

# Success case: H2020 CHARISMA project

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Standardisation in Practice: Towards a CEN-CENELEC Workshop Agreement

2024-03-14



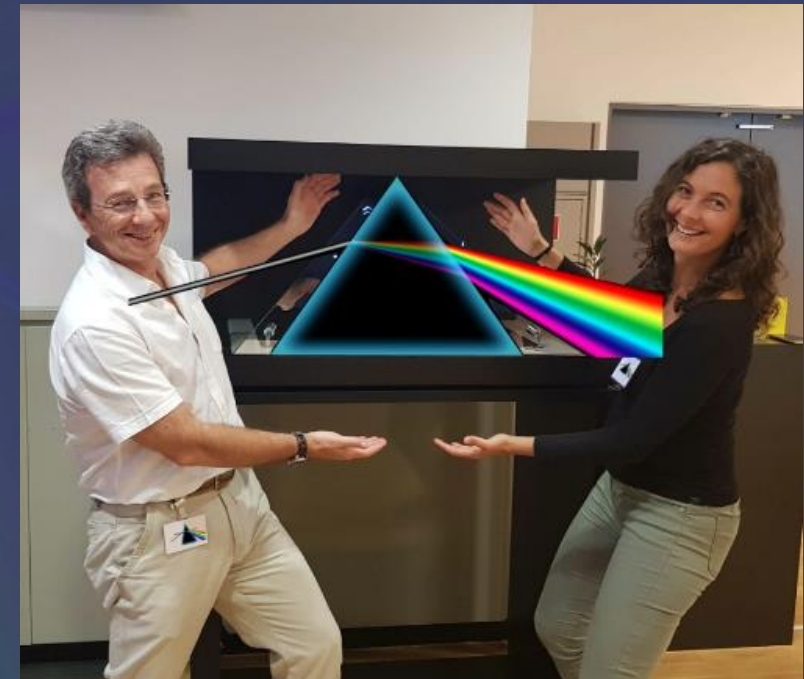
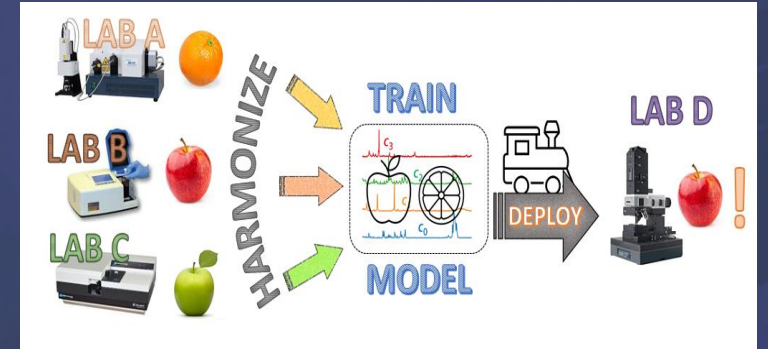
CHARISMA receives funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 952921

# Characterization and HARmonization for Industrial Standardisation of advanced MAterials

## Raman spectroscopy

### Fact sheet:

- Call: H2020-NMBP-TO-IND-2020
- Topic: NMBP-35-2020  
Towards harmonised characterisation protocols in NMBP (RIA)
- Grant agreement: 952921
- Run time: November 2020 – October 2024
- EU grant: 5 M€
- Beneficiaries: 14 (9 countries)
- Coordinator: CSIC: Raquel Portela and Miguel A. Bañares



# Increased industrial and academic use of Raman

## Standards and norms:

- Terminology
- Calibration/Validation
- Data storage and analysis
- SOP / Specific applications

## Realistic conditions:

- Pressure
- Temperature
- Environment
- Sample (shape, size)

## Computational support:

- Sample measurement
- Spectra calculation
- Spectrum processing
- Data analysis and storage

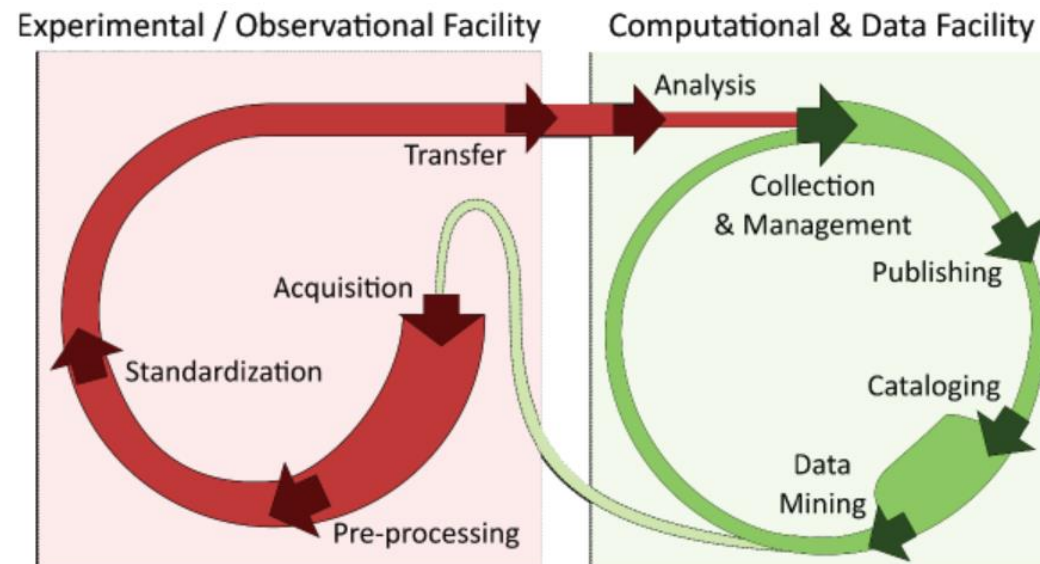
## Data harmonization

### FAIR data

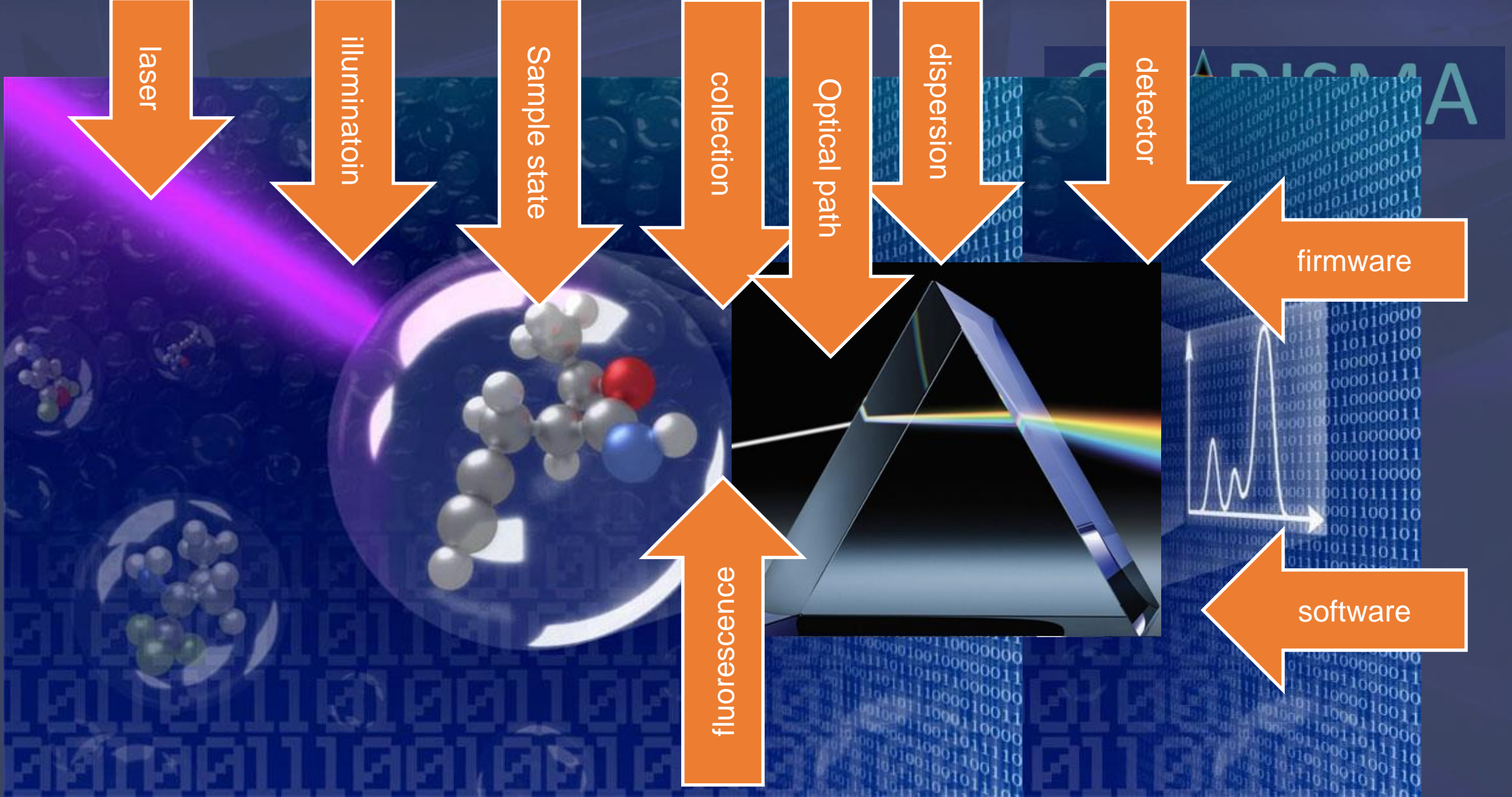
- **F**indability
- **A**ccessibility
- **I**nteroperability
- **R**eusability

Wilkinson *et al. Sci. Data* (2016)

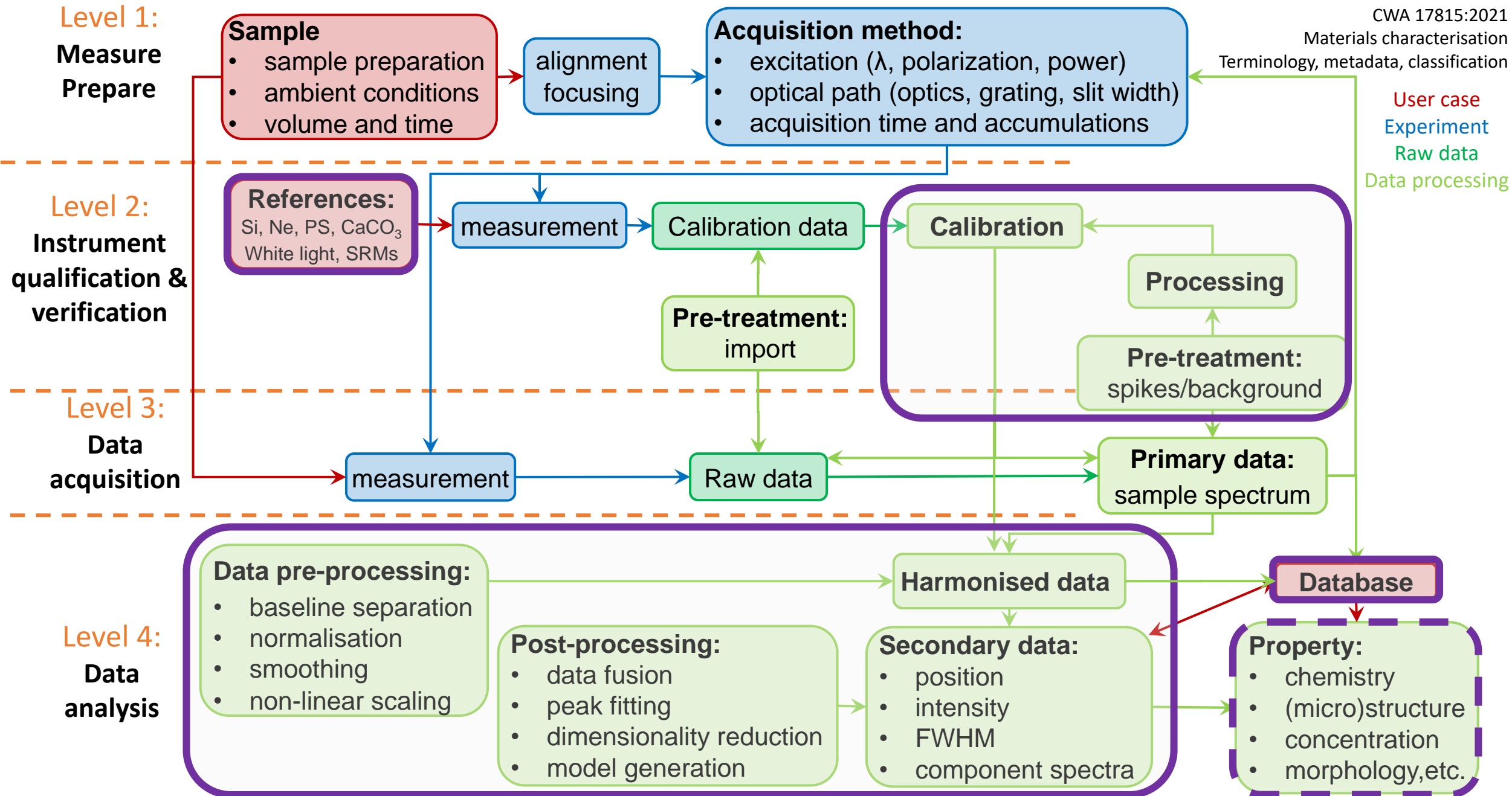
<https://www.go-fair.org/fair-principles>



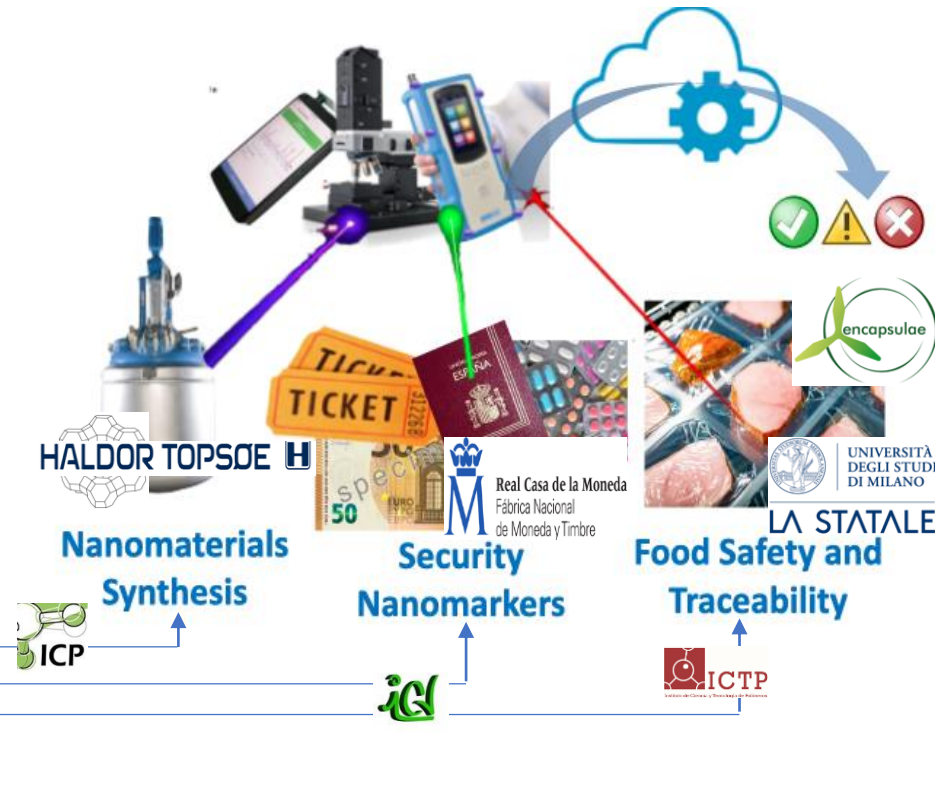
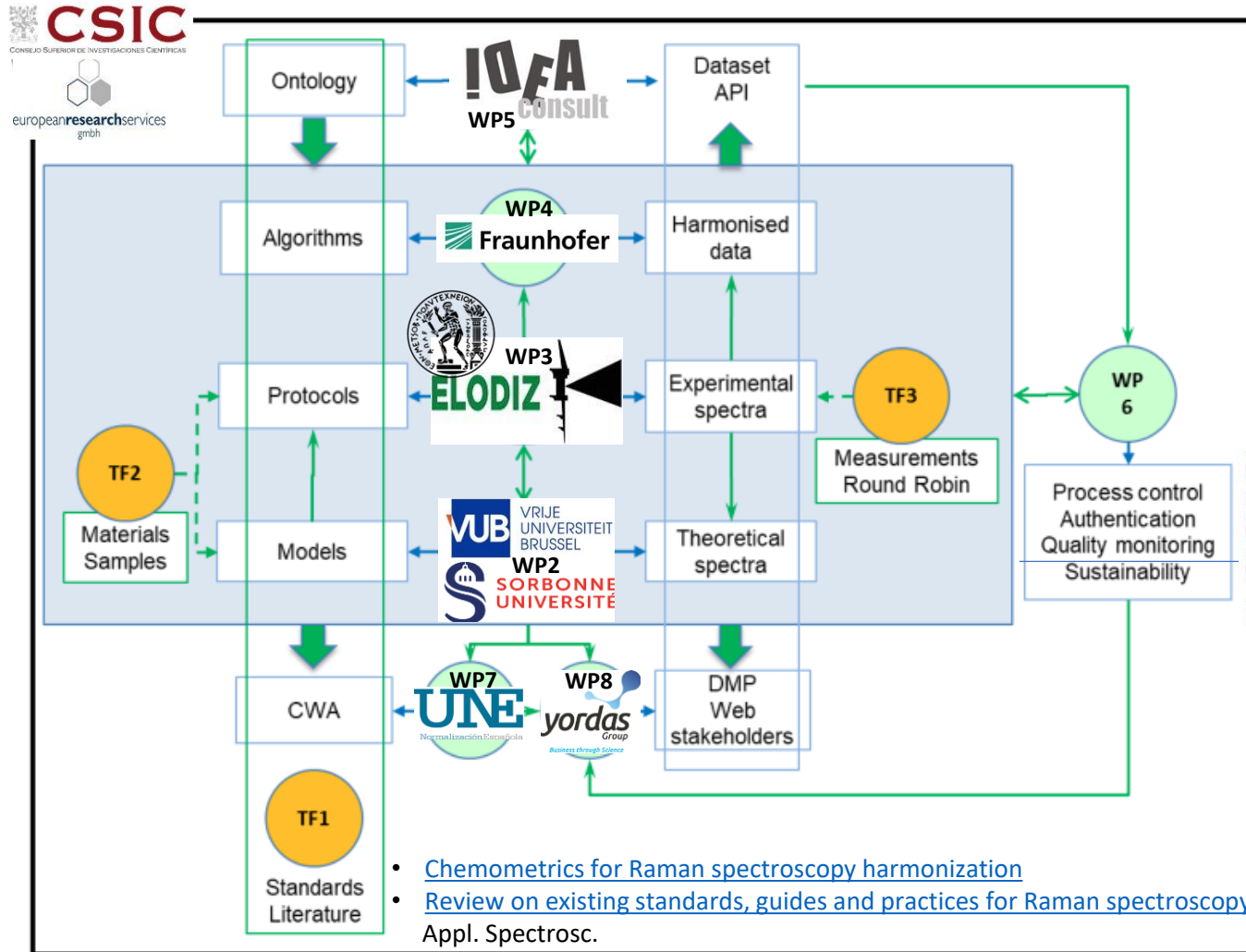
**Figure 6.** Lifecycle of datasets for the proposed future paradigm of research. The complete raw-data stream is acquired from the instruments and written to open and standardized data formats.



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# CHARISMA Objectives and WP



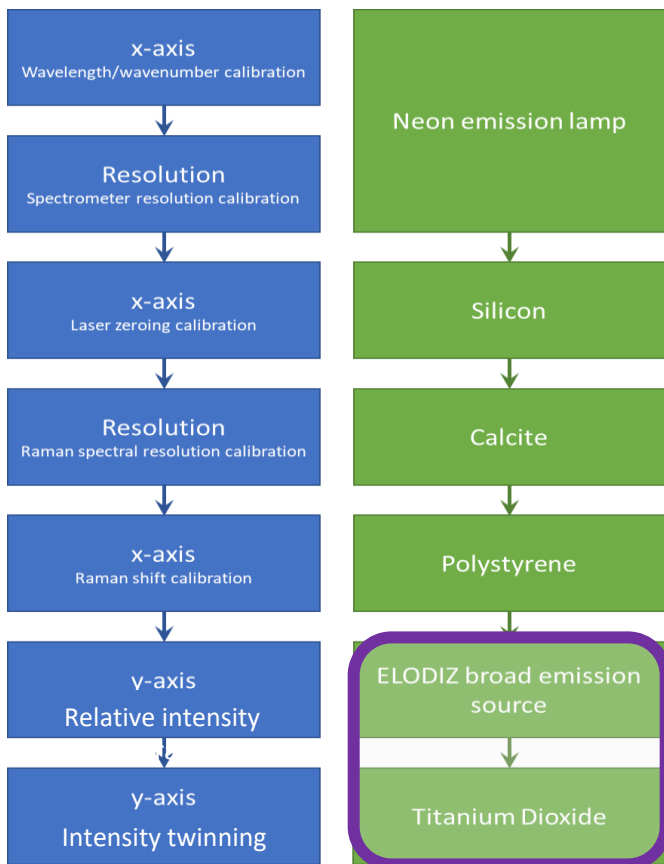
- Lack of interoperability
- Increasingly softer hardware
- Variety of needs
- IoT, AI, etc.



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# CHARISMA impact and tools



## Calibration protocol

Without reinventing the wheel:

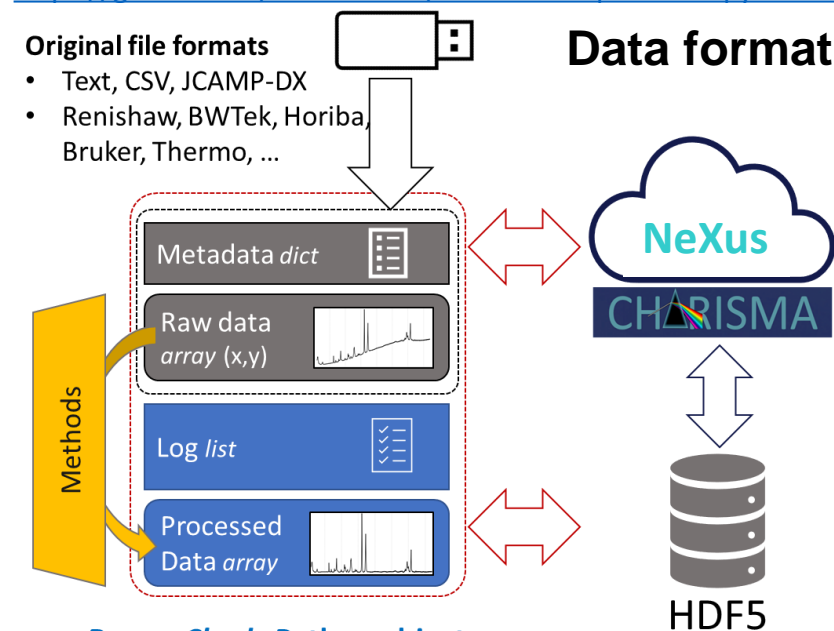
- full calibration
- pre- (device) / post- (data) acquisition
- whole device
- reliable reference spectra generation
- accurate data processing

## Bonus: Raman devices pairing

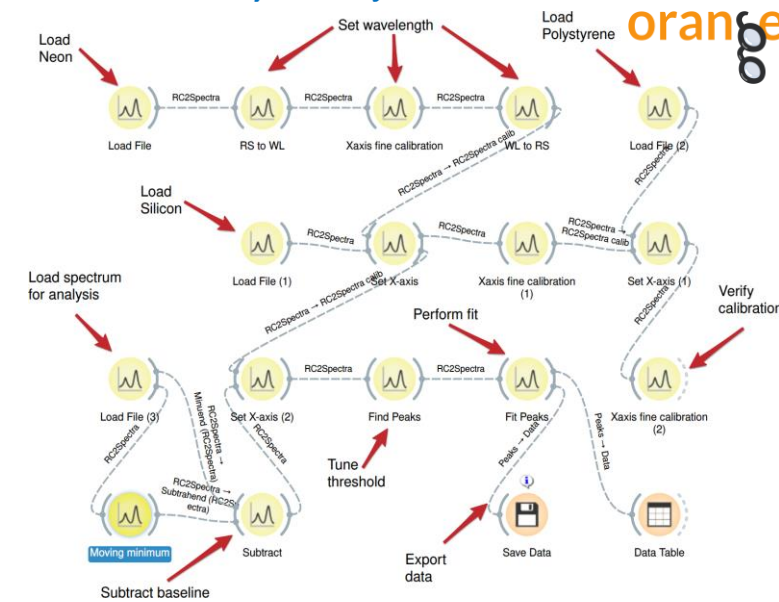
- Support **academic research**  
increased **comparability and exchange** of Raman data
- Foster **industrial implementation**  
real-time, in-line and distributed **monitoring and control/decision tool**
- Improve the **business** of existing and new products/processes  
improved product **quality and trust**

## Ontology (VIBSO)

<https://github.com/NFDI4Chem/VibrationalSpectroscopyOntology>



## RamanChada Python object



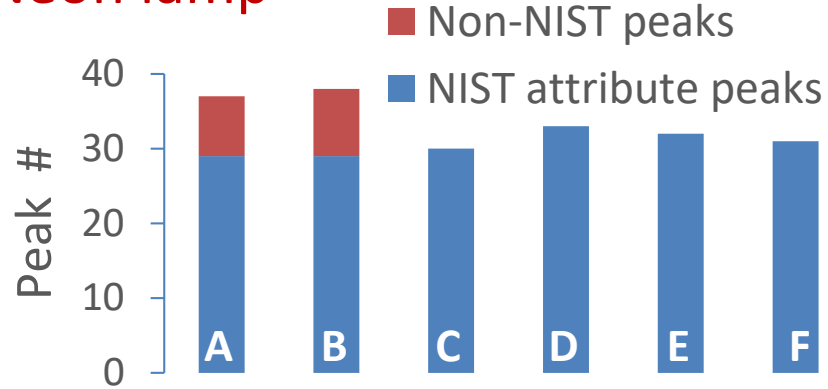
user-friendly wrapper add-on

<https://github.com/h2020charisma/oranchada>

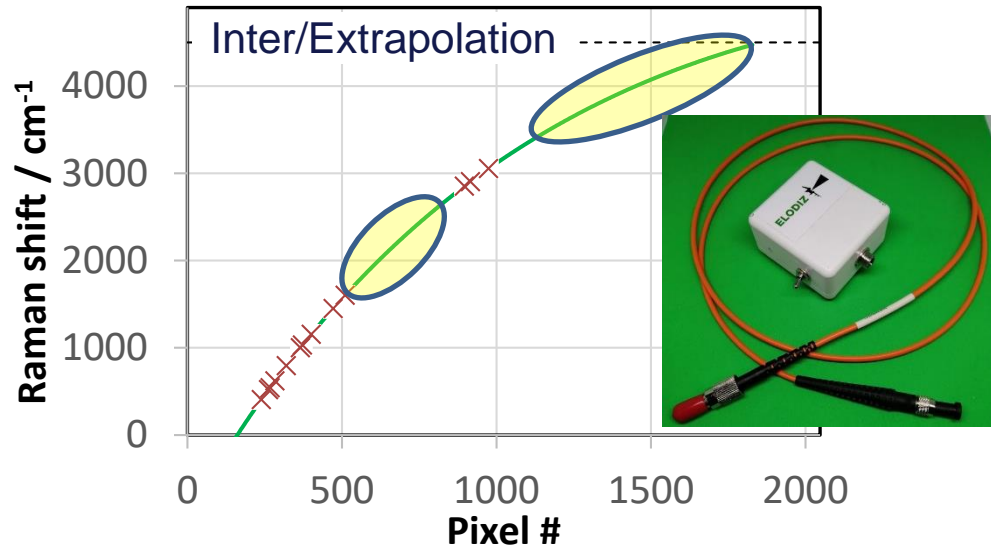
# Reference samples

## Full optical path

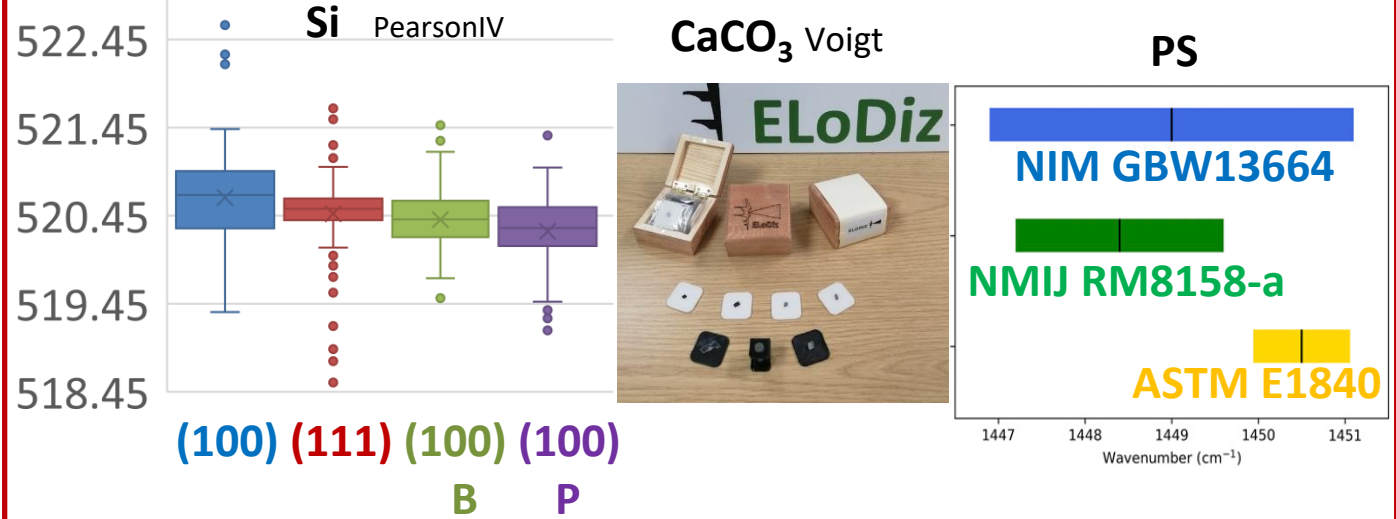
### Neon lamp



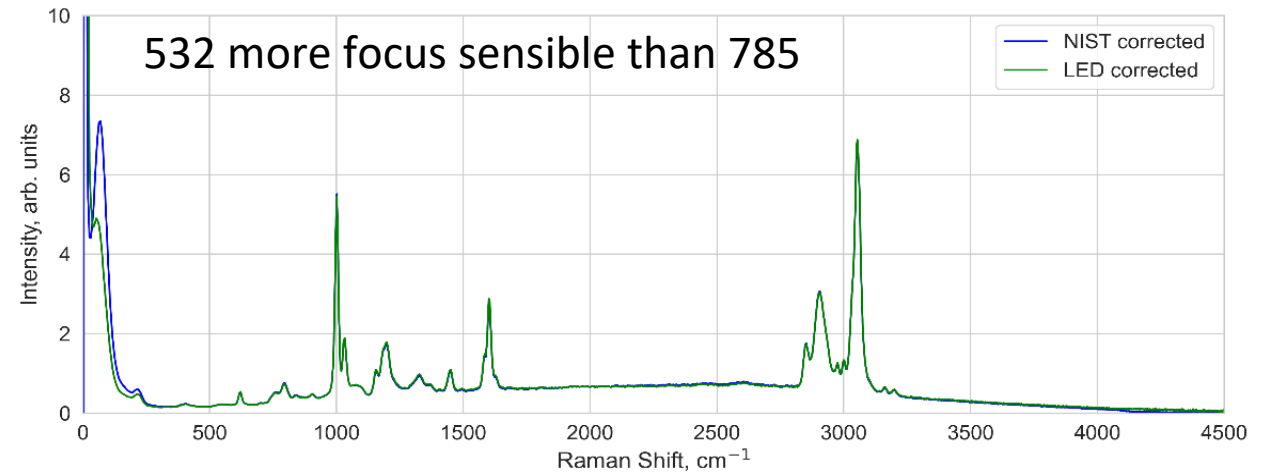
Gaussian + poliharmonic spline



### Sample set



### LED vs NIST SRM 224X





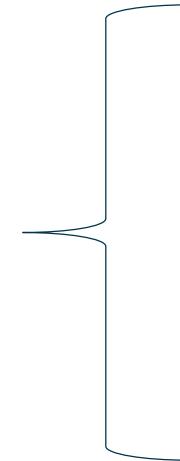
# STANDARDISATION in CHARISMA

<https://www.cencenelec.eu/news-and-events/news/2023/workshop/2023-12-20-raman-devices/>



**CEN-CENELEC  
WORKSHOP**

**Raman devices calibration,  
verification and twinning protocols**  
-KOM February 28<sup>th</sup>-



**CWA 1**

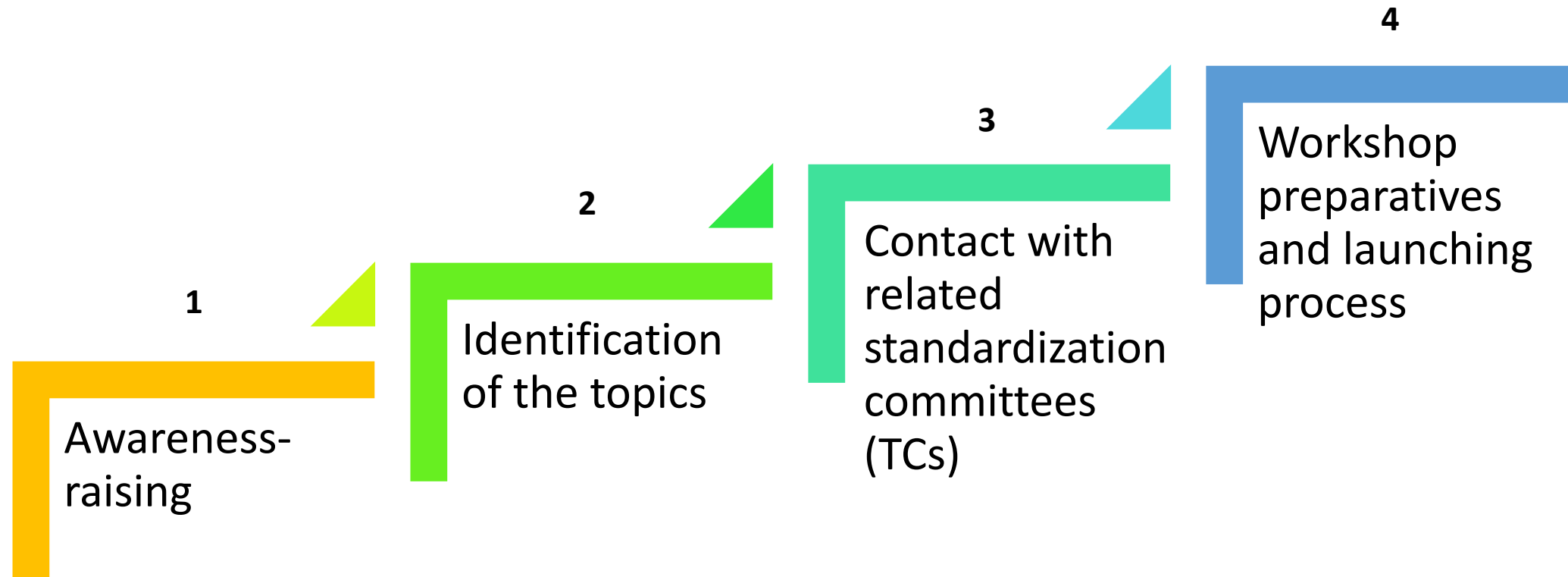
Raman devices calibration  
and verification protocols



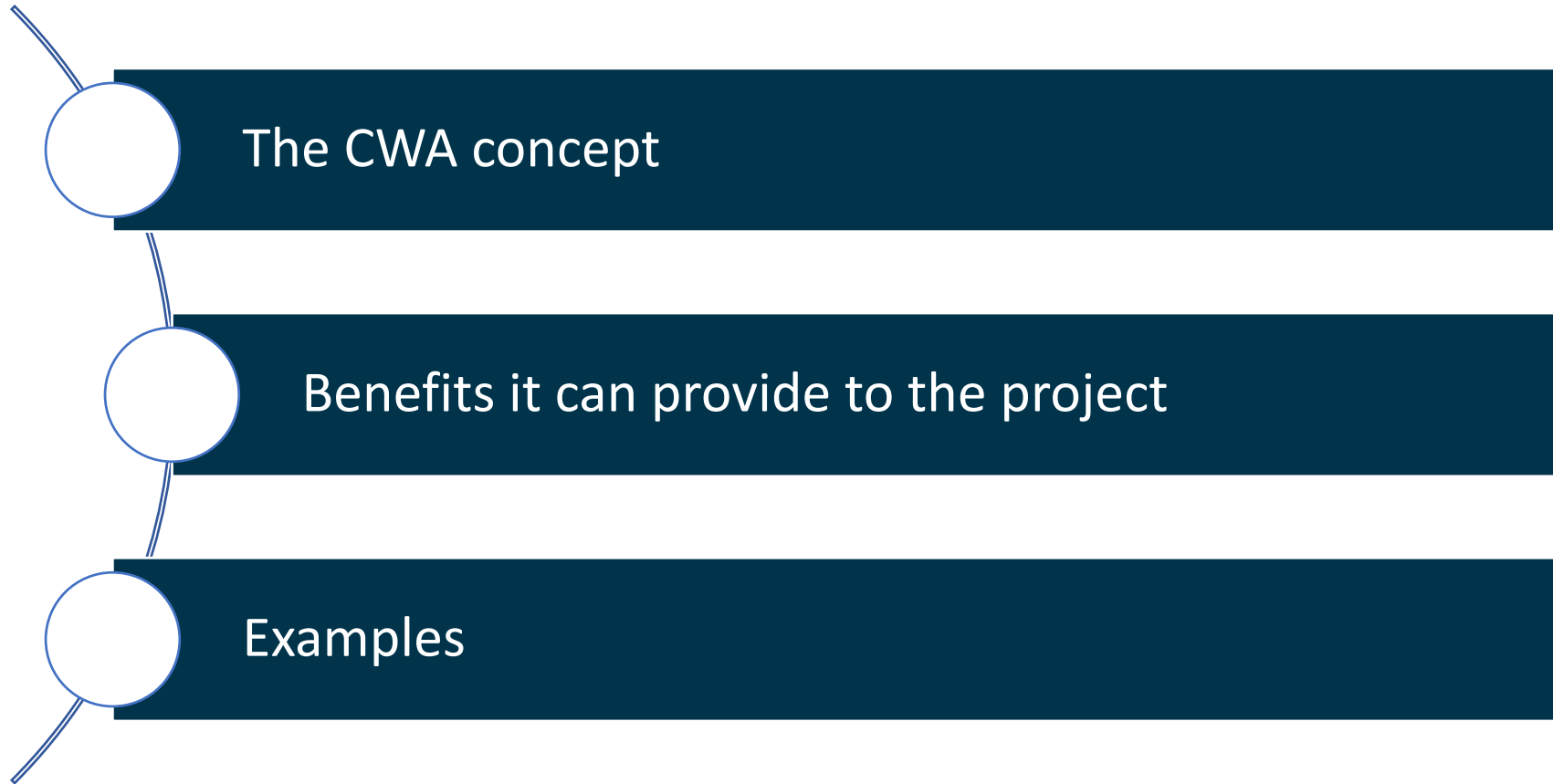
**CWA 2**

Raman devices twinning protocol

# Steps towards a CEN-CENELEC Workshop Agreement



# 1. Awareness-raising



## 2. Identification of the topic

- Start the identification **soon enough** (CHARISMA case: M18/42 first conversations)
- The debate among partners to identify potential topics helps itself to make **common understanding of the impact strategy** of the project

### Topic “requirements”

- Result generated in the project, available and validated, mature enough
- Ideally with high innovation, high impact and core of the project (not mandatory)
- Analysis of the standardization landscape to confirm the Workshop path
- Partners ‘responsible’ of the selected result will have a more active role in the standardization process (CWA leader, Workshop Chair, drafting process, etc.)



### 3. Contact with related standardization Technical Committees (TCs)

#### Why?

- To confirm the standardization **path** (Workshop)
- To use the standardization system as a **dissemination** channel
- To open the door for **future contributions** from the TCs to the CWAs

#### How?

- Selection of TCs** to contact with (scope, structure, standards, projects)
- Define content** to disseminate (brief summary of the Project and available results)
- First contact with TCs **at an early stage of the project** to anticipate potential issues.
- Ask for **feedback** about relevance of the project for their work programme
- Subsequent contacts** with specific TCs when the topic is completely defined.

## 4. Workshop preparation and launching process



**Work previously in a draft CWA as mature as possible**

CHARISMA case: not a direct transformation of a deliverable into a draft CWA  
integration of different areas of the project

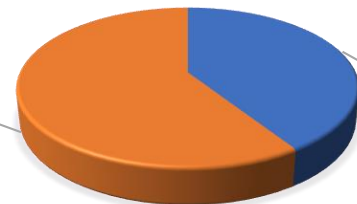


**Very active dissemination actions (invitations)**

CHARISMA case: invitations to manufacturers, Raman communities,  
standardization committees, R&I projects, scientists...

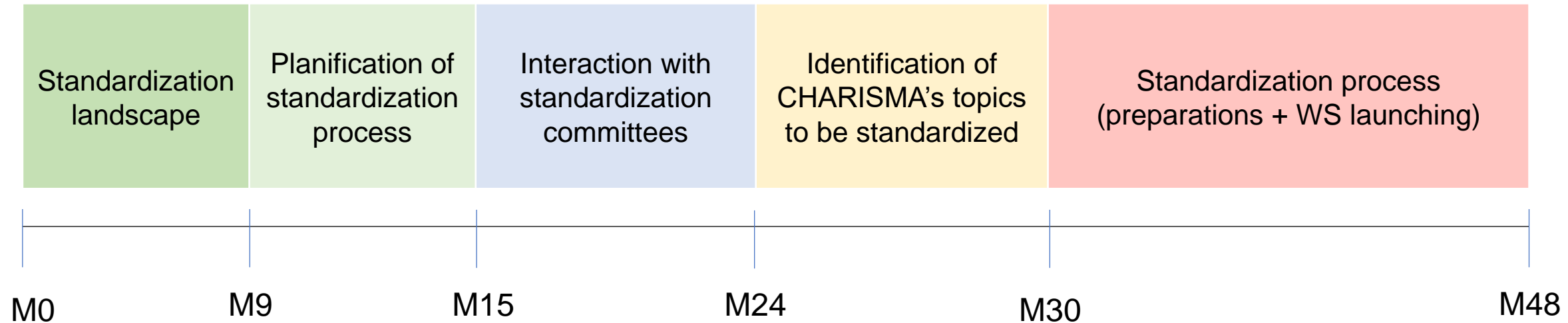
### 22 WORKSHOP PARTICIPANTS

External...



CHARISMA partners - 9

## 5. Standardization activities in CHARISMA



- **Interlaboratory study of Raman harmonisation protocols**  
(to be launched soon)
- **Raman school** (<https://icors2024.org/raman-school/>)  
Rome, July 28-August 2 (satellite event of ICORS conference)

# Raman standardisation landscape: incomplete, complex, and evolving

## **Academia and users:**

- Understand and remove setup-induced variations
- Engagement in standardization development

## **Manufacturers:**

- Access to calibration methods and raw data

## **Standardisation bodies/documents:**

- New/updated/extended standards
- Open-access, easy-to-use documents

## **Metrology institutes/CRMs:**

- Improve accessibility (options, stock, price, multilingual)
- More detailed information



# Thank you!

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