Success case:
H2020 CHARISMA project

Raquel Portela (CSIC)

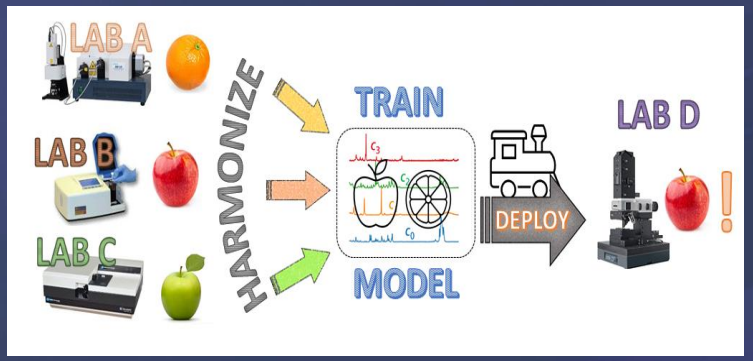
Standardisation in Practice: Towards a CEN-CENELEC Workshop Agreement 2024-03-14

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

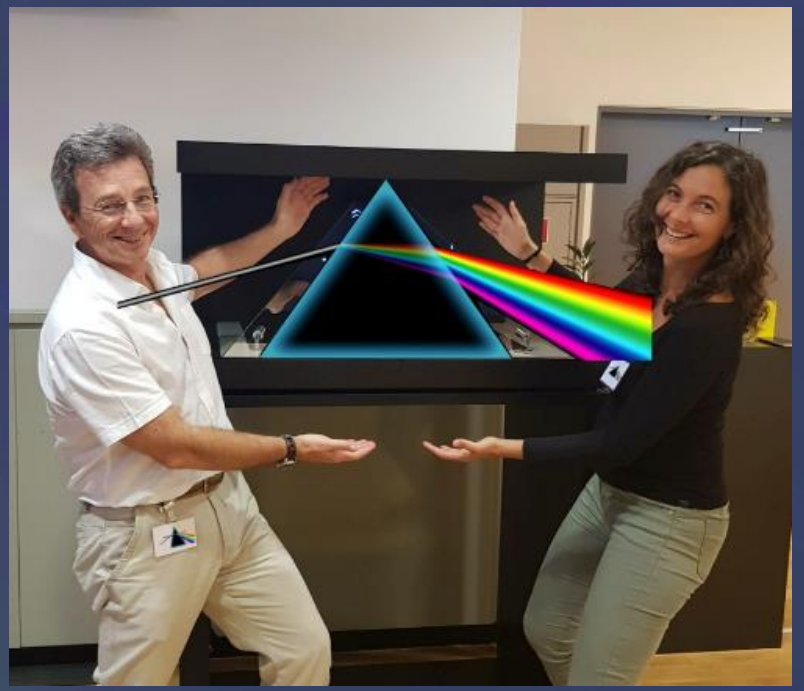
Raman spectroscopy

CHARISMA



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



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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

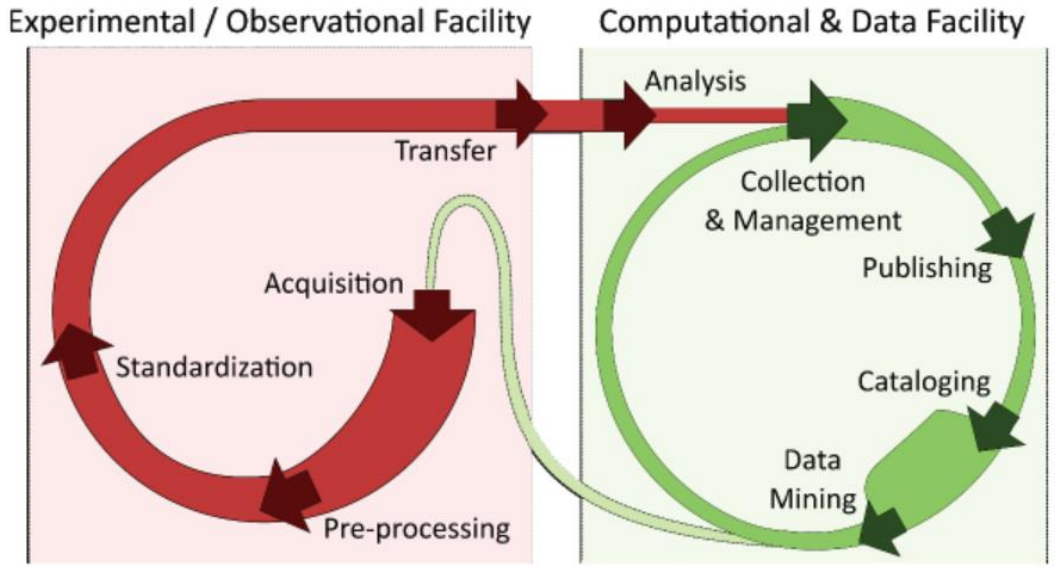

Figure 6. Lifecycle of datasets for the proposed future paradigm of research. The complete raw-data stream is acquired from the instruments and written to open and standardized data formats.

Harmonization

Raquel Portela
Tenured scientist

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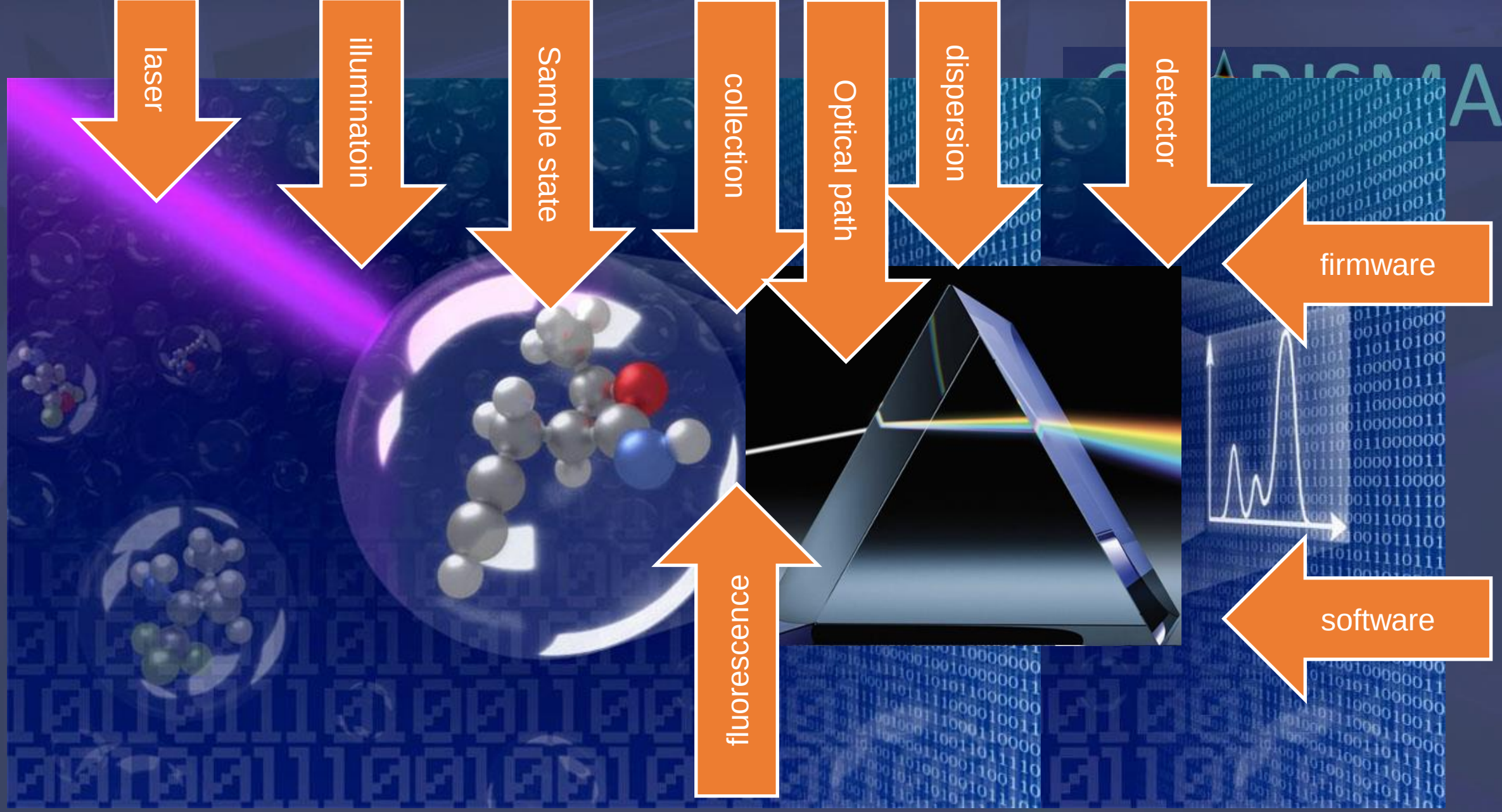

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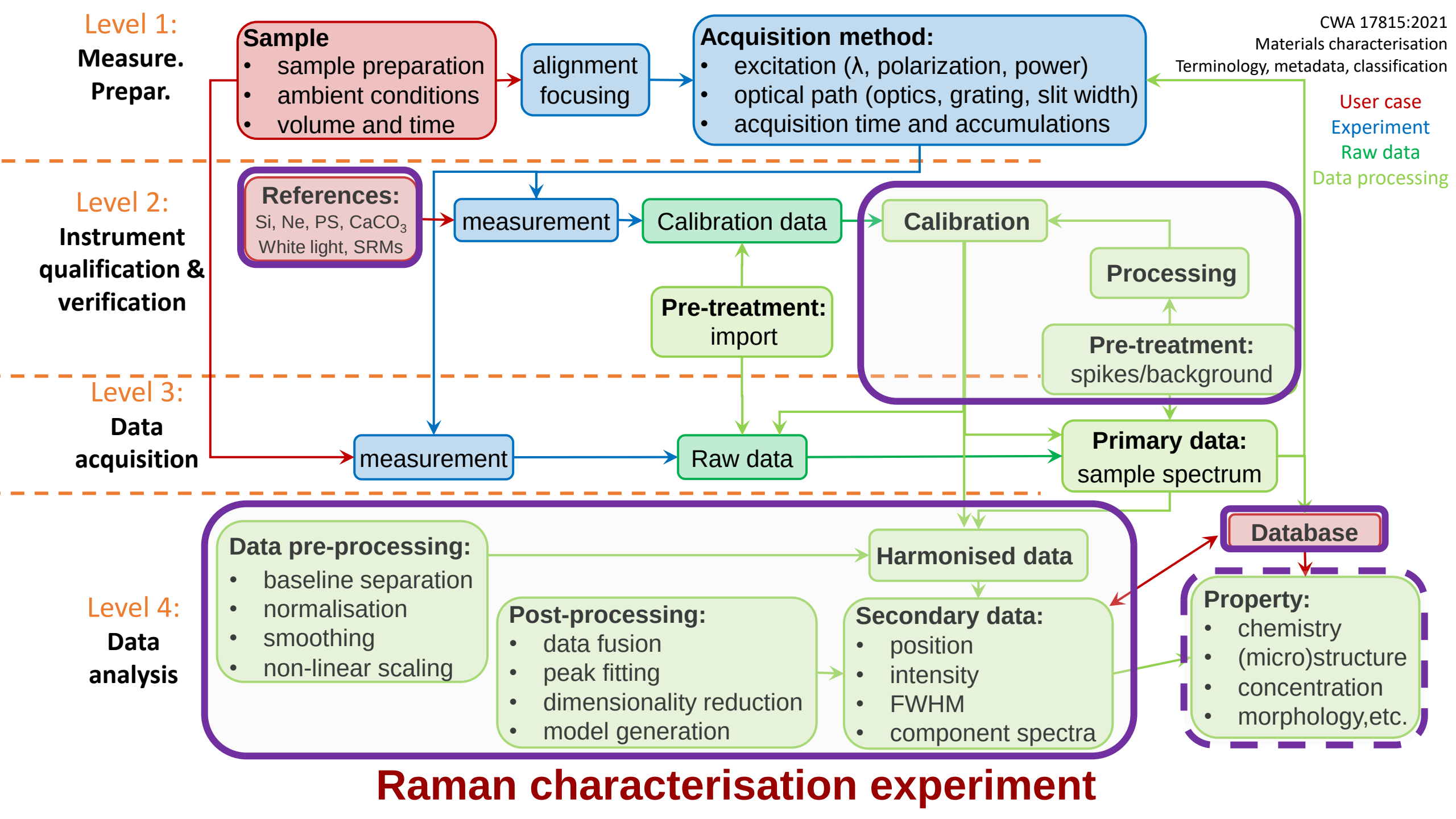
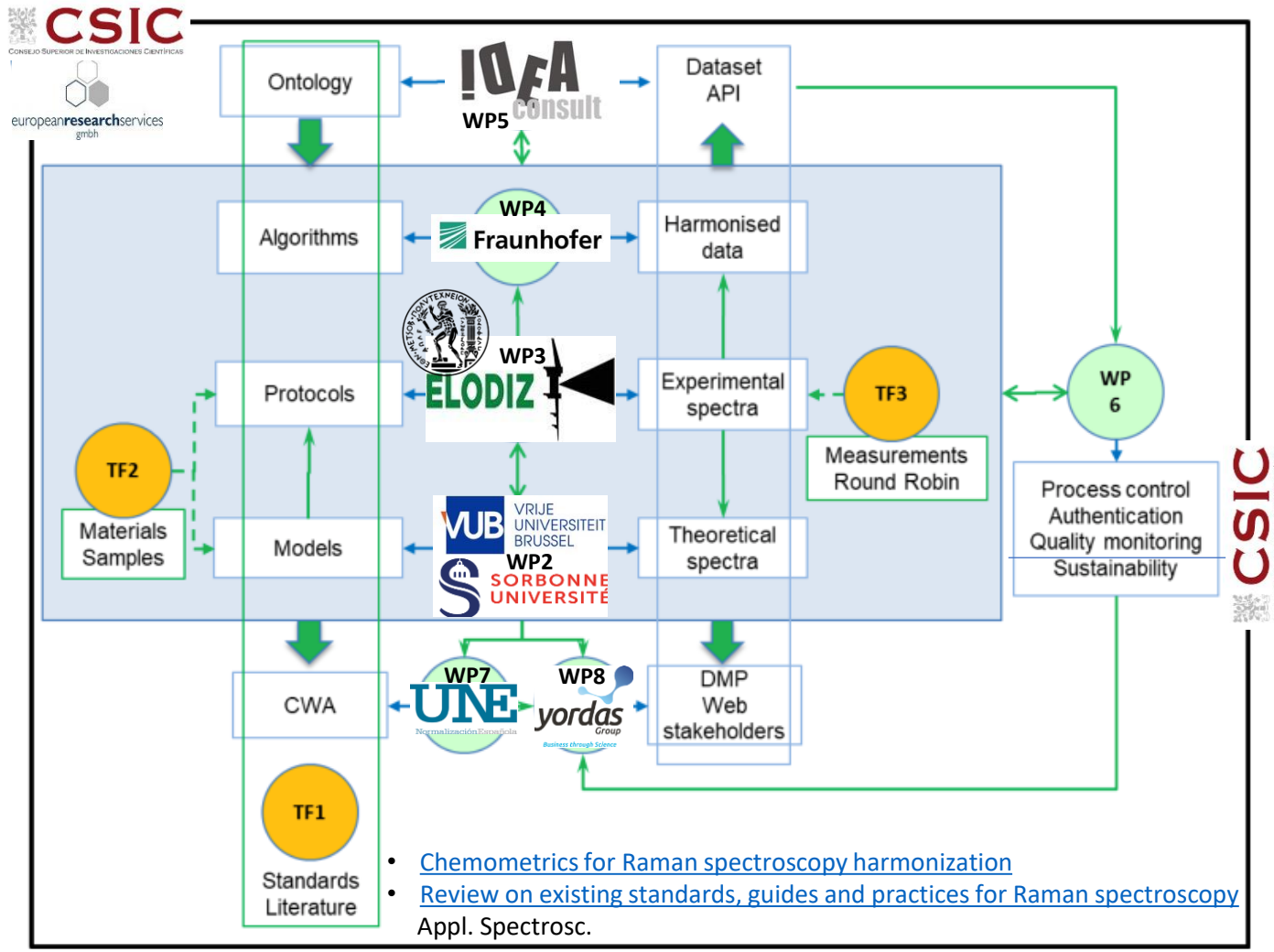
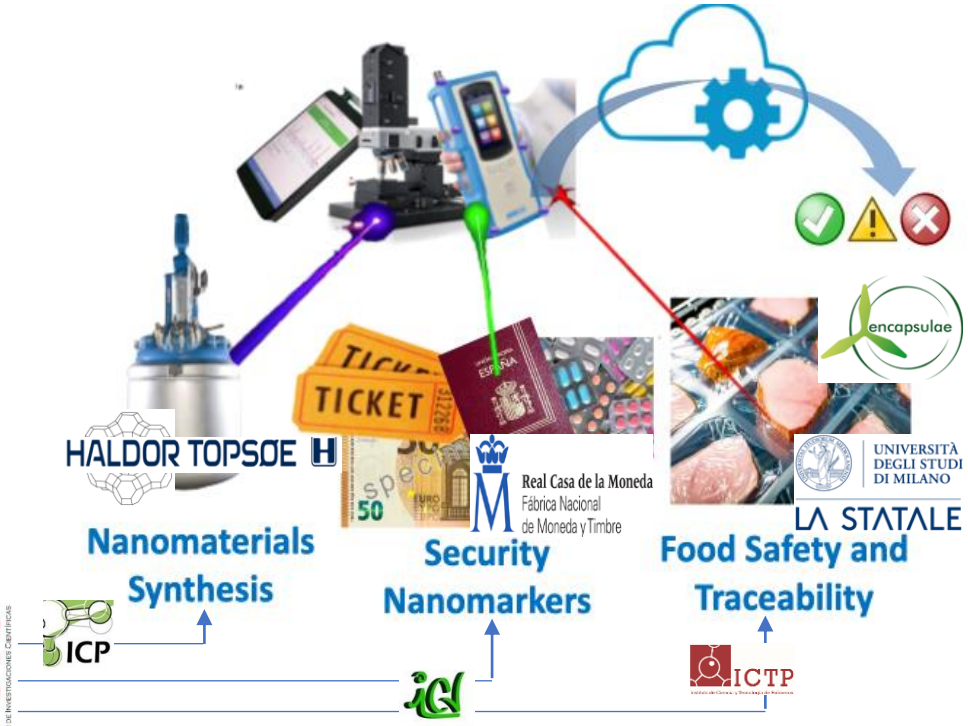

CWA 17815:2021
Materials characterisation
Terminology, metadata, classification
User case
Experiment
Raw data
Data processing
Level 1:
Measure.
Prepar.
Sample
• sample preparation
• ambient conditions
• volume and time
alignment
focusing
Acquisition method:
• excitation (λ, polarization, power)
• optical path (optics, grating, slit width)
• acquisition time and accumulations
Level 2:
Instrument
qualification &
verification
References:
Si, Ne, PS, CaCO3
White light, SRMs
measurement
Calibration data
Calibration
Processing
Pre-treatment:
import
Pre-treatment:
spikes/background
Level 3:
Data
acquisition
measurement
Raw data
Primary data:
sample spectrum
Level 4:
Data
analysis
Data pre-processing:
• baseline separation
• normalisation
• smoothing
• non-linear scaling
Harmonised data
Database
Post-processing:
• data fusion
• peak fitting
• dimensionality reduction
• model generation
Secondary data:
• position
• intensity
• FWHM
• component spectra
Property:
• chemistry
• (micro)structure
• concentration
• morphology,etc.
Raman characterisation experiment

CHARISMA Objectives and WP



- Chemometrics for Raman spectroscopy harmonization
- Review on existing standards, guides and practices for Raman spectroscopy

Appl. Spectrosc.



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

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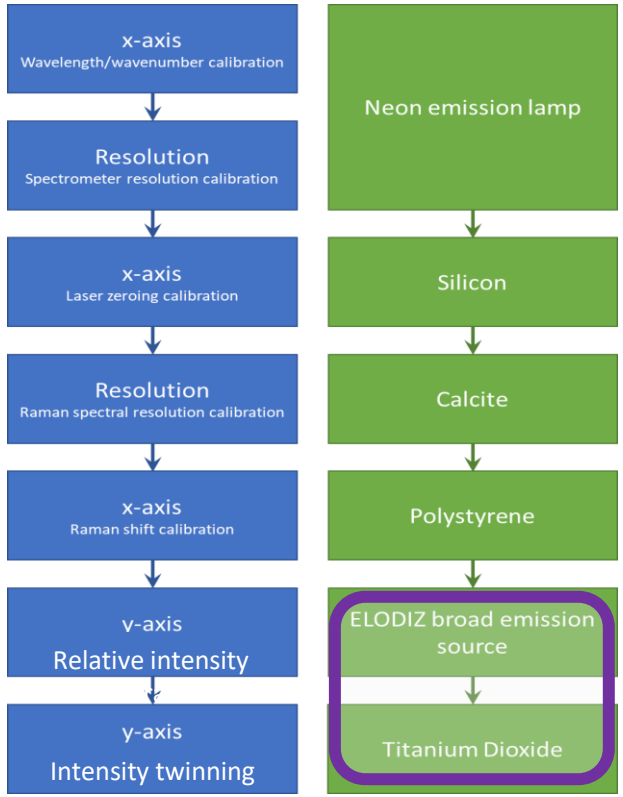
CHARISMA impact and tools



Calibration protocol

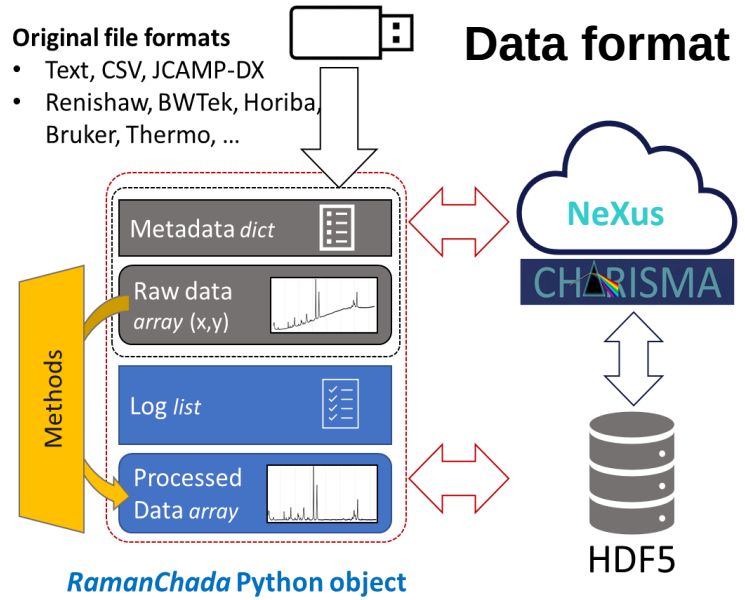
Without reinventing the wheel:

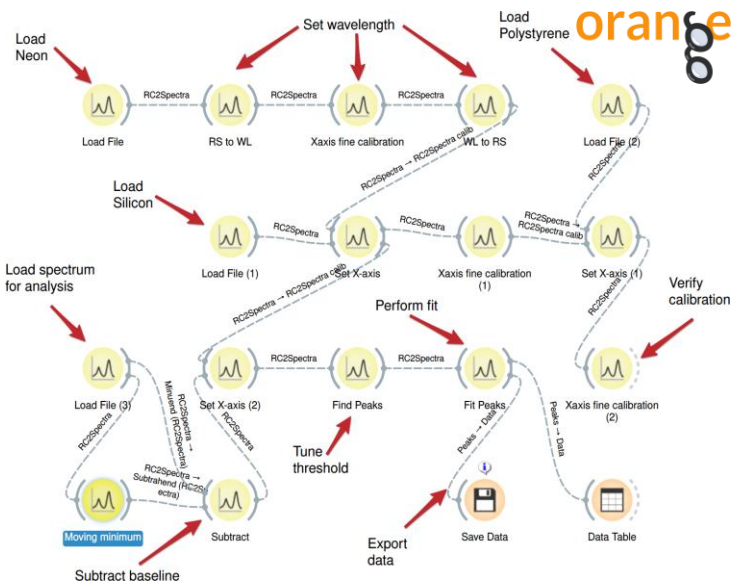
- full calibration
- pre- (device) / post- (data) acquisition
- whole device
- reliable reference spectra generation
- accurate data processing

Bonus: Raman devices pairing

Ontology (VIBSO)

https://github.com/NFDI4Chem/VibrationalSpectroscopyOntology





user-friendly wrapper add-on

https://github.com/h2020charisma/oranchada

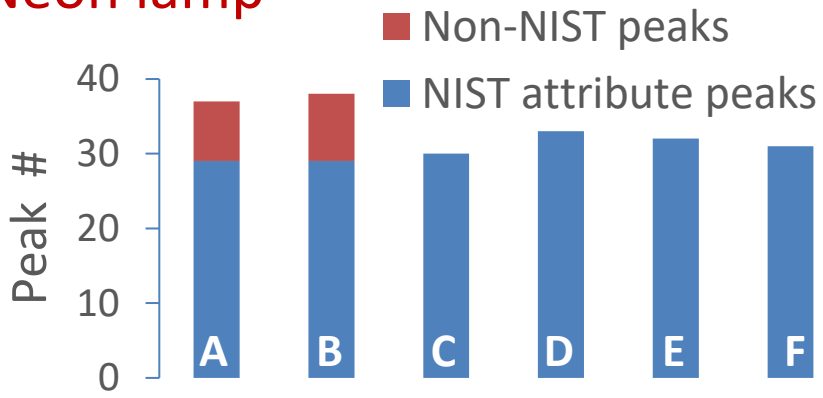
- Support **academic research**
  increased comparability and exchange of Raman data
- Foster **industrial implementation**
  real-time, in-line and distributed monitoring and control/decision tool
- Improve the **business** of existing and new products/processes
  improved product quality and trust

CHARISMA

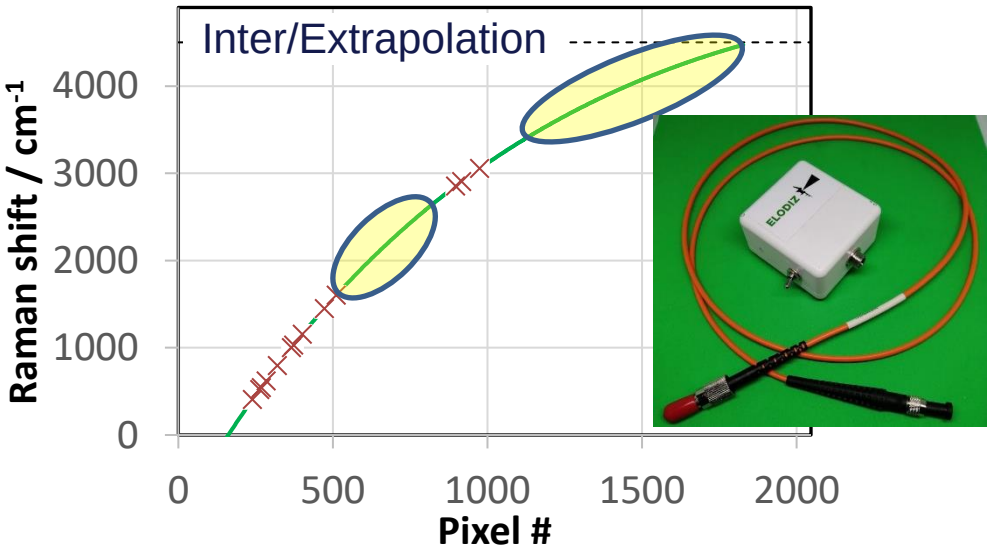
Reference samples

Full optical path

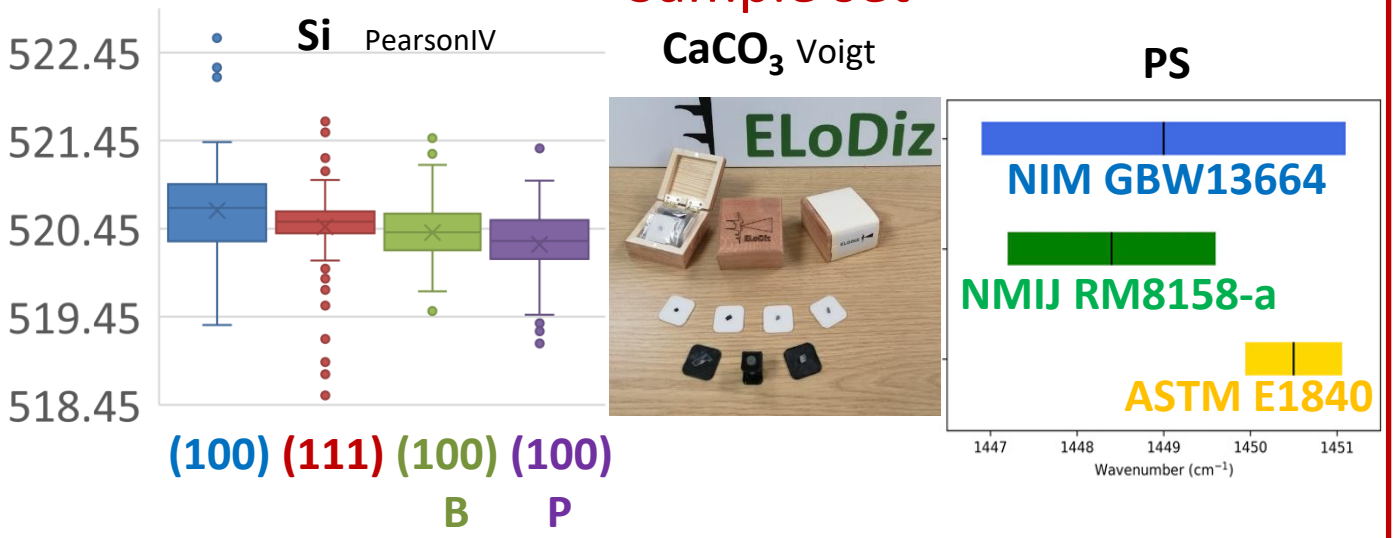
Neon lamp



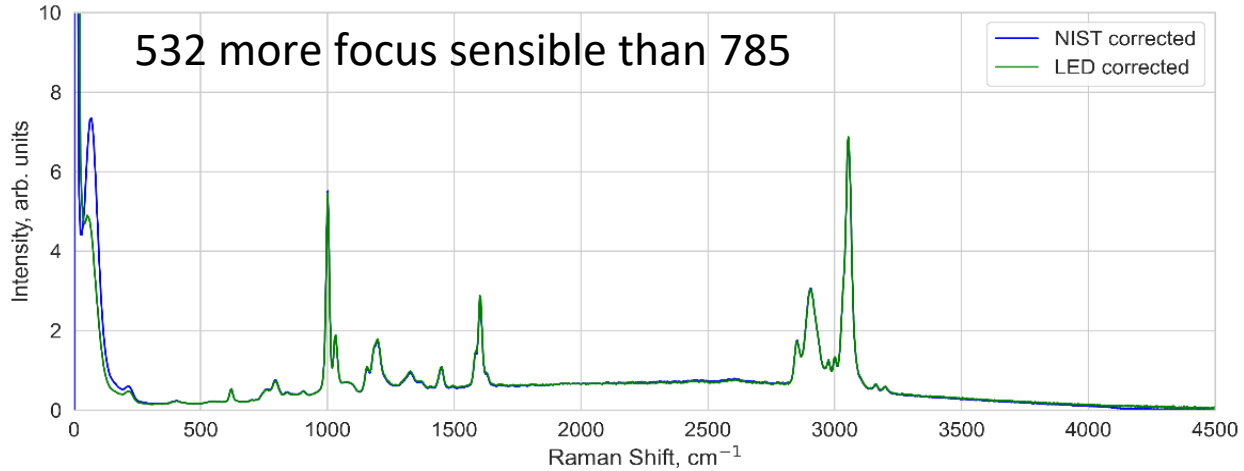
Gaussian + poliharmonic spline



Sample set



LED vs NIST SRM 224X



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CHARISMA

Realistic and FAIR Raman characterization

- **Relevant reactor-cells**

Measure the performance

- **Relevant operating conditions**

Gradients?

- **Industrially relevant**

Final shape, size

- **Harmonized data**

Calibration, SOPs, traceability

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

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Tenured scientist

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CHARISMA project

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 28th-

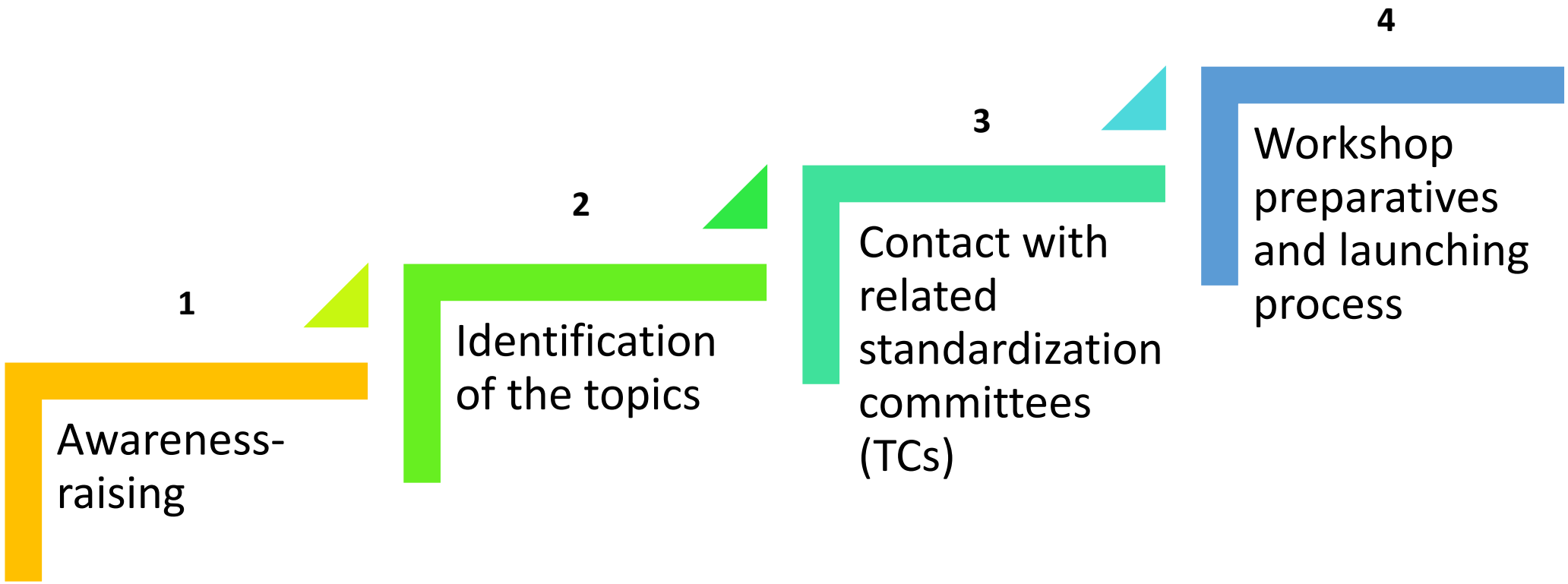
CWA 1

Raman devices calibration and verification protocols

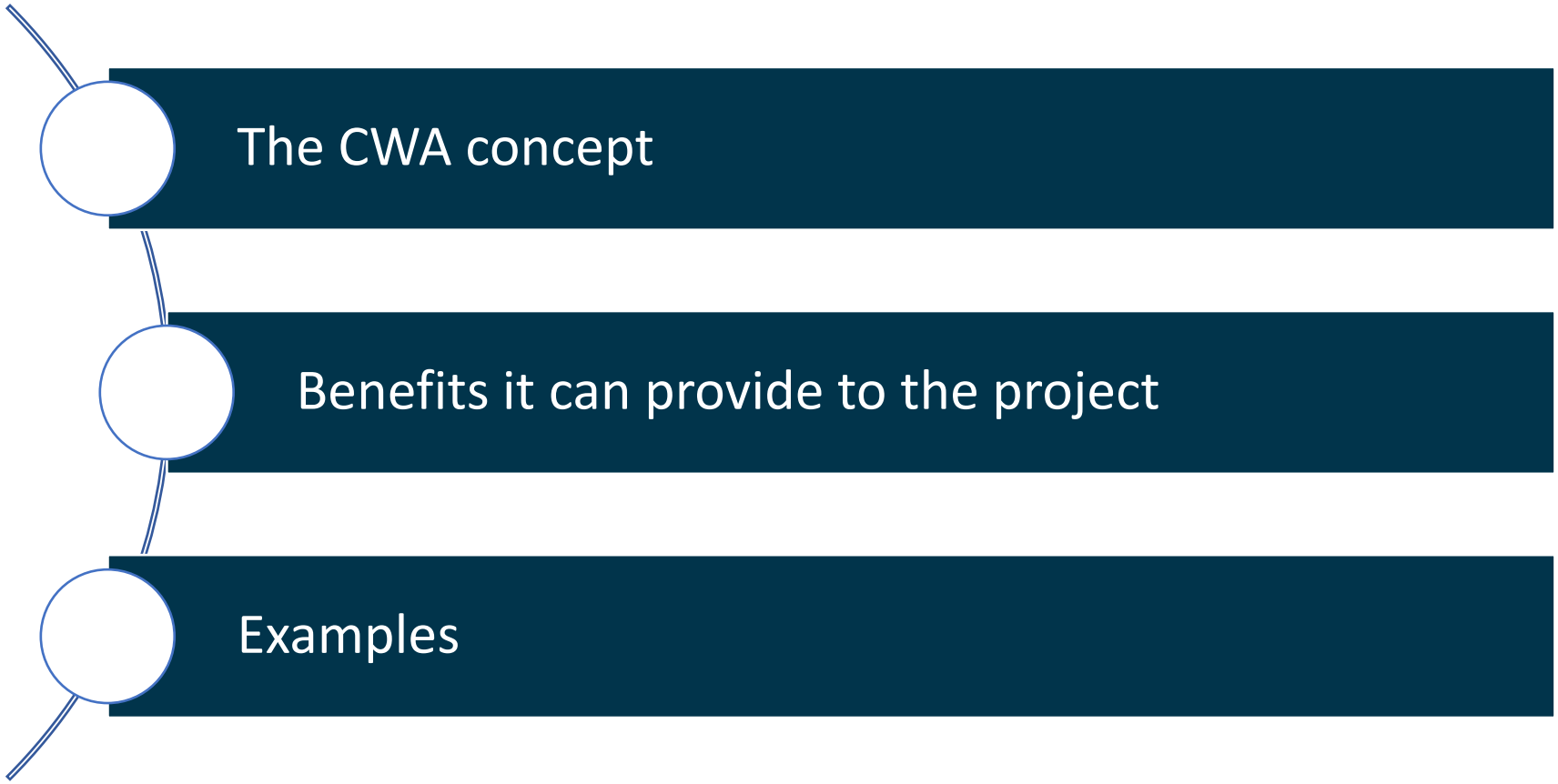
CWA 2

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 to identify potential topics helps itself to make **common understanding of the impact strategy** of the project among partners

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 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.

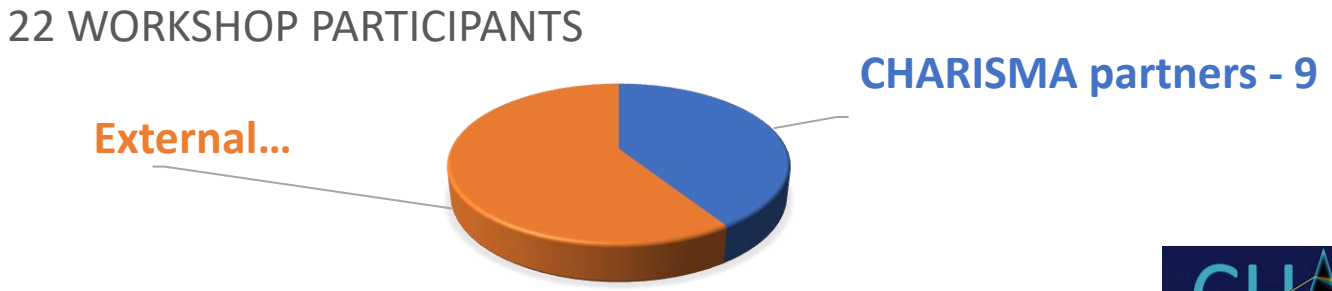
4. Workshop preparations and launching process

Work previously in a draft CWA <u>as mature as possible</u>

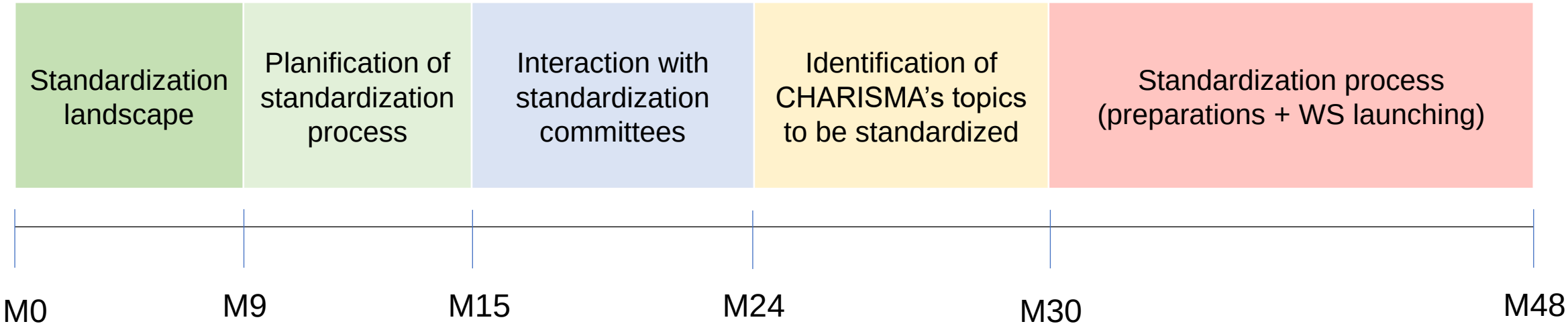
CHARISMA case: not a direct transformation of a deliverable into a draft CWA
integration of different areas of the project

Very active dissemination actions (invitations)

CHARISMA case: invitations to manufacturers, Raman communities, standadization committees, R&I projects, scientists…



5. Standardization activities in CHARISMA



- **Raman school** (https://icors2024.org/raman-school/)

  Rome, July 28-August 2 (satellite event of ICORS conference)

Thank you!

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OUR VIDEO

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