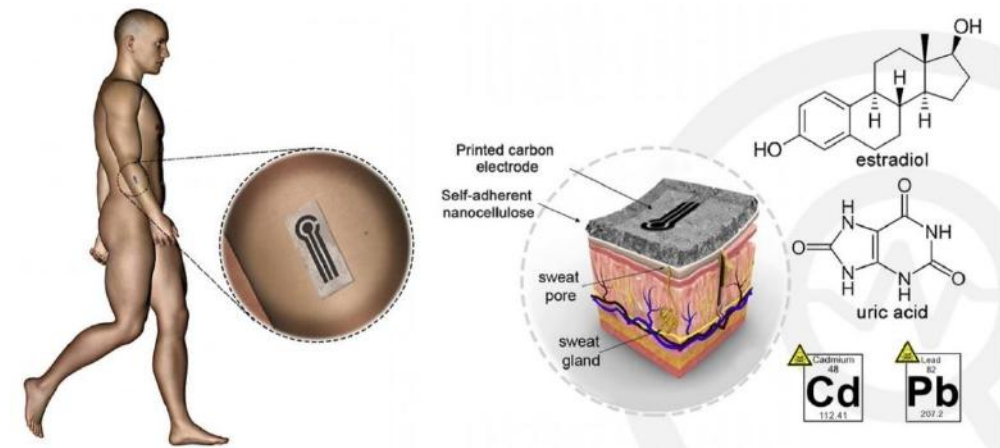
CA 19-9 Biomarker



Microbial nanocellulose adherent to human skin used in electrochemical sensors to detect metal ions and biomarkers in sweat



Robson R. Silva^{a,1,*}, Paulo A. Raymundo-Pereira^{a,1}, Anderson M. Campos^b, Deivy Wilson^a, Caio G. Otoni^c, Hernane S. Barud^d, Carlos A.R. Costa^e, Rafael R. Domenequetti^f, Debora T. Balogh^a, Sidney J.L. Ribeiro^f, Osvaldo N. Oliveira Jr.^a



Biomarkers, range of detection and type of sample.

Glucose:	$1.0 - 30 \times 10^{-3} \text{ mol L}^{-1}$	sweat and saliva
Lactic acid:	$1.0 - 24 \times 10^{-3} \text{ mol L}^{-1}$	sweat and saliva
Uric acid:	$0 - 70 \times 10^{-6} \text{ mol L}^{-1}$	sweat and saliva
Estradiol:	$0 - 3.0 \times 10^{-6} \text{ mol L}^{-1}$	sweat and saliva
Lead:	$1.0 - 10 \times 10^{-6} \text{ mol L}^{-1}$	sweat and saliva
Cadmium:	$4.5 - 14 \times 10^{-6} \text{ mol L}^{-1}$	sweat and saliva
Sodium:	under development	sweat and saliva
Potassium:	under development	sweat and saliva
Creatinine:	under development	sweat and saliva
Urea:	under development	sweat and saliva

Electrochemical detection
Adherent to human skin
Biocompatible
Biodegradable
Mechanically resistant
Permeable to sweat

Features

cost-effective, rapid response,
robust and high stability

Selective and sensitive multiplexed detection of pesticides in food samples using wearable, flexible glove-embedded non-enzymatic sensors

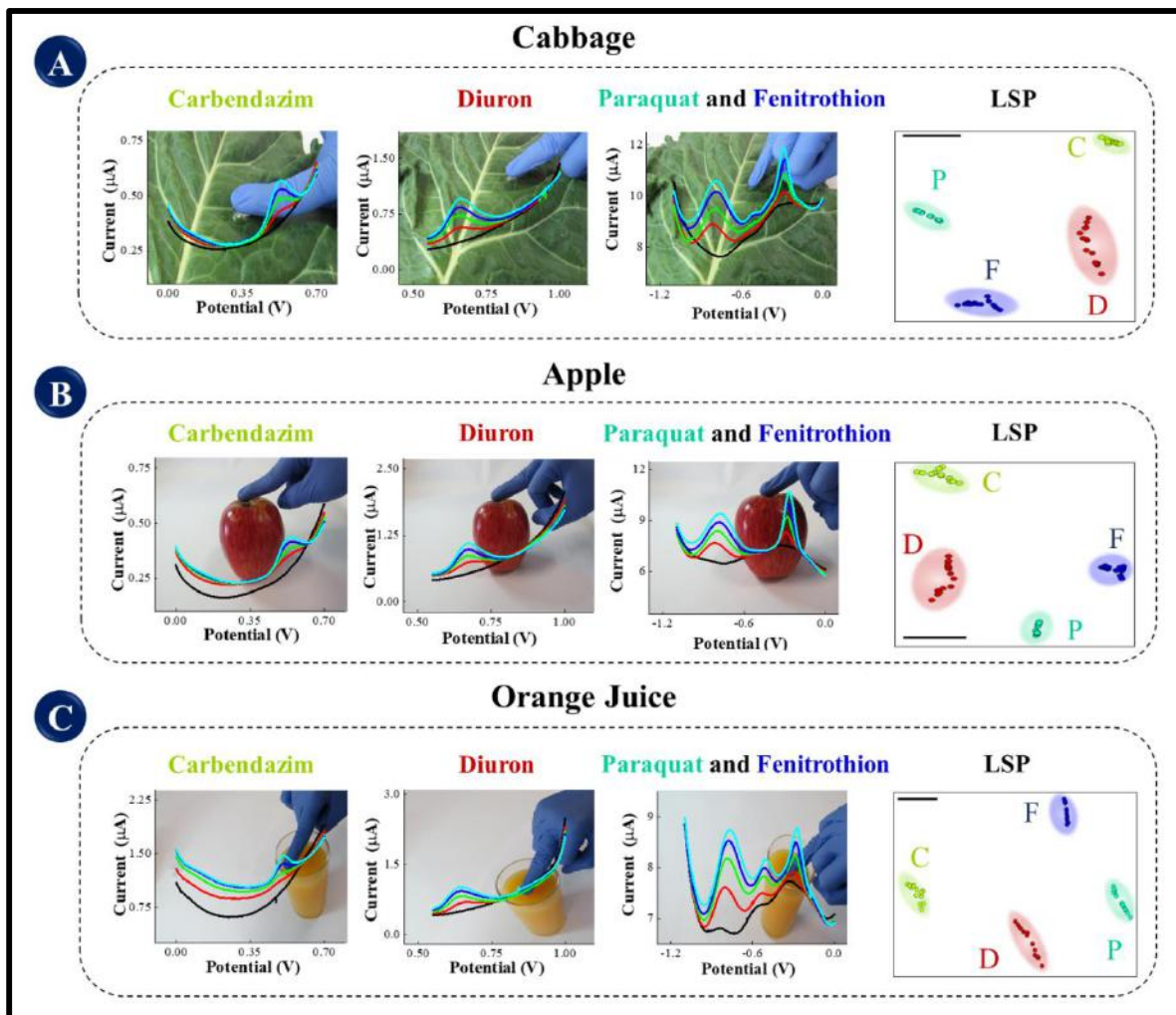
Paulo A. Raymundo-Pereira^{a,*}, Nathalia O. Gomes^b, Flávio M. Shimizu^{a,1}, Sergio A. S. Machado^b, Osvaldo N. Oliveira Jr.^a

On-site chemical analysis of hazardous materials

Security applications for a rapid decision-making process in the field

Screening of several analytes in a decentralized chemical analysis

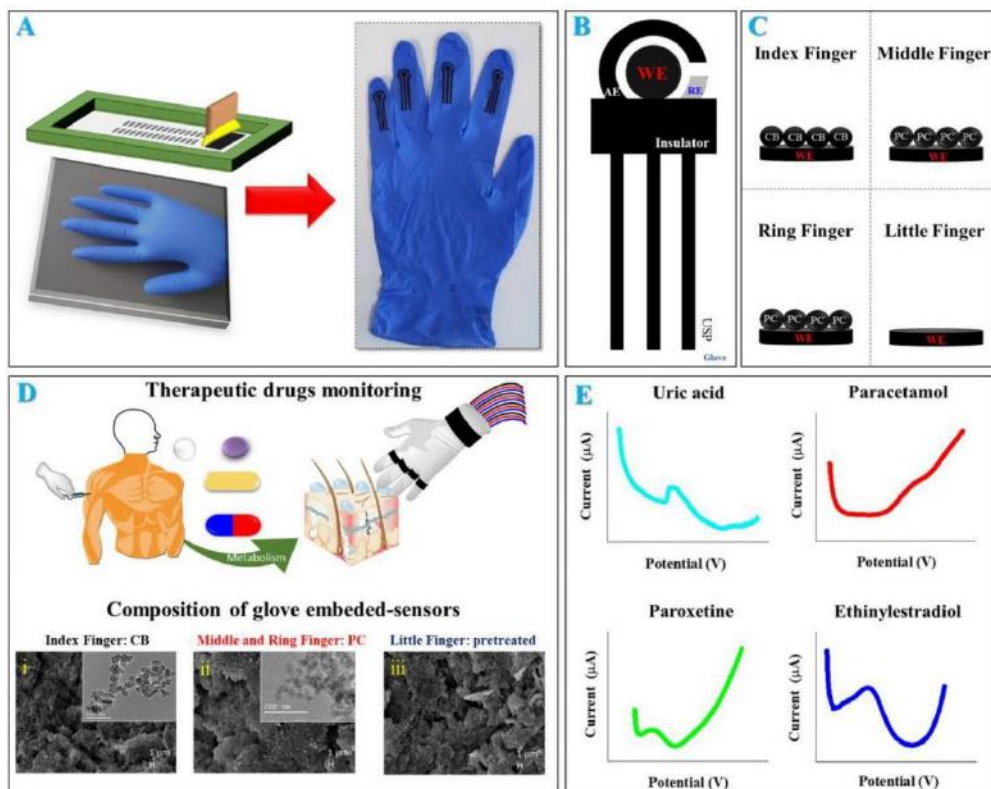
Sensors on a rubber glove





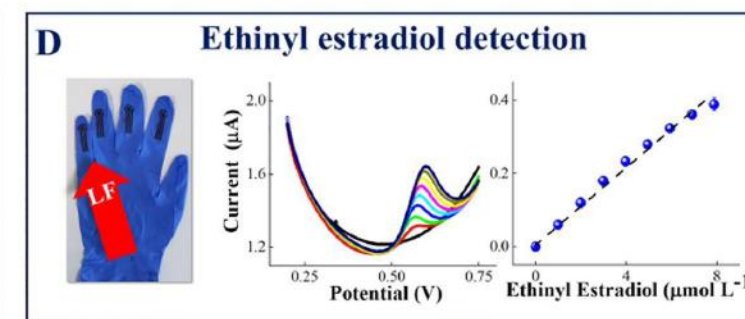
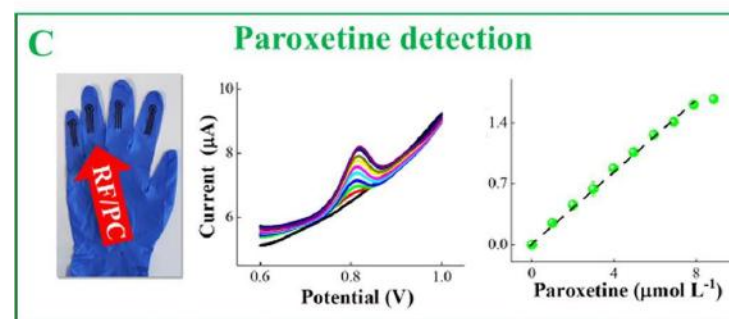
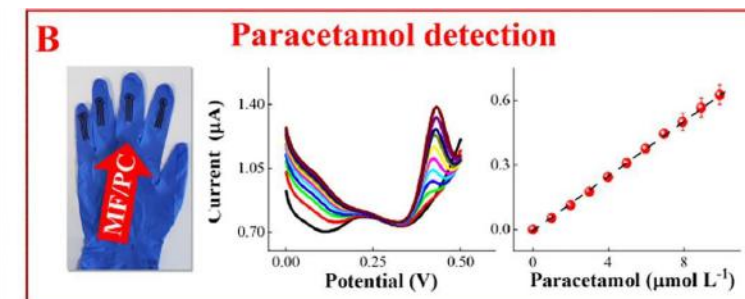
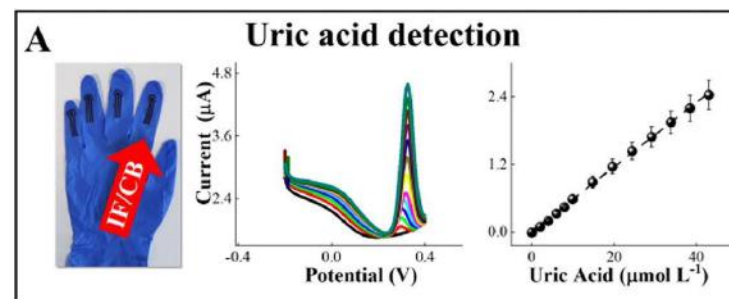
ELSEVIER

Chemical Engineering Journal

 journal homepage: www.elsevier.com/locate/cej


Wearable glove-embedded sensors for therapeutic drug monitoring in sweat for personalized medicine

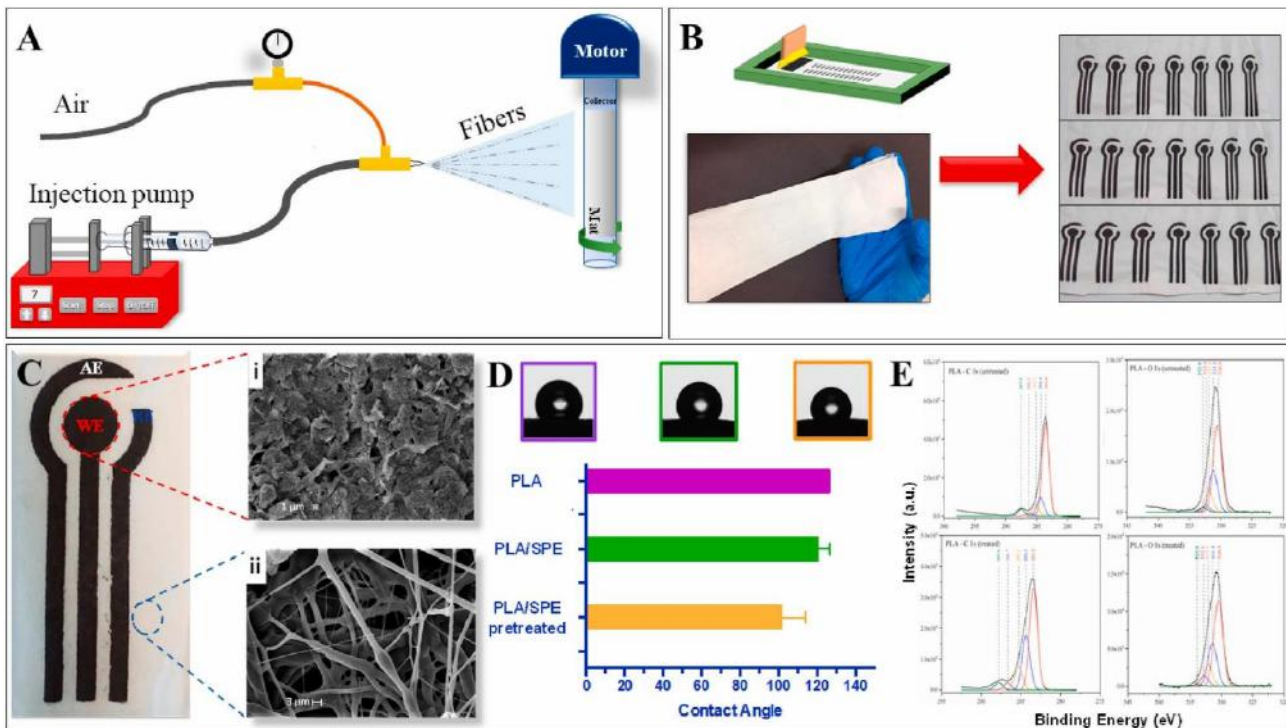
Paulo A. Raymundo-Pereira^{a,1,*}, Nathalia O. Gomes^{b,1}, Sergio A.S. Machado^b, Osvaldo N. Oliveira Jr.^a



Glove-embedded sensors
 Four sensors in 4 fingers
 Carbon balls, electrode pre-treatment and method tailored for the analytes
 Artificial sweat

Towards personalized medicine

PLA fibers produced with solution-blow spinning



Low-cost carbon nanomaterials for screen printed electrodes, optimized with the electrochemical method

Quality control and precision agriculture

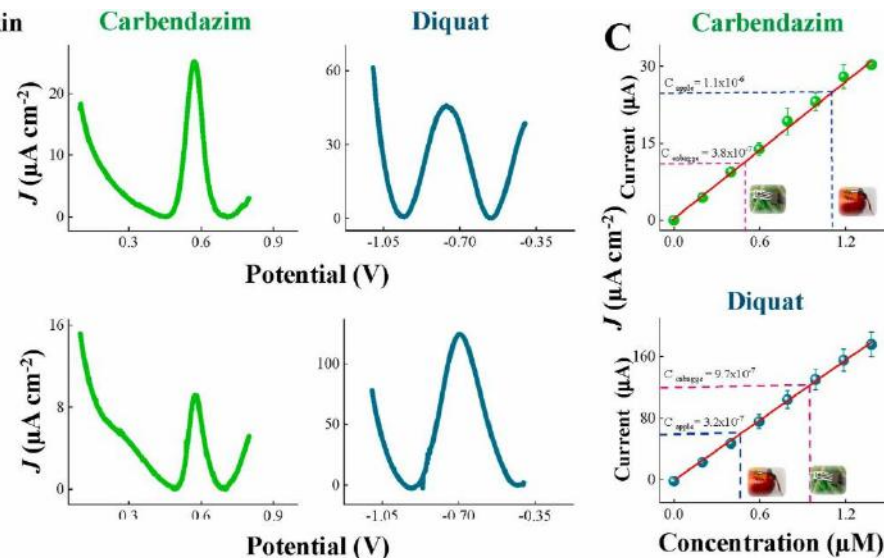
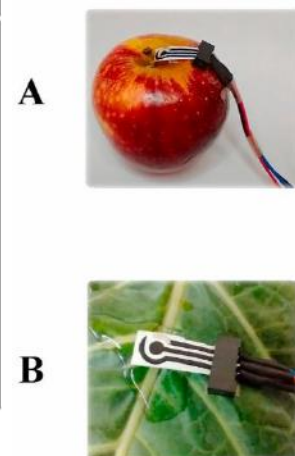
VSI: Wearables

Wearable sensors made with solution-blow spinning poly(lactic acid) for non-enzymatic pesticide detection in agriculture and food safety

Rafaella T. Paschoalin^{a,1}, Nathalia O. Gomes^{b,1}, Gabriela F. Almeida^c, Stanley Bilatto^c, Cristiane S. Farinas^c, Sergio A.S. Machado^b, Luiz H.C. Mattoso^c, Osvaldo N. Oliveira Jr.^a, Paulo A. Raymundo-Pereira^{a,*}



Detection on contaminated skin

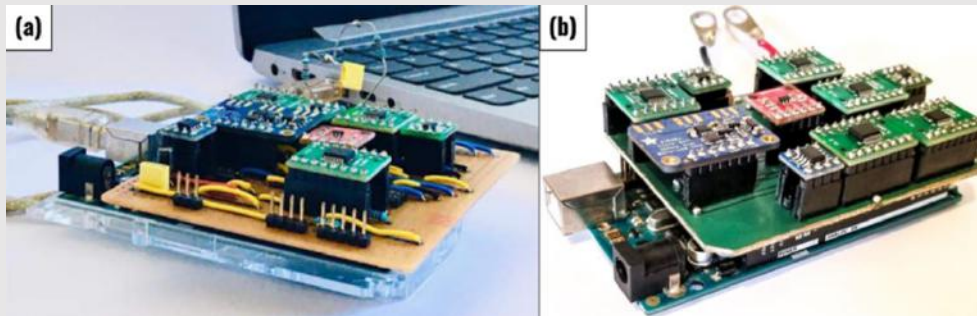
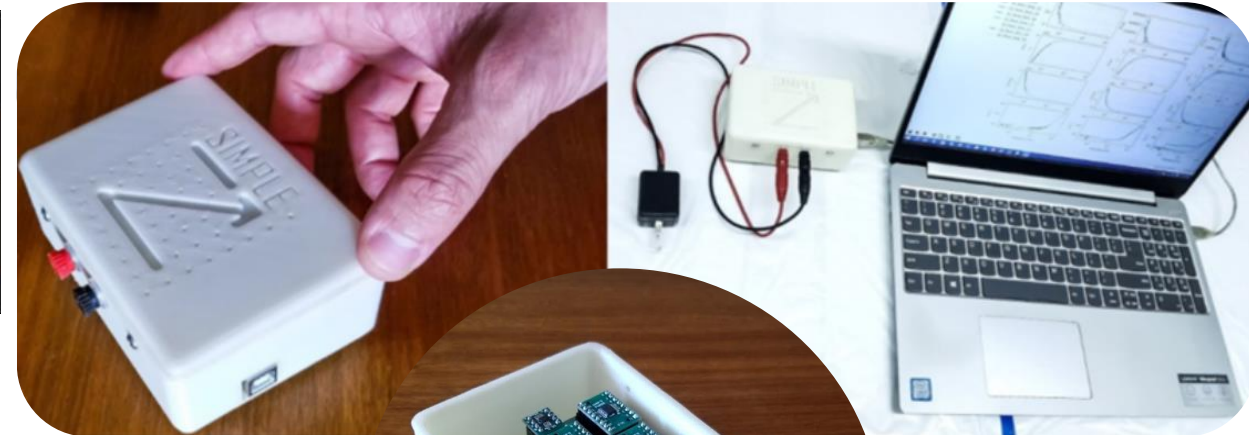
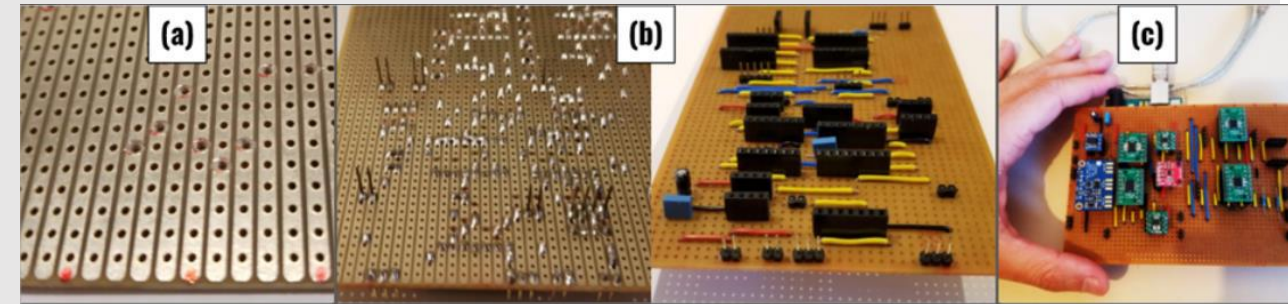


Measurements made on site by touching the fruits and vegetables

Low-cost impedance analyser

Electronic Circuits

Protection Casing



Simple-Z, Buscaglia et al.

Moisture + Dust + Unwanted Contacts + Small Impacts

3D-Printing with Polylactic Acid (PLA)

Low Relief Logo

85x120x50 mm

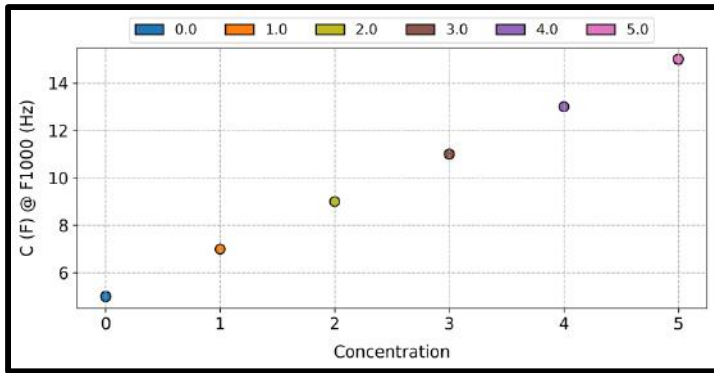
- **Calibration curve replaced by multidimensional space**
- **Equation replaced by rules from Decision Trees or Random Forests**
- **Number of dimensions is the number of features**
- **Minimum number of rules is number of classes**
- **Rule coverage – 1 if all instances are classified correctly**
- **Feature importance – percentage of samples explained**

Popolin et al., Bull. Japanese Chem. Soc. 2021

Machine Learning Used to Create a Multidimensional Calibration Space for Sensing and Biosensing Data



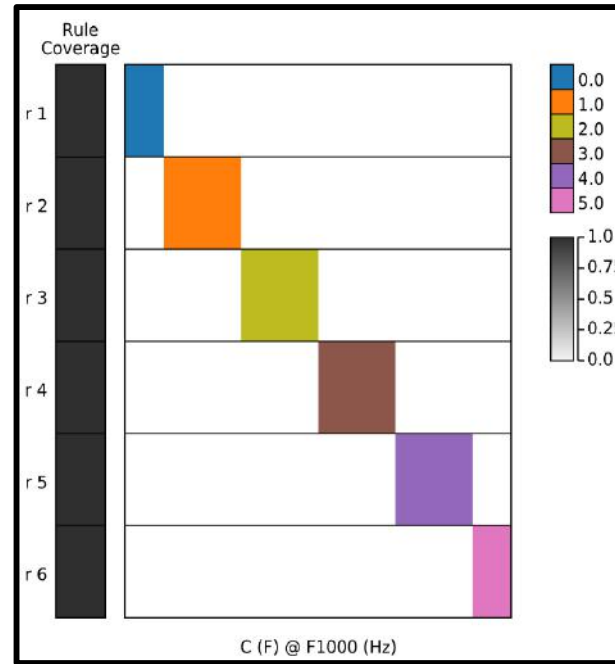
Multidimensional calibration space



Rule r1: Coverage 1.0 (supporting all instances)

IF $5.0 \leq C(F) @ F1000 (Hz) < 6.0$

THEN Class 0.0

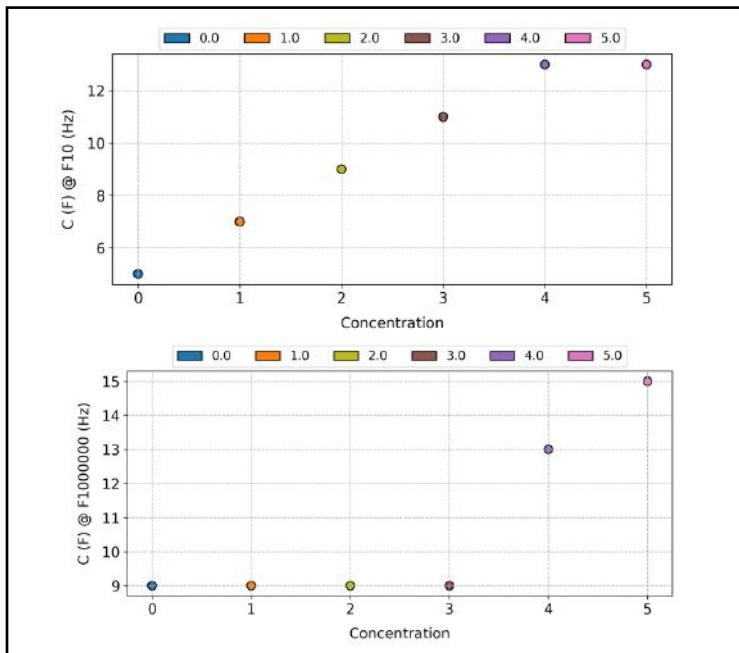


1D MCS

**6 rules
(minimum)**

Full coverage

Same feature importance

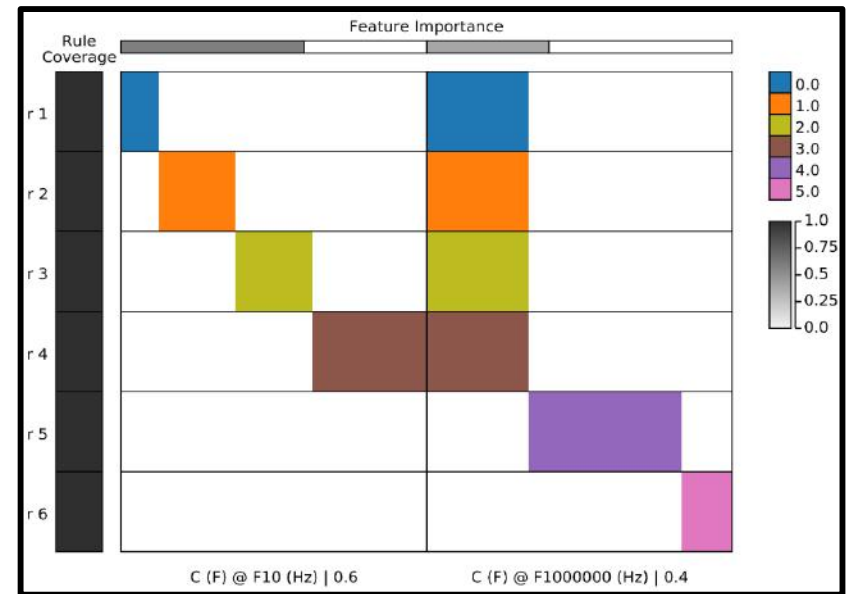


Distinction:

**4 samples at
10 Hz.**

**higher
feature
importance**

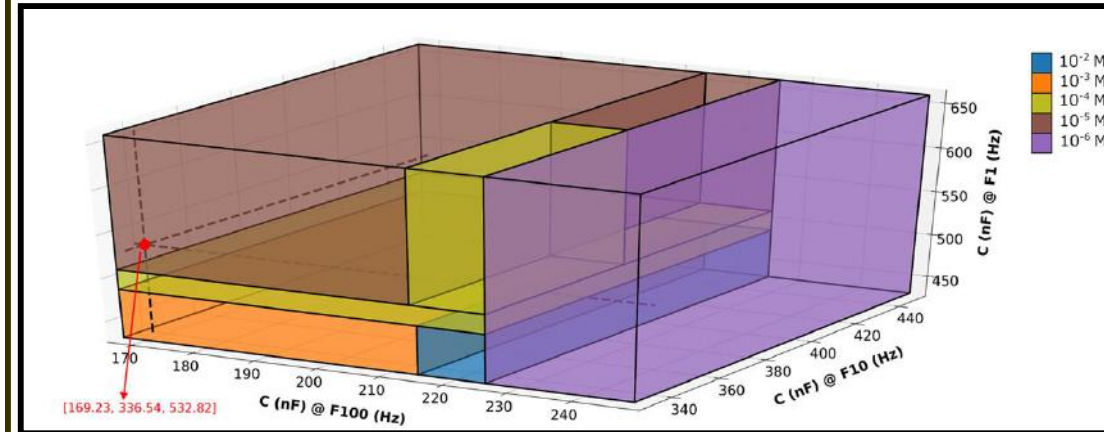
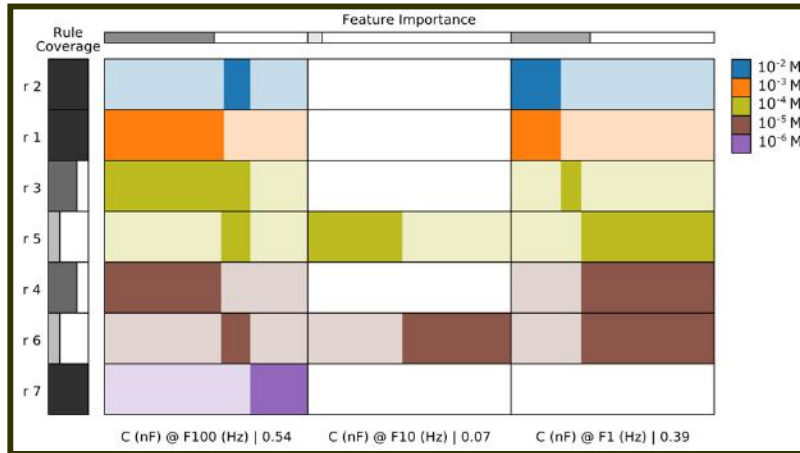
**2 samples at
1MHz**



2D MCS

Multidimensional calibration space

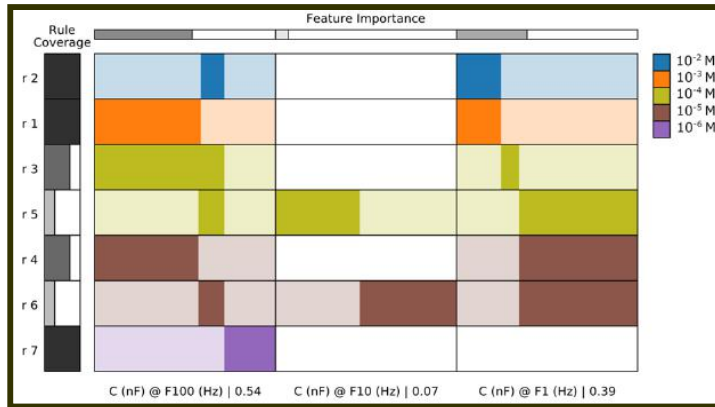
Detection of phytic acid with a bad sensor. Capacitance at three frequencies to generate MCS (3D)



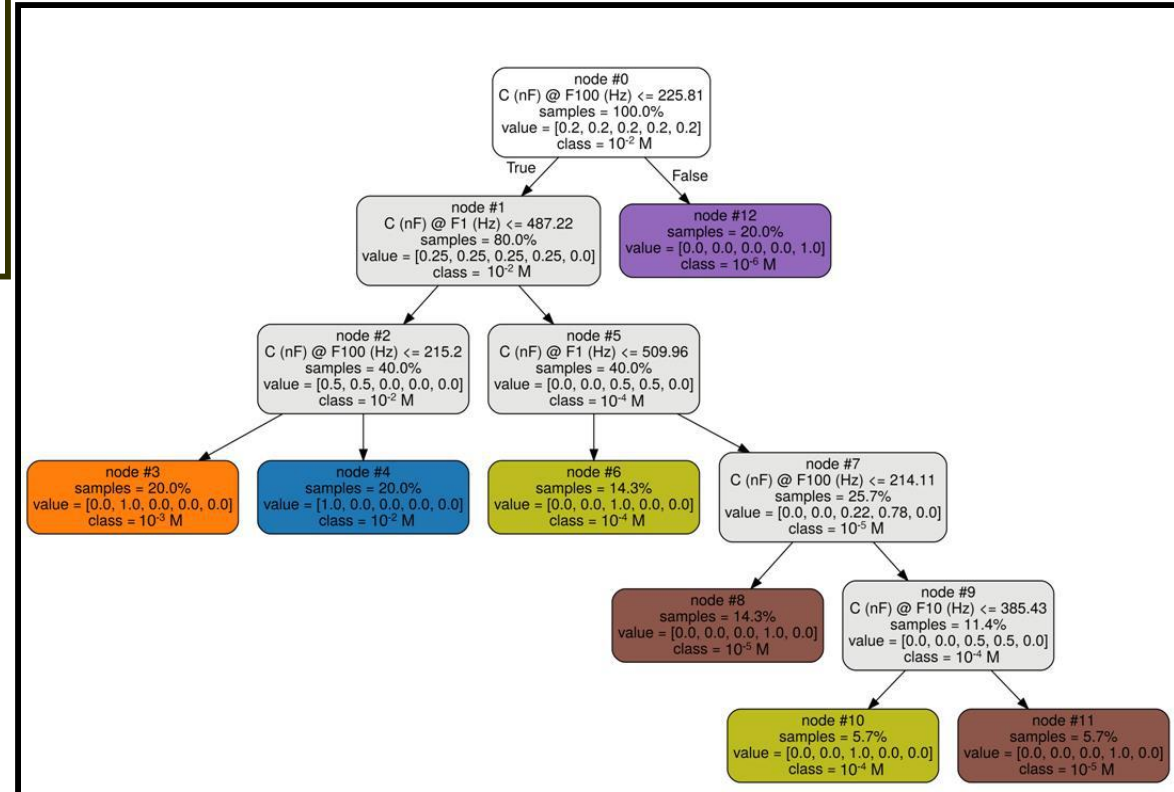
Seven rules used to classify samples with 5 concentrations. Rule coverage was usually lower than one, and the highest feature importance applied to F100

Popolin et al., Bull. Japanese Chem. Soc. - 2021
Machine Learning Used to Create a Multidimensional Calibration Space for Sensing and Biosensing Data

Multidimensional calibration space

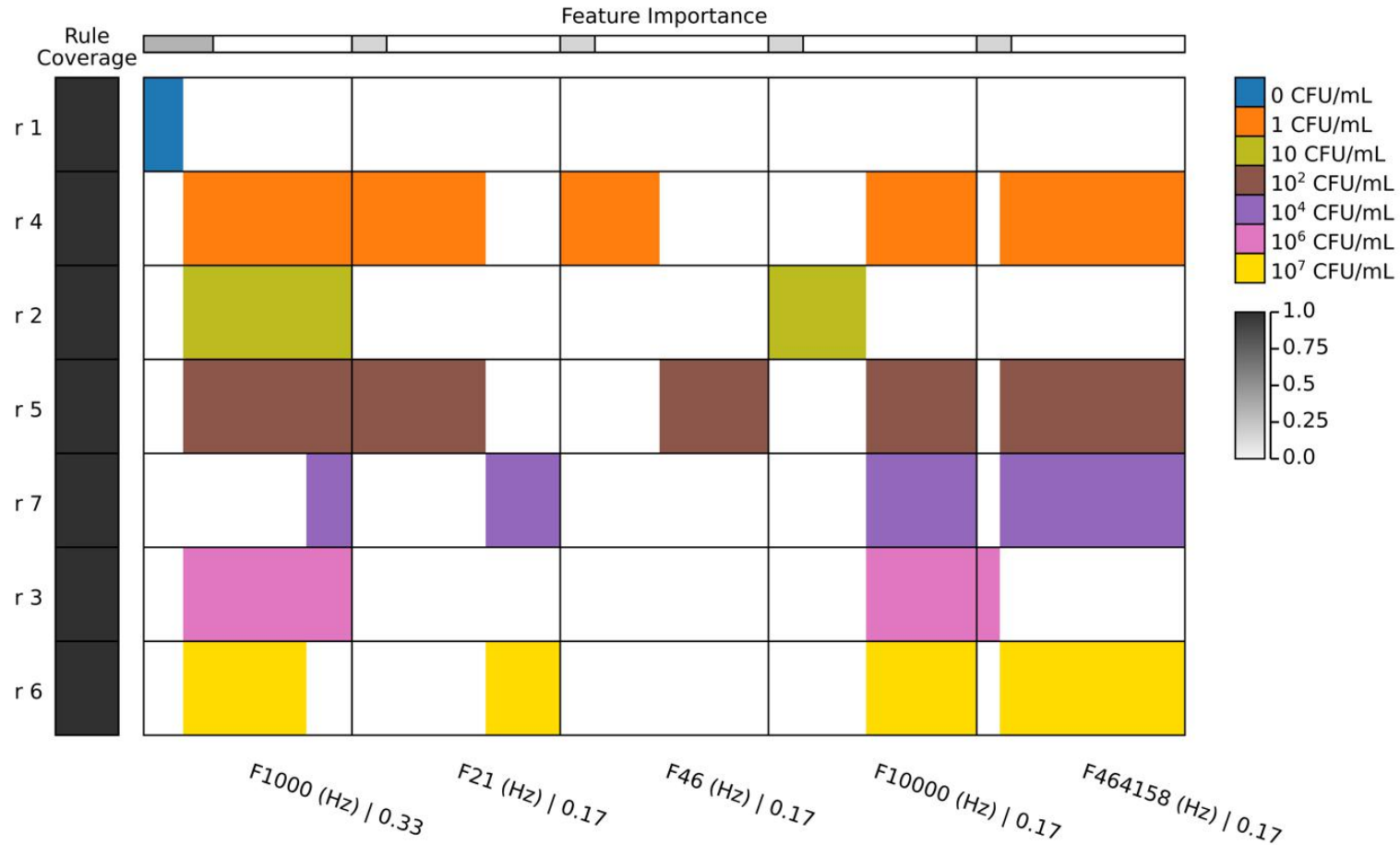


**Rules from
Decision
Trees**



Popolin et al., Bull. Japanese Chem. Soc. - 2021
*Machine Learning Used to Create a Multidimensional Calibration
 Space for Sensing and Biosensing Data*

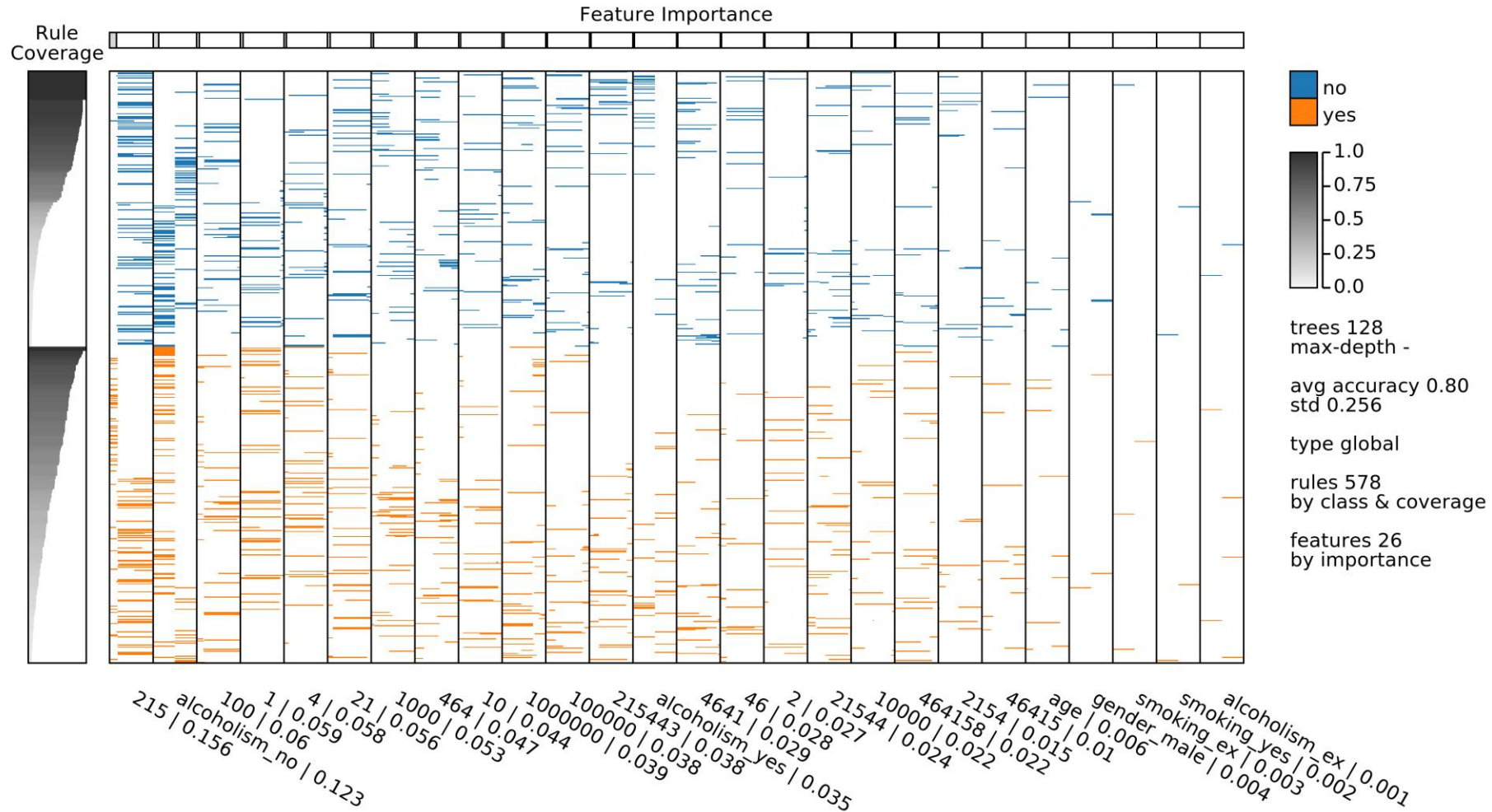
Immunosensor to detect bacteria in milk



Milk samples: *S.aureus* concentrations: 0 - 10⁷ CFU/mL discretized as classes. MCS has 5 dimensions (F1000, F21, F46, F10000 and F464158). Most important feature: F1000 with importance value of 0.33.

Soares et al. Detection of *Staphylococcus aureus* in milk samples using impedance spectroscopy and data processing with information visualization and machine learning (Sensors & Actuators Reports, 2022)

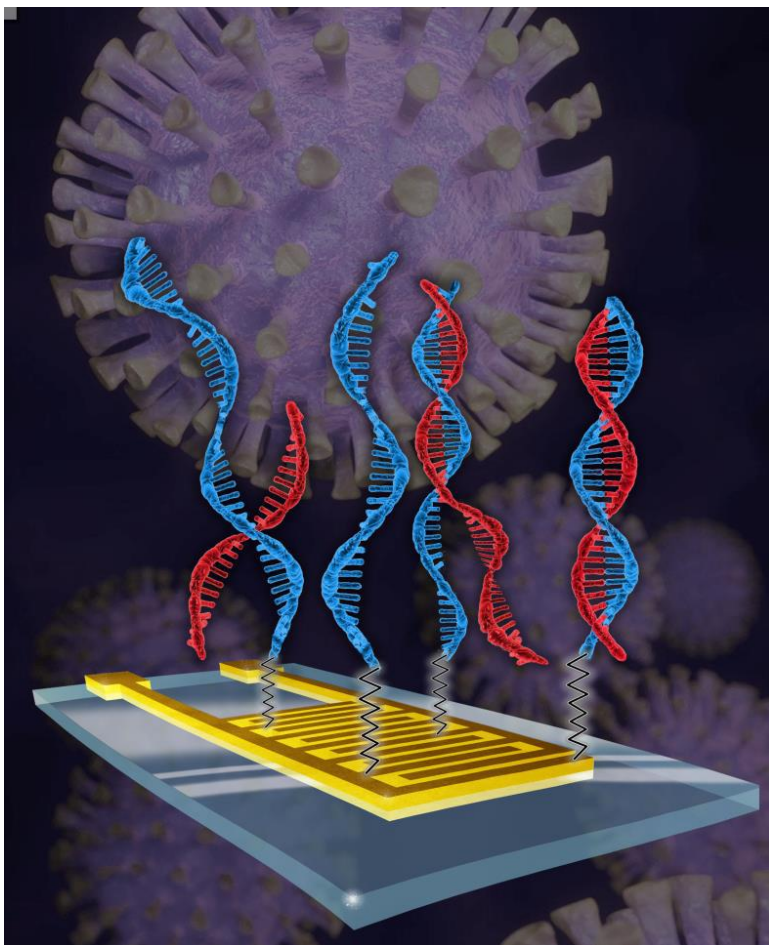
E-tongue for cancer diagnosis



MCS: 26 dimensions - 19 frequencies and 7 clinic features. Most important features: 2 first columns, frequency 215 Hz and "alcoholism_no".

Braz et al. Using machine learning and an electronic tongue for discriminating saliva samples from cancer patients and healthy individuals (Talanta, 2022)

Genosensor to detect SARS-CoV-2



Impedance spectroscopy (IS)
Electrochemical IS
Optical – LSPR
Image analysis

**Gold electrodes coated with SAM
 functionalized with EDC/NHS and a
 layer of ssDNA sequences**

**Probe: cp DNA SARS-CoV-2: 5'-5AmMC6/-
 ATTTCGCTGATTTTGGGGTC-3'**

Positive Control: ssDNA SARS-CoV-2

**5'-
 TGATAATGGACCCCAAATCAGCGAAATGC
 ACCCCGCATTACGTTTGGTGGACCCTCAGA
 TTCAACTGGCAGTAACCAGA-3'**

Negative control: From TP53 gene

**5' - CCCATCCTCACCATCATCACA
 CTGGAAGACTCCAGTGGTAATCTACTGGGA
 CGGAACAGCTTTGAGGTGCGGTTTGTG - 3'**

Image Analysis

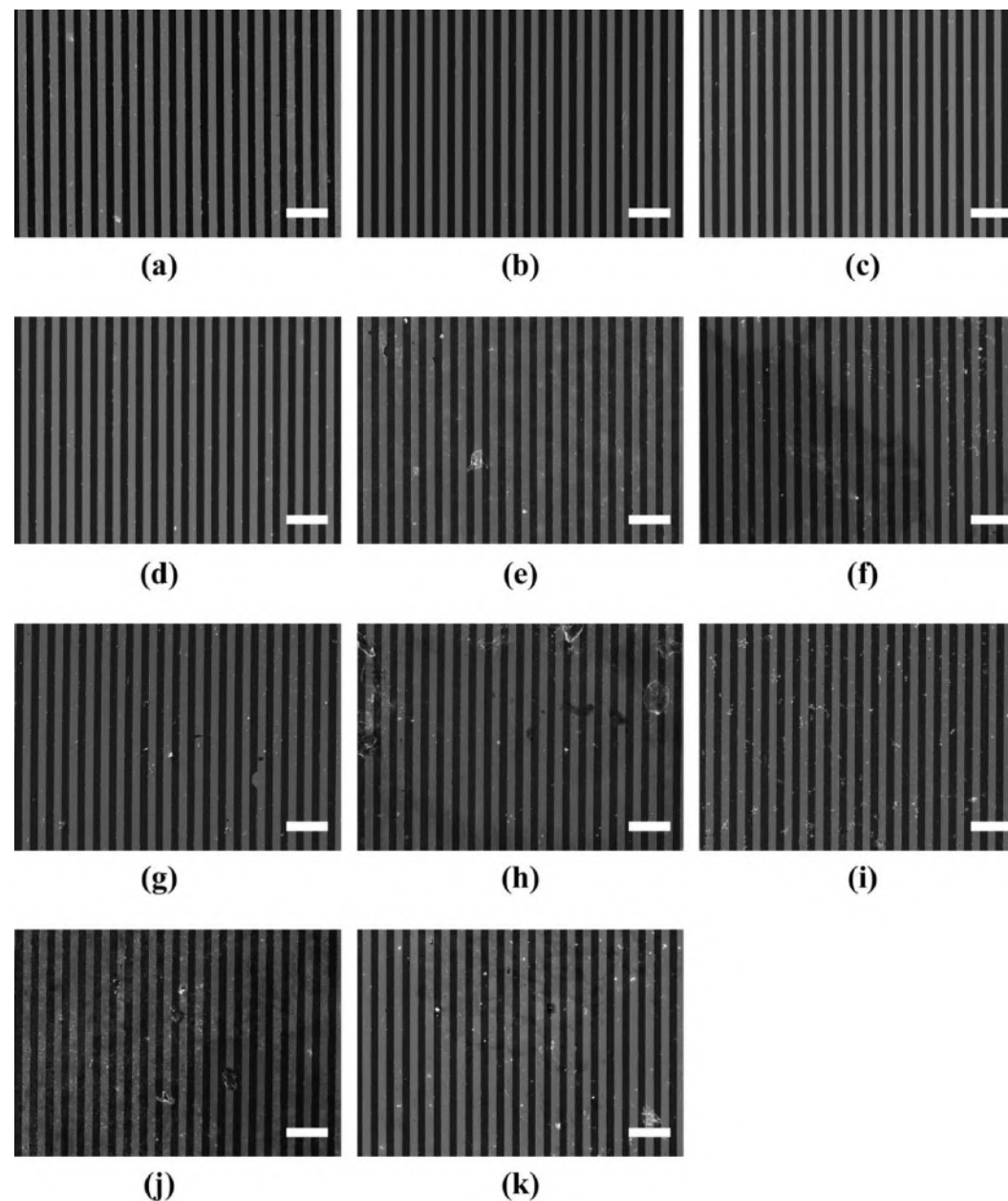
- (a) blank
- (b) negative control
- (c) HPV16
- (d) PCA3
- (e) 10^{-18} mol L⁻¹
- (f) 10^{-16} mol L⁻¹
- (g) 10^{-14} mol L⁻¹
- (h) 10^{-12} mol L⁻¹
- (i) 10^{-10} mol L⁻¹
- (j) 10^{-8} mol L⁻¹
- (k) 10^{-6} mol L⁻¹

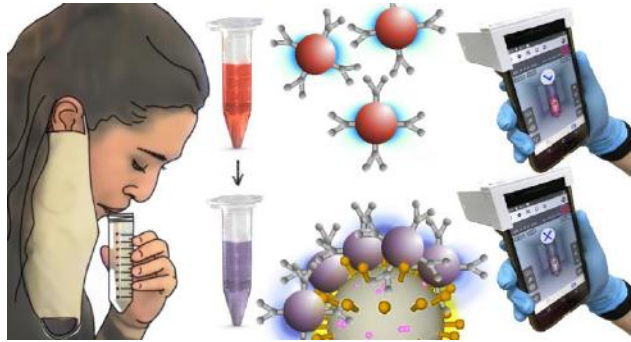
Scale bar: 50 μ m.

Supervised machine learning

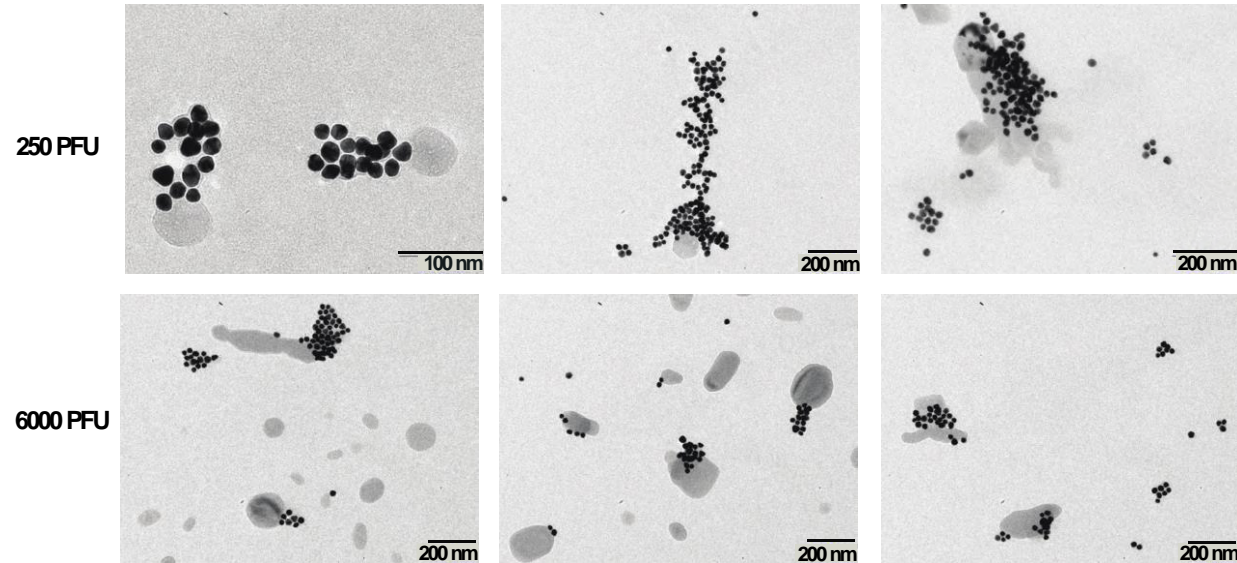
**99.7% accuracy in binary
classification with SVM**

**95.8% accuracy in multiclass
with LDA**

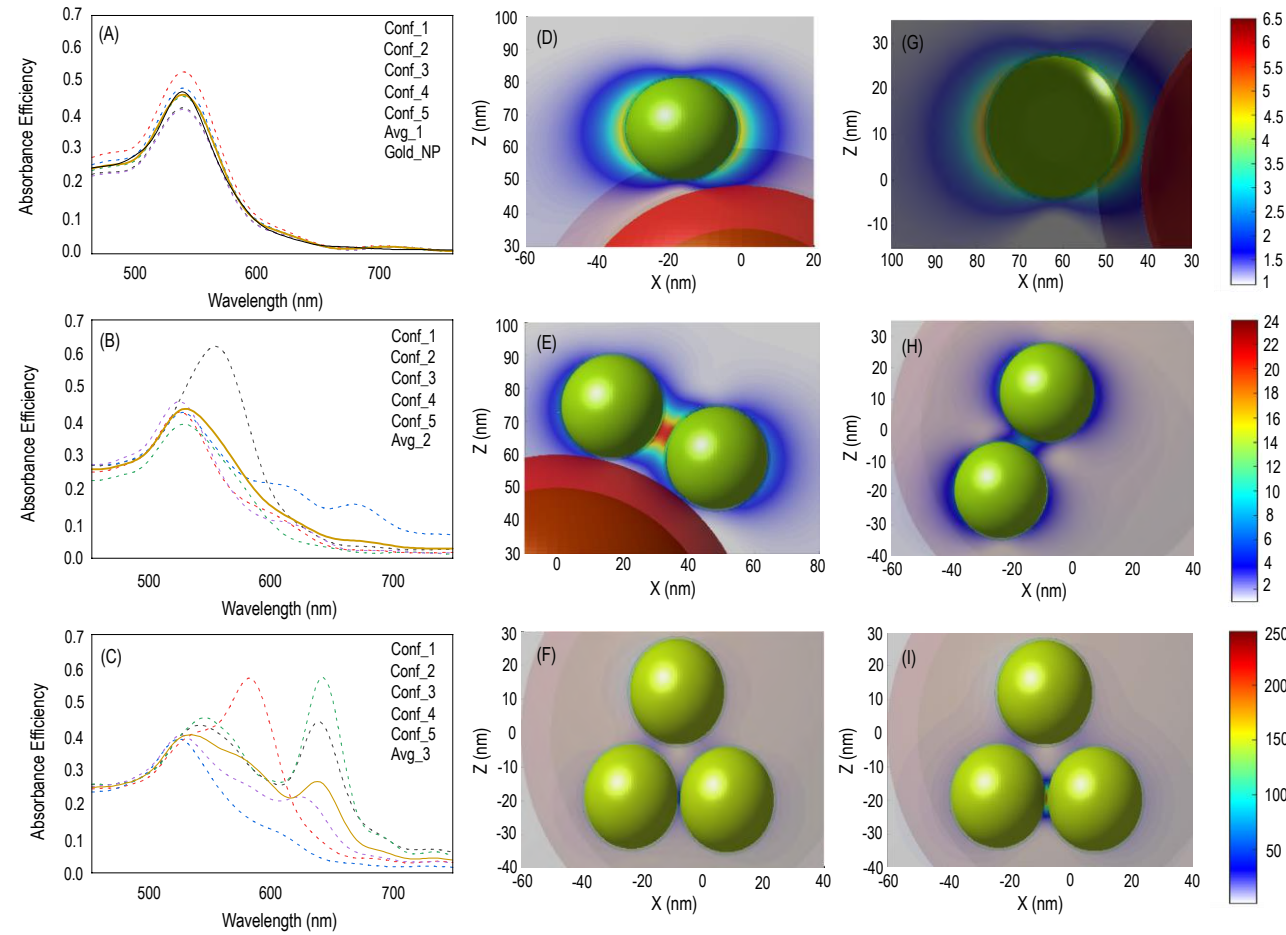




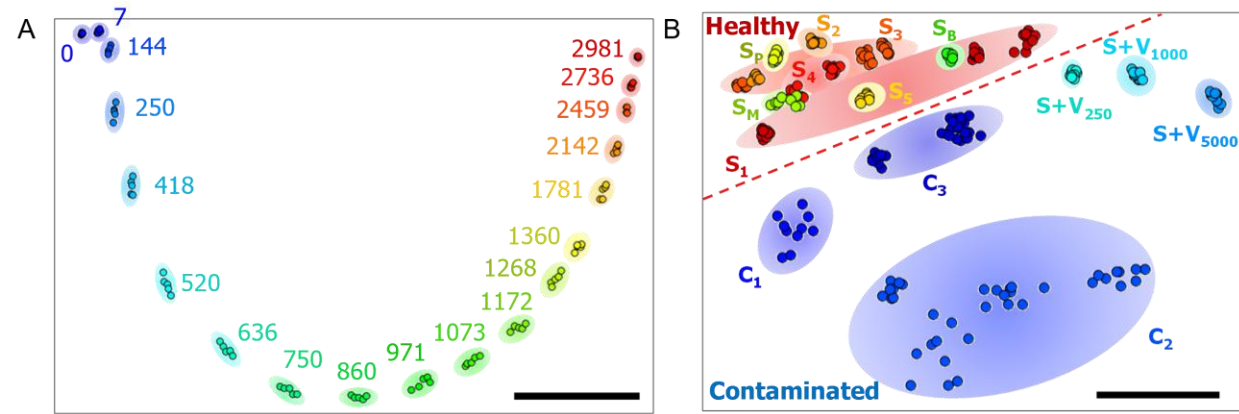
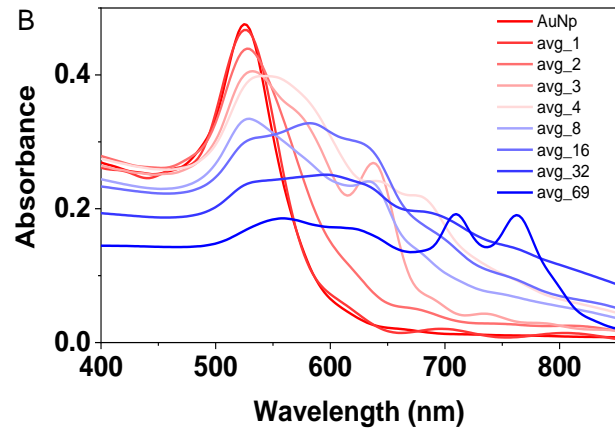
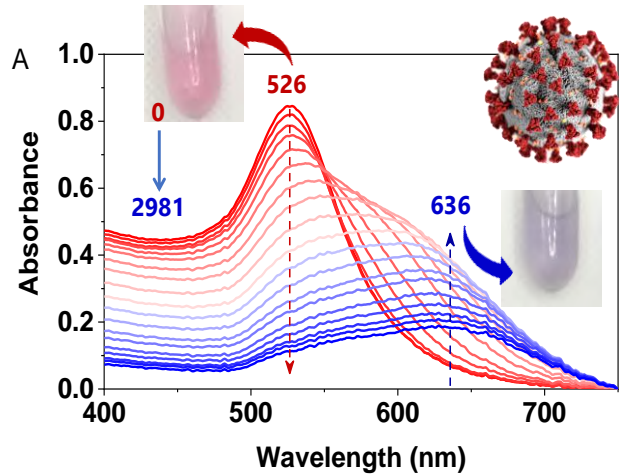
Detection in 5 min



Functionalized AuNPs aggregate after exposure to 250 and 6000 PFU of inactivated SARS-CoV-2.

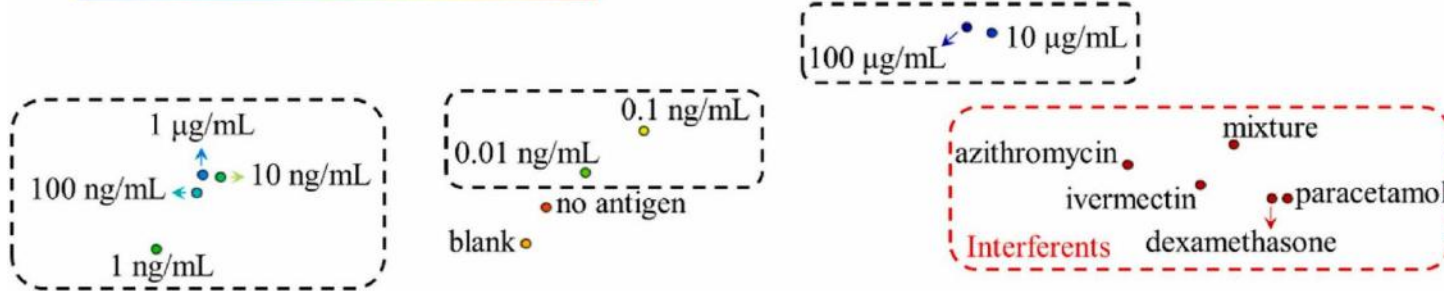


Computer simulations indicate that clustering of the functionalized AuNPs is essential for detection

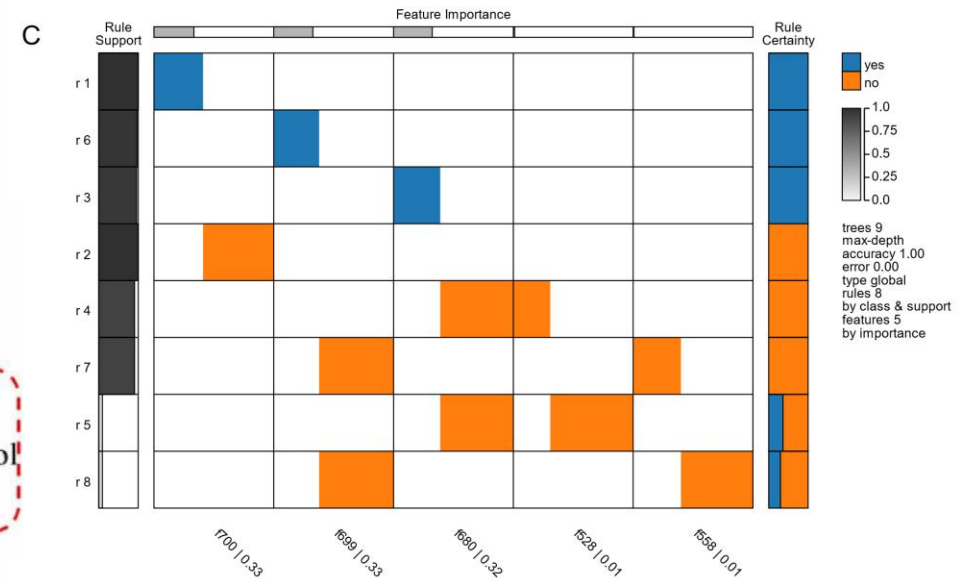


f-AuNPs with SARS-CoV-2 (0 - 2980 PFU mL⁻¹). Spectral absorption efficiency clusters (FDTD simulations).

Min Max



Distinction of SARS-CoV-2 at various concentrations.
No effects from interferents



Inactivated SARS-CoV-2 and tests with human saliva.

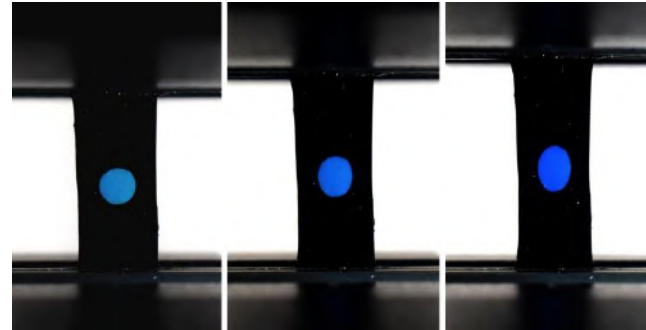
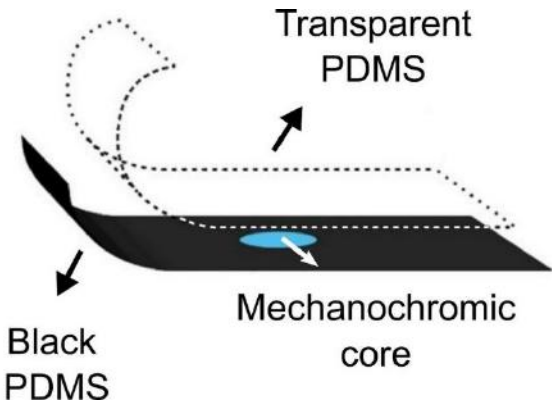
Mechanochromic sensors

Silica Nanoparticle/Polymer Film-Based Soft Mechanochromic Devices for Detecting Mechanical Deformation and Stress Cycles in Varied Environments

Lucas D. C de Castro and Osvaldo N. Oliveira, Jr*

Cite This: *ACS Appl. Nano Mater.* 2022, 5, 2906–2911

Read Online



Color changes during stretching/releasing cycles

Color change is reversible

Works under sunlight and under water

