NANOMATERIALREGISTRY

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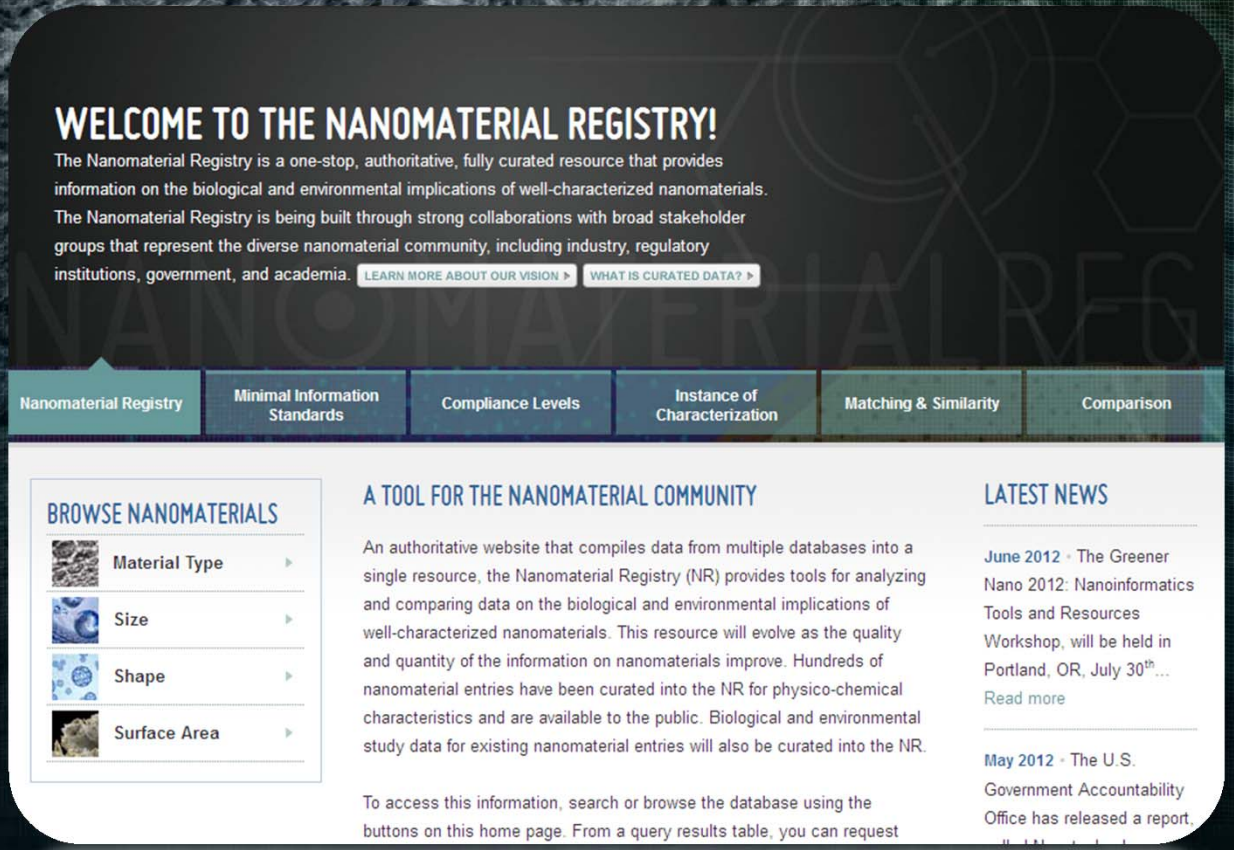
RTI International

NANOMATERIALREGISTRY

Funded by:

NIEHS NIBIB NATIONAL CANCER INSTITUTE

Comprehensively curated, validated data on a scale suitable for decision making



Web Address:

www.nanomaterialregistry.org

RTI INTERNATIONAL

Federal Initiatives

The NNI Coordinates R&D in nanoscale science, engineering, and technology

"NNI recognizes the **potential of nanomaterials** to

- collect and store energy
- reinforce materials
- sense contaminants
- enable life-saving drugs
- shrink and accelerate computational device"

NNI — National Nanotechnology Initiative

- An interagency effort that was launched in 2001
- 25 Federal agencies
- Informs and influences the Federal budget for Nanotechnology R&D

NKI — Nanotechnology Knowledge Infrastructure

- NNI Signature Initiative for sustainable design of nanomaterials
- NKI THRUST 4: robust digital nanotechnology data and information infrastructure to support effective data sharing, collaboration, and innovation across disciplines and applications

NIH — Nanomaterial Registry

- NIH funded project
- Web-based Registry of characterizations and biomedical and environmental applications of nanomaterials
- Launched in 2012, led by RTI International

http://nano.gov/sites/default/files/pub_resource/nki_nsi_white_paper_-_final_for_web.pdf

NANOMATERIALREGISTRY

NANOMATERIAL REGISTRY MISSION

Create a central authoritative data source for the nanomaterial community

- ✓ Integrate data from multiple public data sources
- ✓ Access the data
- ✓ Facilitate improvement in data quality
- ✓ Facilitate development of new models
- ✓ Engage the community

Target User Groups

- ✓ Nanomaterial researchers who generate or analyze data for biological, medical, or environmental implications and applications
- ✓ SME's who make research decisions/guide research
- ✓ Groups that want to share data globally

Challenges

- Archiving **BROAD** data into a single integrated repository (scope, application of data)
- Developing an **EFFICIENT** data curation process and tools
- **SHARING** the data in a effective way
- Staying **CURRENT** with relevant information and standards

NANOMATERIALREGISTRY

The Approach

1. **Define a scope - The Domain of the Registry**
   - ✓ nanoparticles, materials with nano-features, nano-enabled products, and nano-formulations
   - ✓ Physico-chemical characteristics
   - ✓ Data that describes how these materials interact in environmental (air, water, soil) or biological (in vitro, in vivo, in silico) systems
2. **Identify the relevant information**
3. **Develop a process for systematic data archiving**
4. **Evaluate information in a systematic way**
5. **Disseminate the information**
6. **Hands on analysis**

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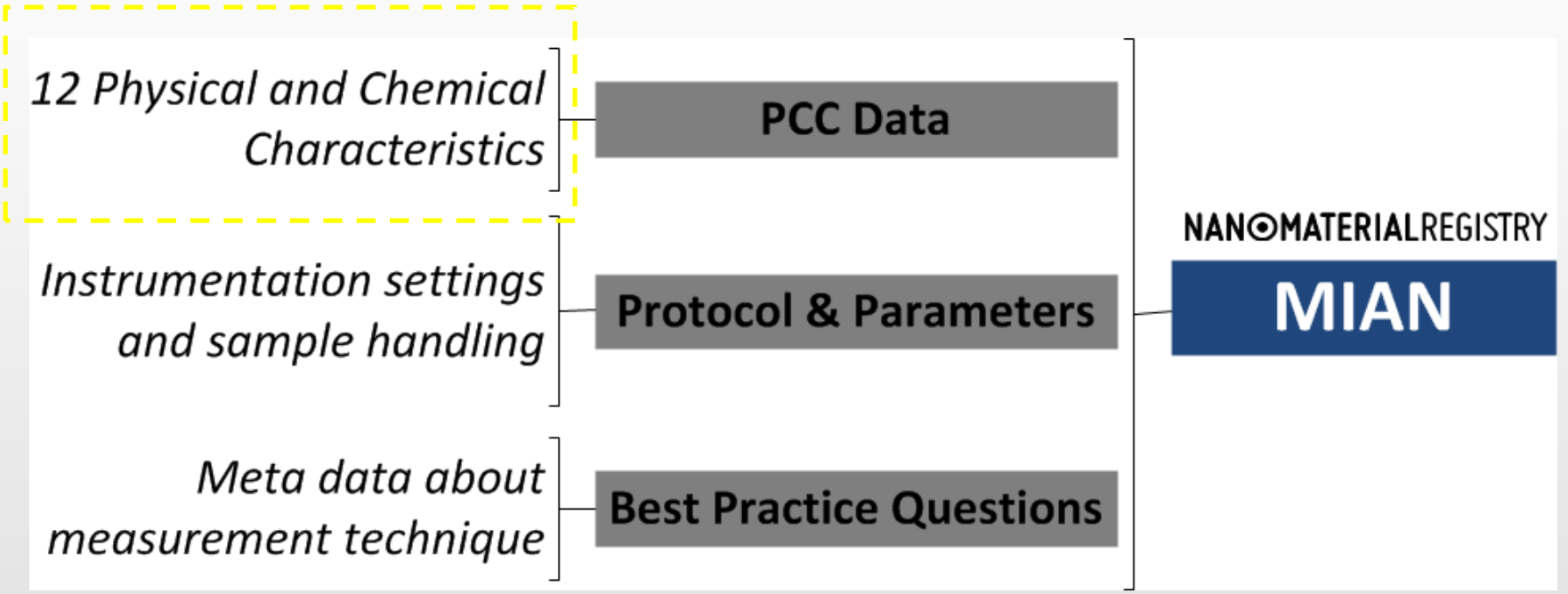
Data for decision making

IDENTIFYING RELEVANT INFORMATION

Relevant Information

Minimal **I**nformation **A**bout **N**anomaterials for **P**hysico-**C**hemical **C**haracteristics



A **controlled vocabulary** of PCC & measurands have been identified (https://www.nanomaterialregistry.com/resources/**Glossary**.aspx)

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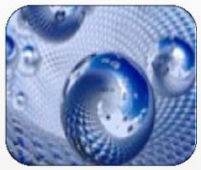
Relevant Information

Minimal **I**nformation **A**bout **N**anomaterials for **P**hysico-**C**hemical **C**haracteristics

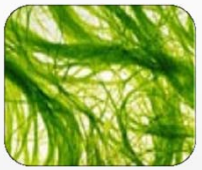
12 Physical and Chemical Characteristics ("PCC MIAN")

Composition



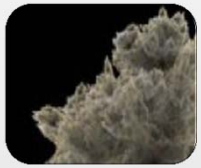
Size

Size Distribution



Shape

Aggregation/ Agglomeration State



Surface Area

Surface Charge

Surface Chemistry

Surface Reactivity

Purity

Solubility

Stability

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Relevant Information

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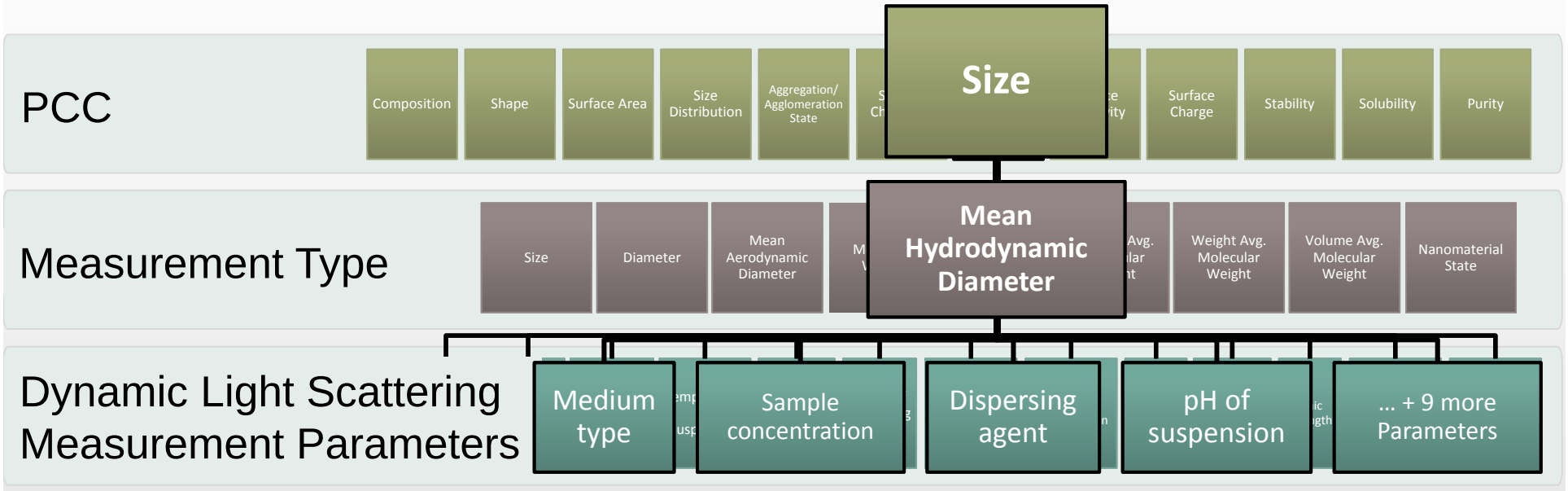

Measurement Best Practice Questions

- Raw data provided?
- Proper controls used?
- Instrument within calibration?
- Replicates used?
- Experimental protocol reported?

Minimal Information = PCC data + Metadata

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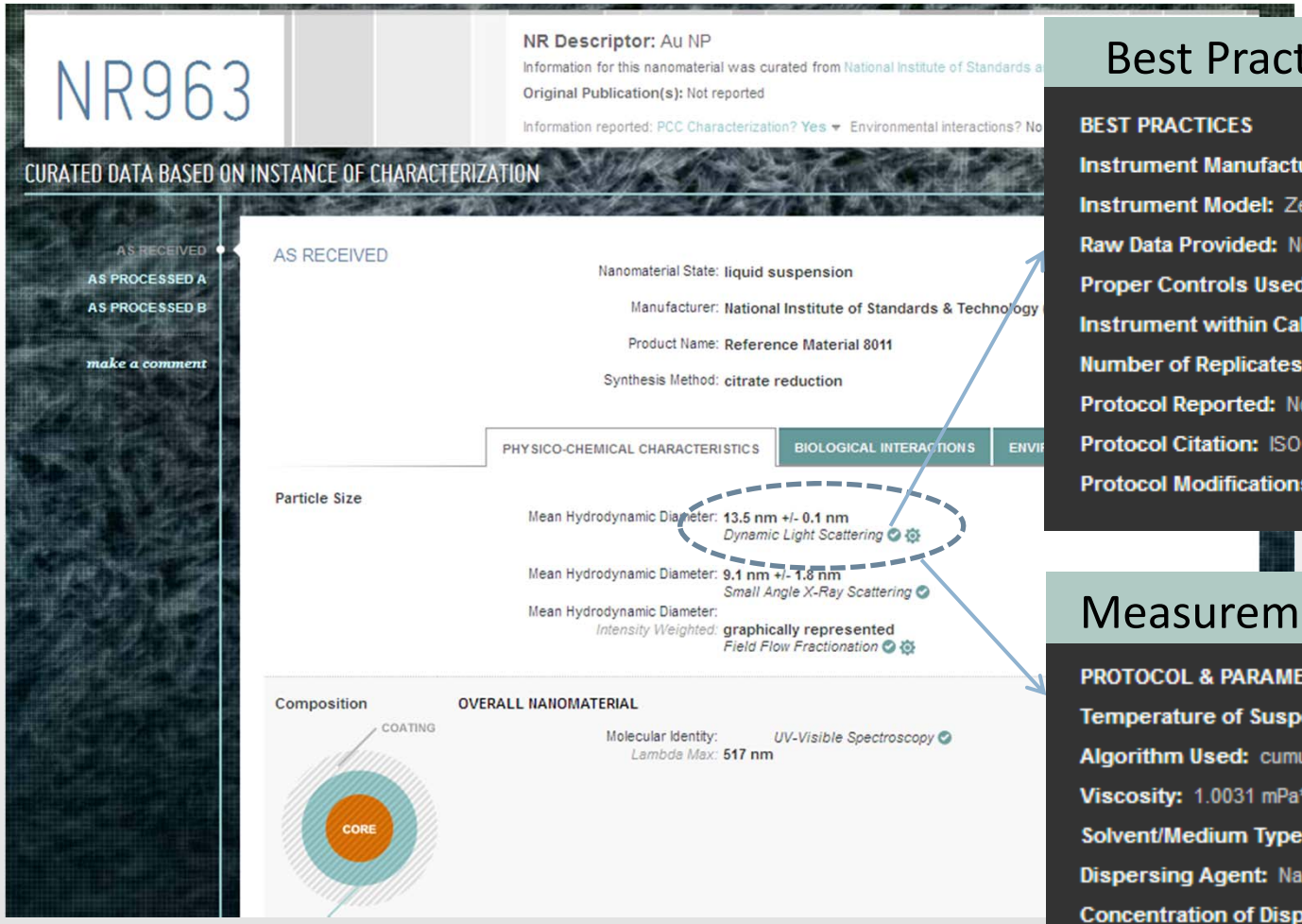
Relevant Information

Minimal **I**nformation **A**bout **N**anomaterials for **P**hysico-**C**hemical **C**haracteristics



Best Practice Questions

BEST PRACTICES

Instrument Manufacturer: Malvern

Instrument Model: Zetasizer Nano ZS

Raw Data Provided: Not reported

Proper Controls Used: Not reported

Instrument within Calibration: Yes

Number of Replicates: 40

Protocol Reported: Not reported

Protocol Citation: ISO 13321:1996(E)

Protocol Modifications: Not Reported

Measurement Parameters

PROTOCOL & PARAMETERS

Temperature of Suspension: 20 +/- 0.1 C

Algorithm Used: cumulants

Viscosity: 1.0031 mPa*s

Solvent/Medium Type: water

Dispersing Agent: NaCl

Concentration of Dispersing Agent: 2 mM

Sample Concentration: diluted 6-fold

Sonication/Milling Power: none

Sonication/Milling Time: none

NIST Reference Material 8011 – Citrate stabilized Au NP

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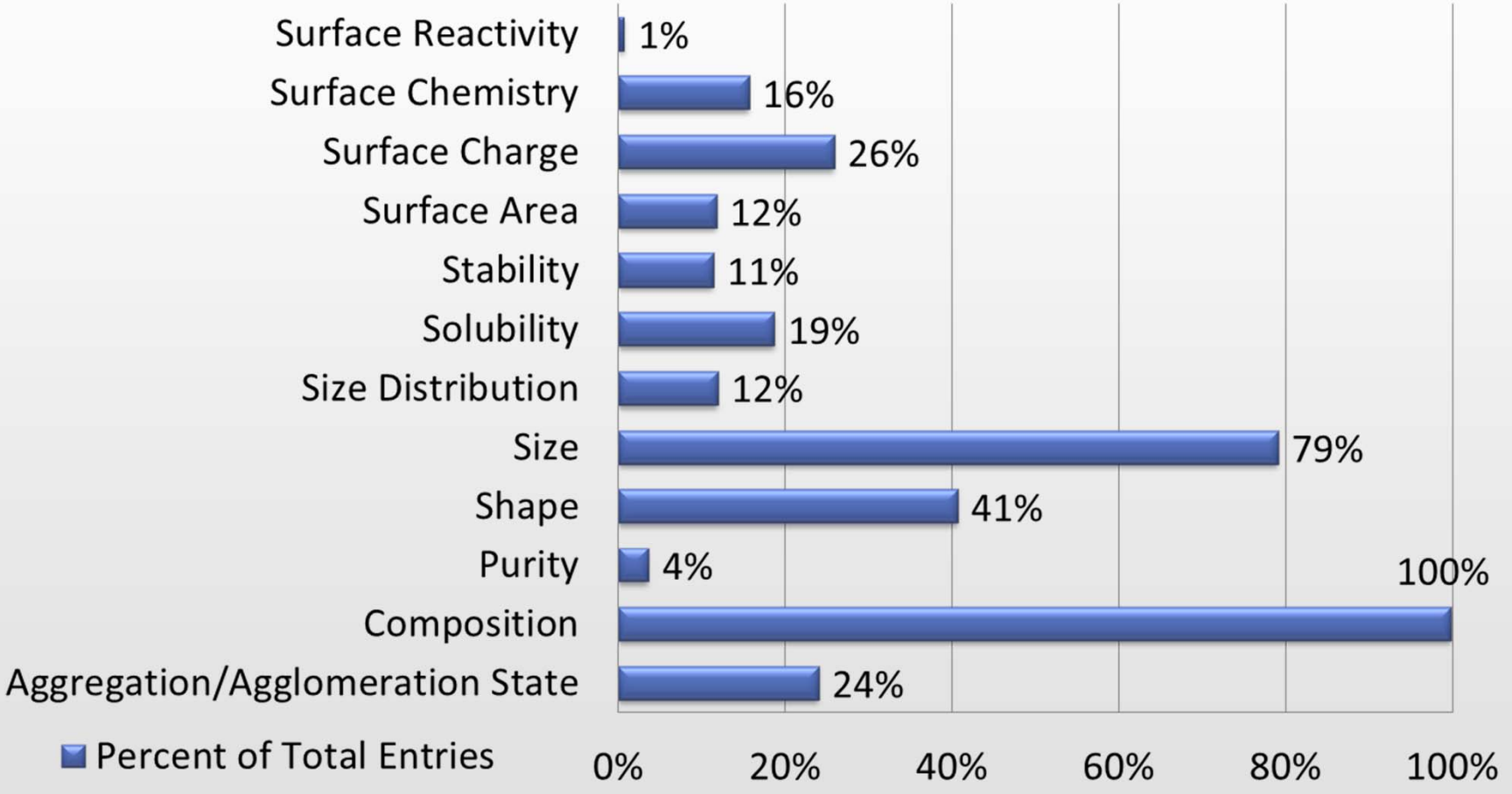
Minimal **I**nformation **A**bout **N**anomaterials for **P**hysico-**C**hemical **C**haracteristics

Current Characterization Profile for NR Records



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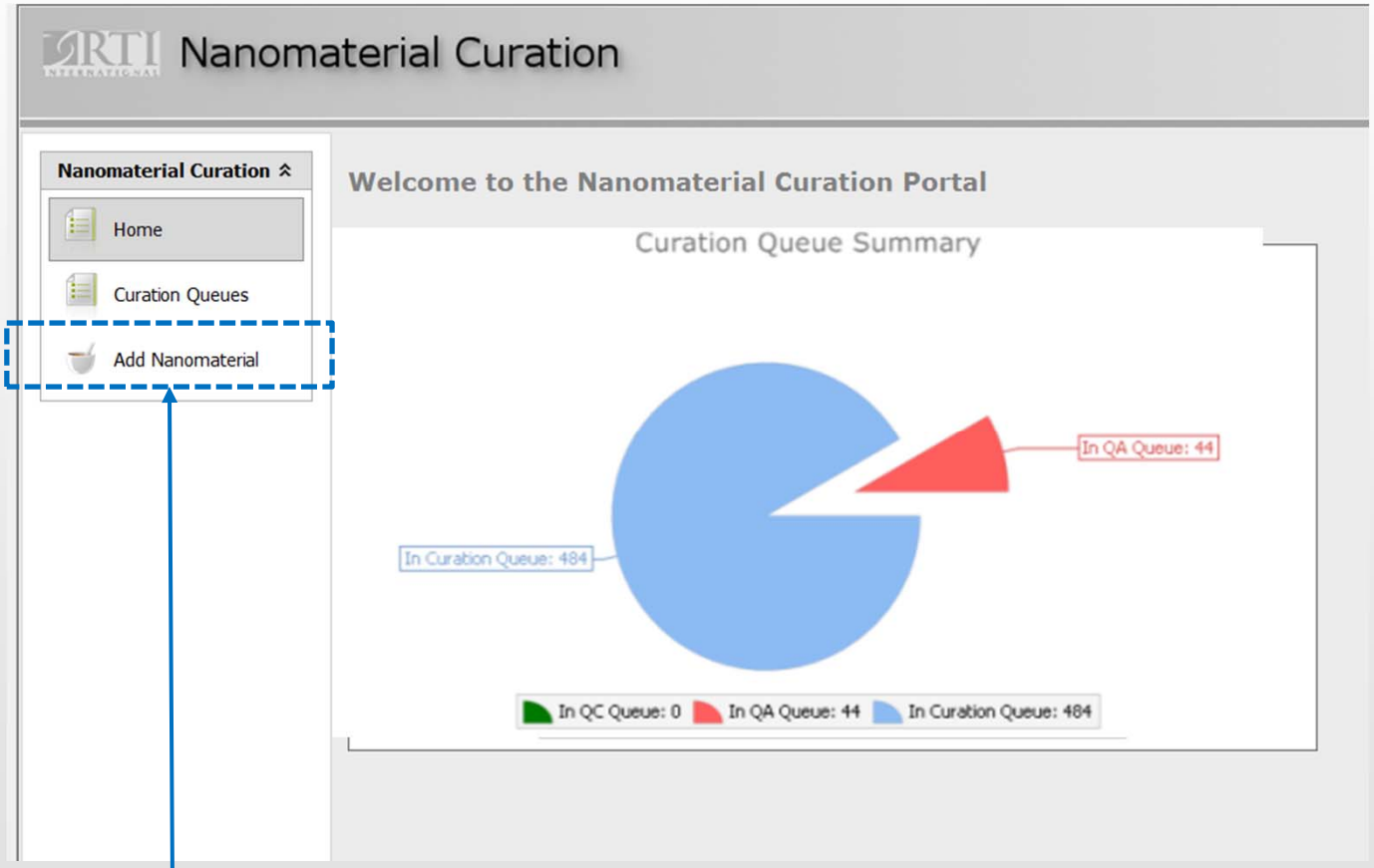
Data for decision making

A PROCESS FOR SYSTEMATIC DATA ARCHIVING

Systematic Data Archiving

*A **DATA CURATION TOOL** facilitates the progression of nanomaterial entries through the curation process to the Nanomaterial Registry website*



Curation tool workflow starts with the creation of a nanomaterial record

DATA ENTRY

- ✓ identifies, evaluates, and enters data

QUALITY ASSURANCE

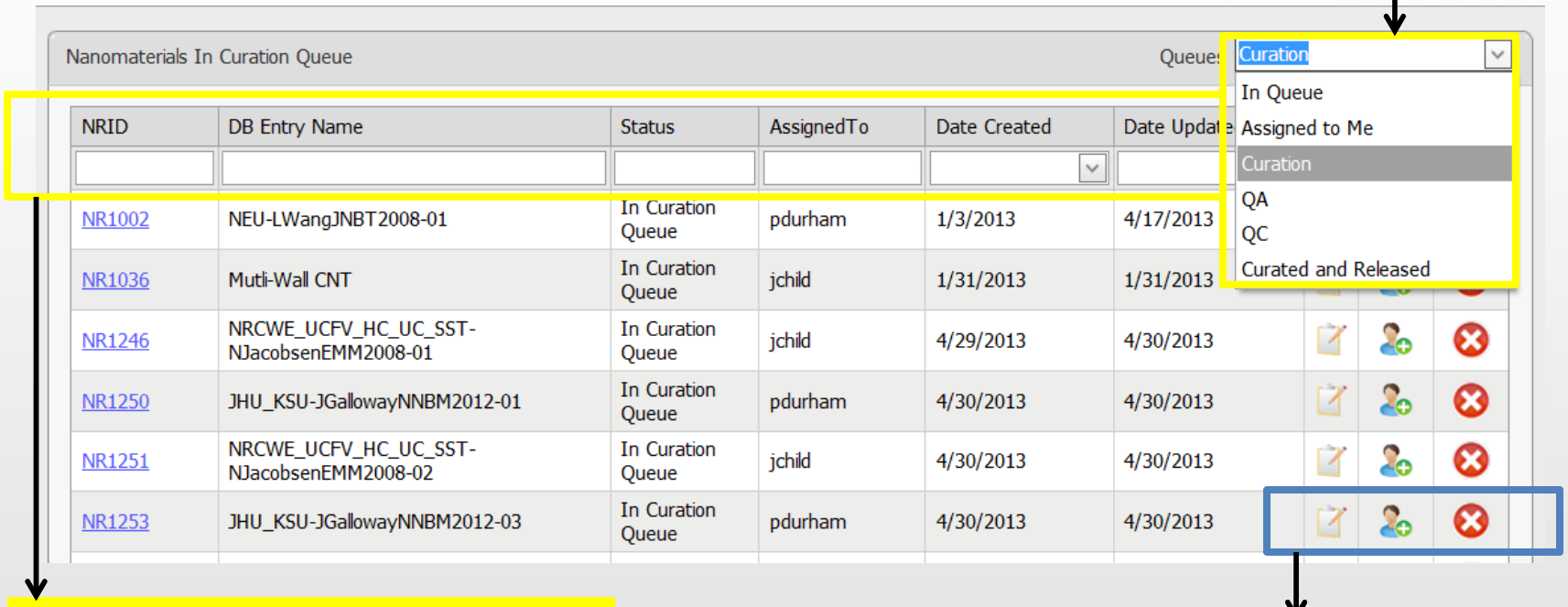
- ✓ check for transcription errors

QUALITY CONTROL

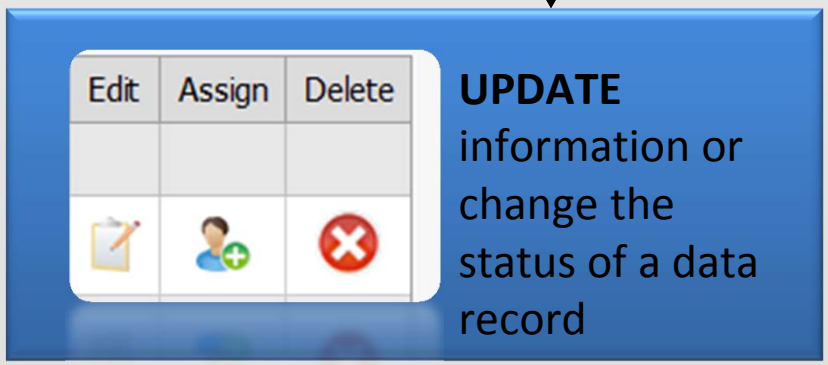
- ✓ correct any errors or inconsistencies in the scientific interpretation

Systematic Data Archiving:
DATA CURATION TOOL

Data records are promoted through **QUEUES**



SEARCH and **SORT** options for data in queues



UPDATE information or change the status of a data record

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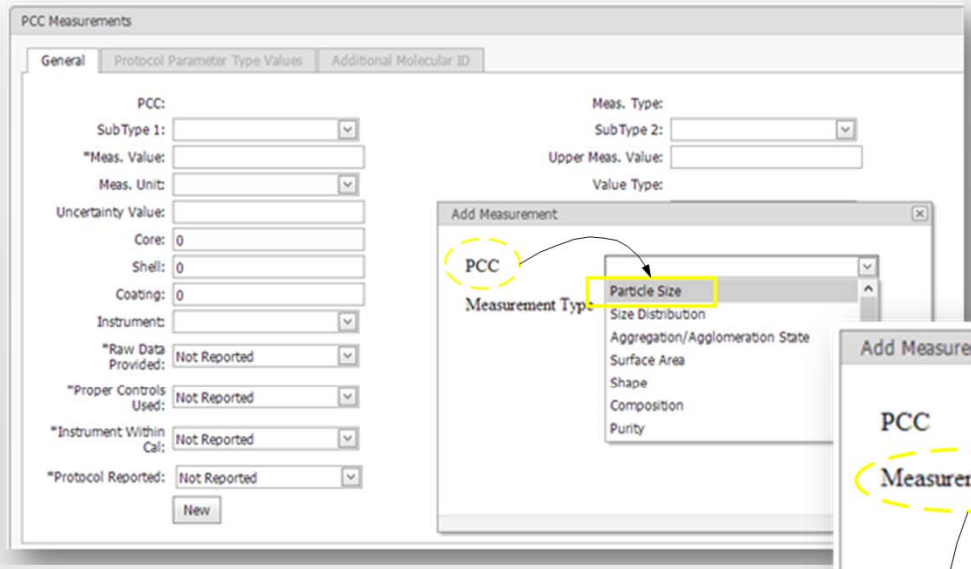
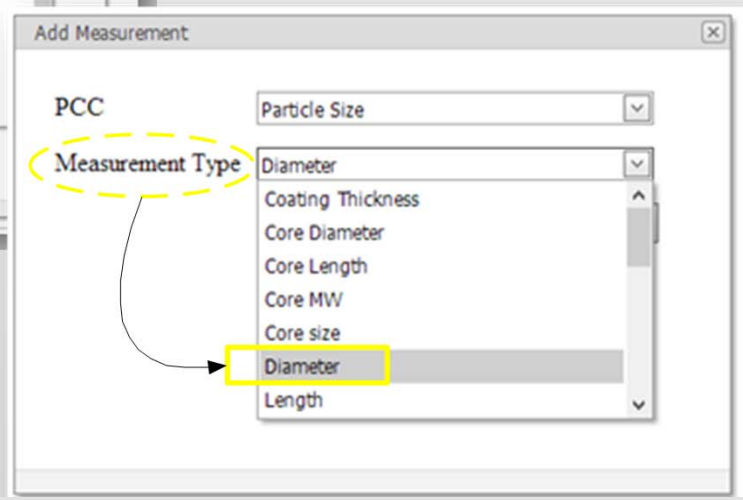
Systematic Data Archiving:
DATA CURATION TOOL

- ✓ **STEP 1**: **PCC** "Particle Size" is selected from a list of the 12 MIAN PCCs



An example of SMART CURATION:

- ✓ Drop downs in data entry fields are populated with selection lists that are valid according to the fields already entered



- ✓ **STEP 2**: **Measurement Type** drop down is populated with options relevant to "Particle Size"

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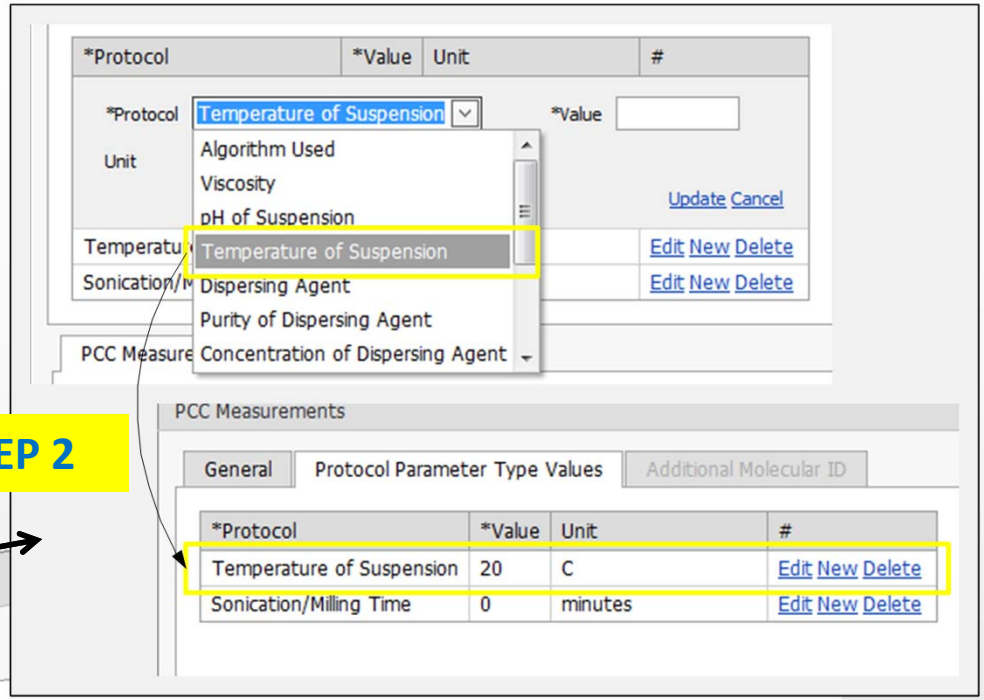
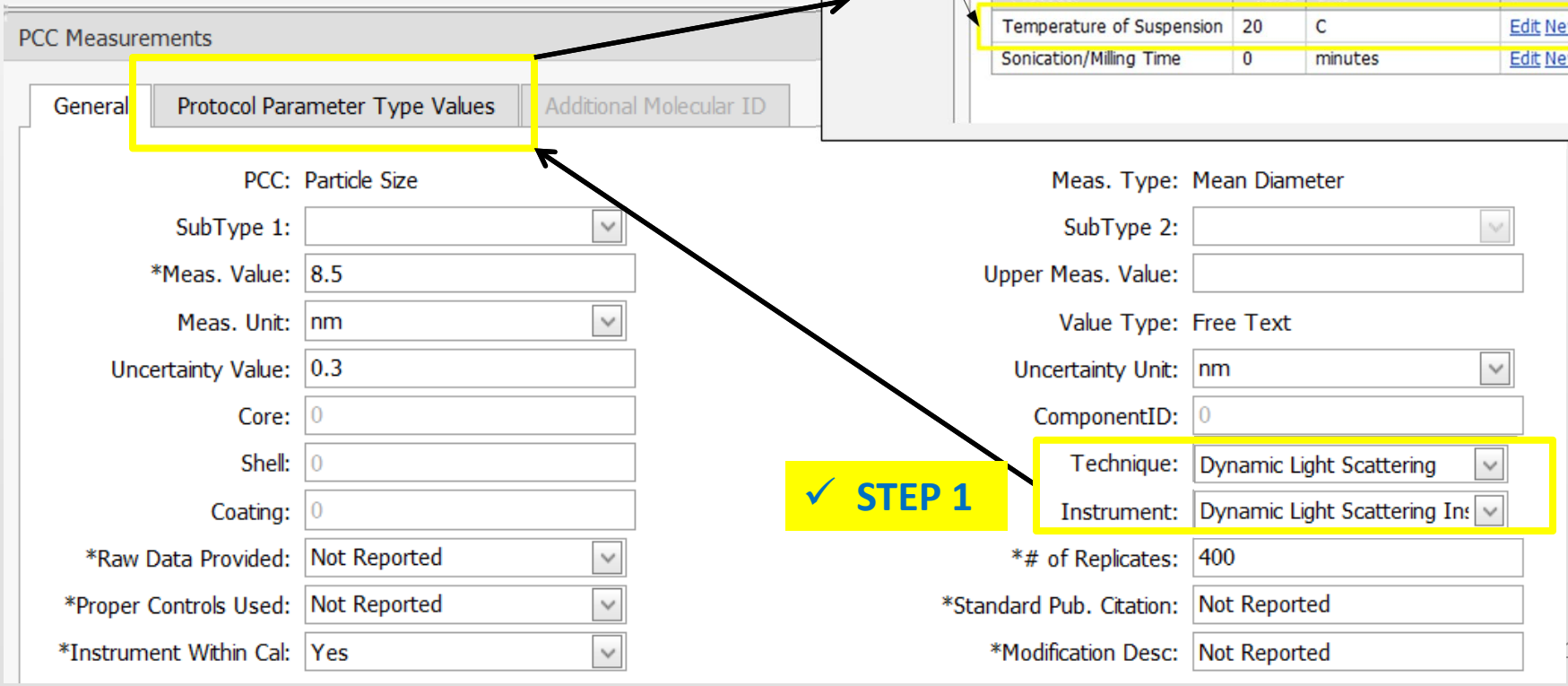
Systematic Data Archiving: *DATA CURATION TOOL*

An example of SMART CURATION:

- ✓ **STEP 1**: **MEASUREMENT** technique is selected from a list of options relevant to "particle size"
- ✓ **STEP 2**: **PROTOCOL** tab is populated with options relevant to "Dynamic Light Scattering"



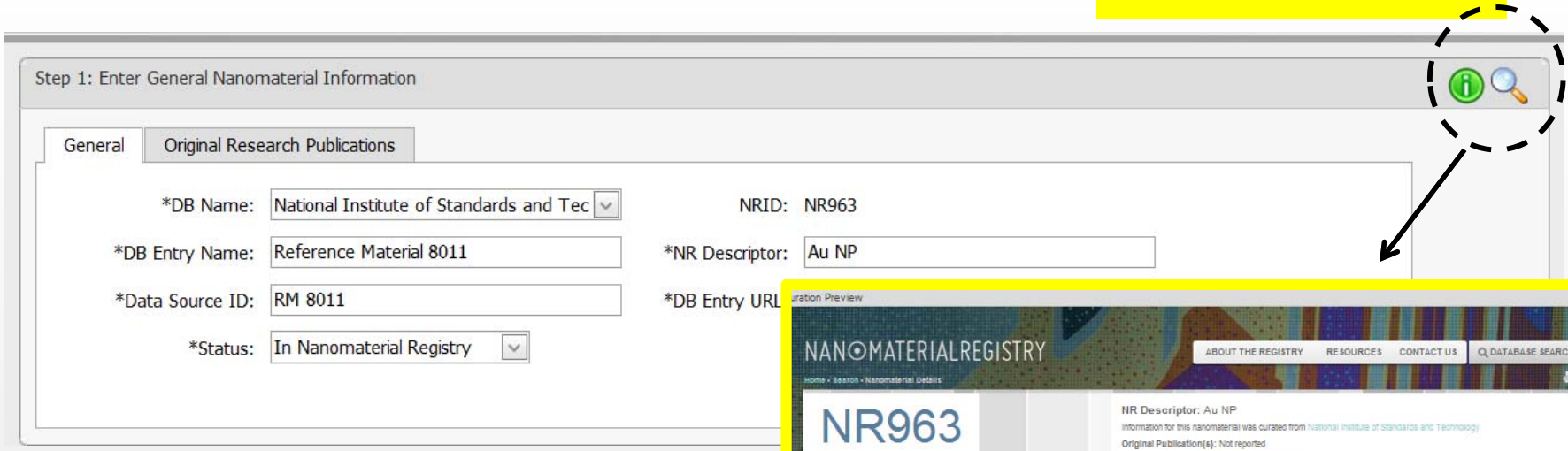
✓ STEP 2

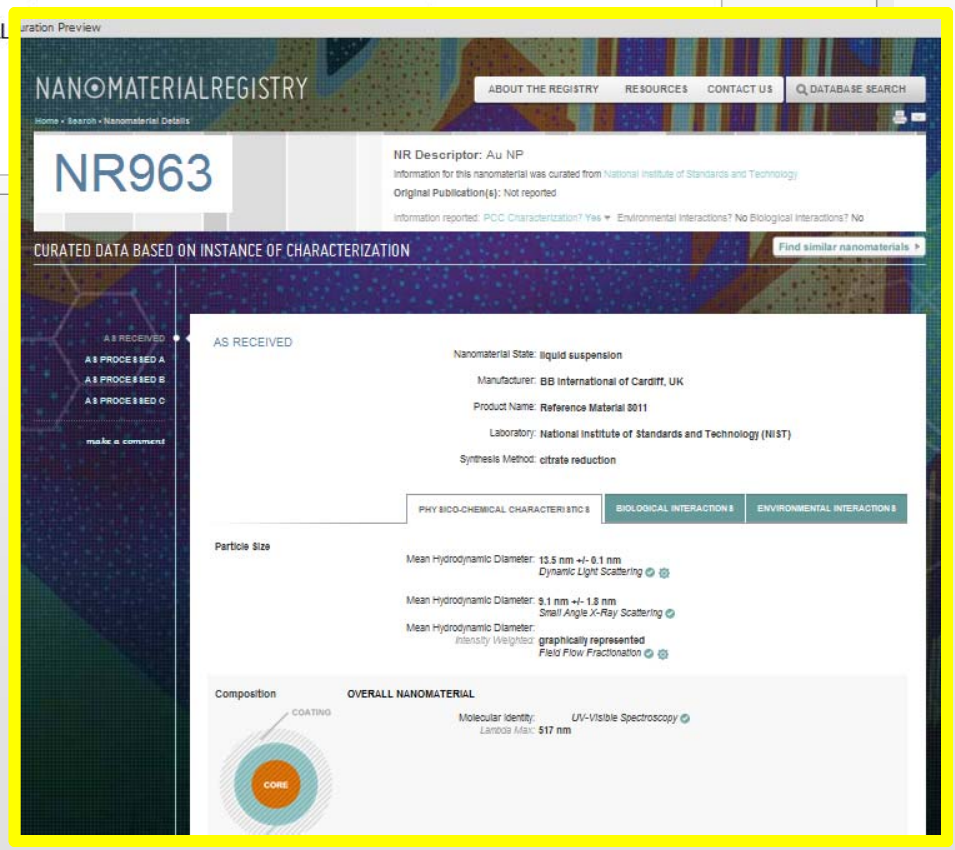


✓ STEP 1

Systematic Data Archiving: *DATA CURATION TOOL*

Preview Data Tool





The curation team can use the PREVIEW tool to quickly see how the data will display on the website

NANOMATERIALREGISTRY

Data for decision making

EVALUATING THE INFORMATION

Evaluating the Information

Compliance Level

The Nanomaterial Registry's **COMPLIANCE LEVEL FEATURE** provides a **METRIC** on the **QUALITY** of characterization of a nanomaterial entry

Compliance Level	Score	Medal
Gold	76-100	
Silver	51-75	
Bronze	26-50	
Merit	0-25	

COMPLIANCE LEVELS are broken into **MERIT**, **BRONZE**, **SILVER**, and **GOLD** and represent increasing quality of characterization based on our evaluation criteria

$$CL_{IPCC} = \sum_{i=1}^{M} \frac{W_i}{(M * N)}$$

A COMPLIANCE LEVEL SCORE is a quantitative value calculated by assigning a weight (W) to each value reported in the curated entry (M)

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Evaluating the Information

Compliance Level

COMPLIANCE LEVEL WEIGHTING FACTOR IS HIGHER WHEN:

- Terms with **greater specificity** are used
- **Well-established techniques** are used
- **Protocols are adequately described**
- **Standard protocols** are used
- Values are measured with **multiple techniques**
- **Good laboratory practices** are reported

Example: Particle Size reported as

- Diameter
- Mean aerodynamic diameter

$$CL_{IPCC} = \sum_{i=1}^{M} \frac{W_i}{(M * N)}$$

Example:

- Instruments within calibration and proper controls were used
- replicate measurements were taken

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Evaluating the Information

Compliance Level

COMPLIANCE LEVEL is higher when more Meta-data about a characterization are reported

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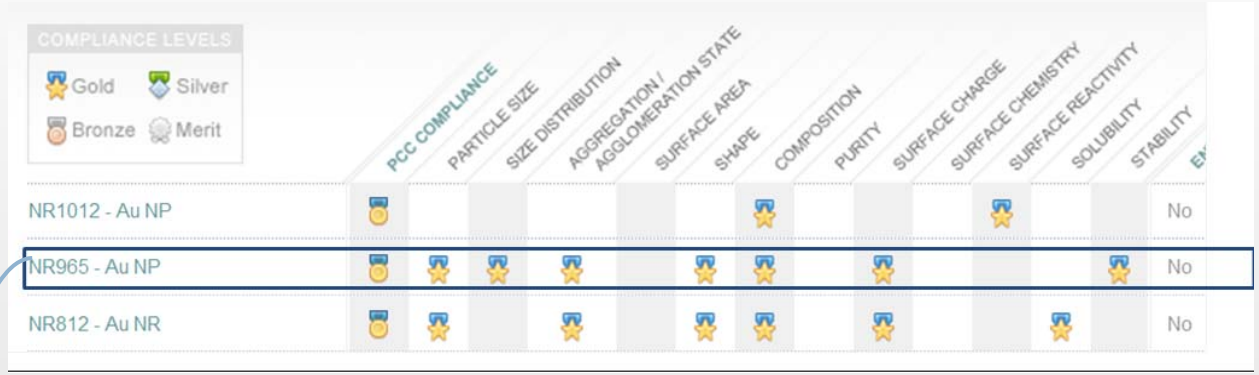
Evaluating the Information

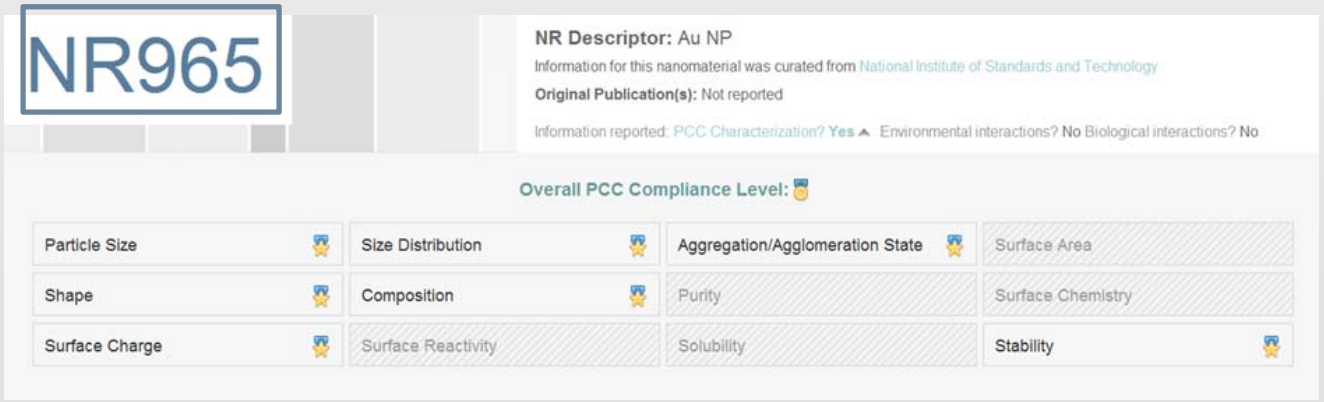
Compliance Level on the Registry

COMPLIANCE LEVEL for individual characterizations are displayed



✓ On the SEARCH RESULTS page

✓ On the DETAILS PAGE

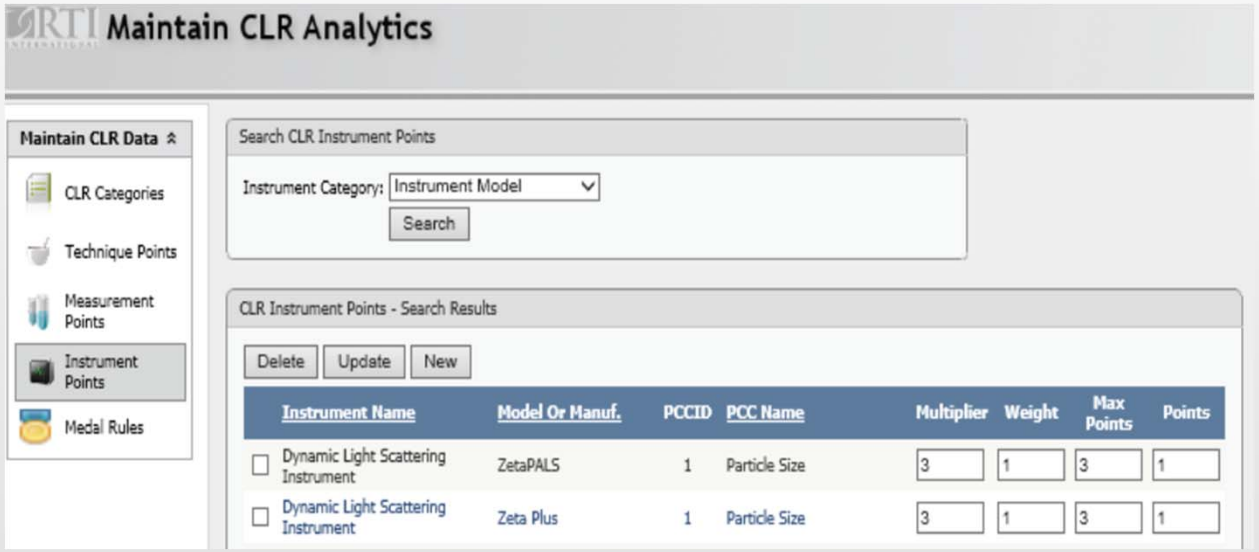


Evaluating the Information

Compliance Level - work is ongoing

The **COMPLIANCE LEVEL** was designed as a **FLEXIBLE** tool

As terminology, standards, and techniques become relevant and/or obsolete, the terms and weighting factors behind the ***compliance level score can be updated***.



Implementation of new algorithms can be tested on actual data sets

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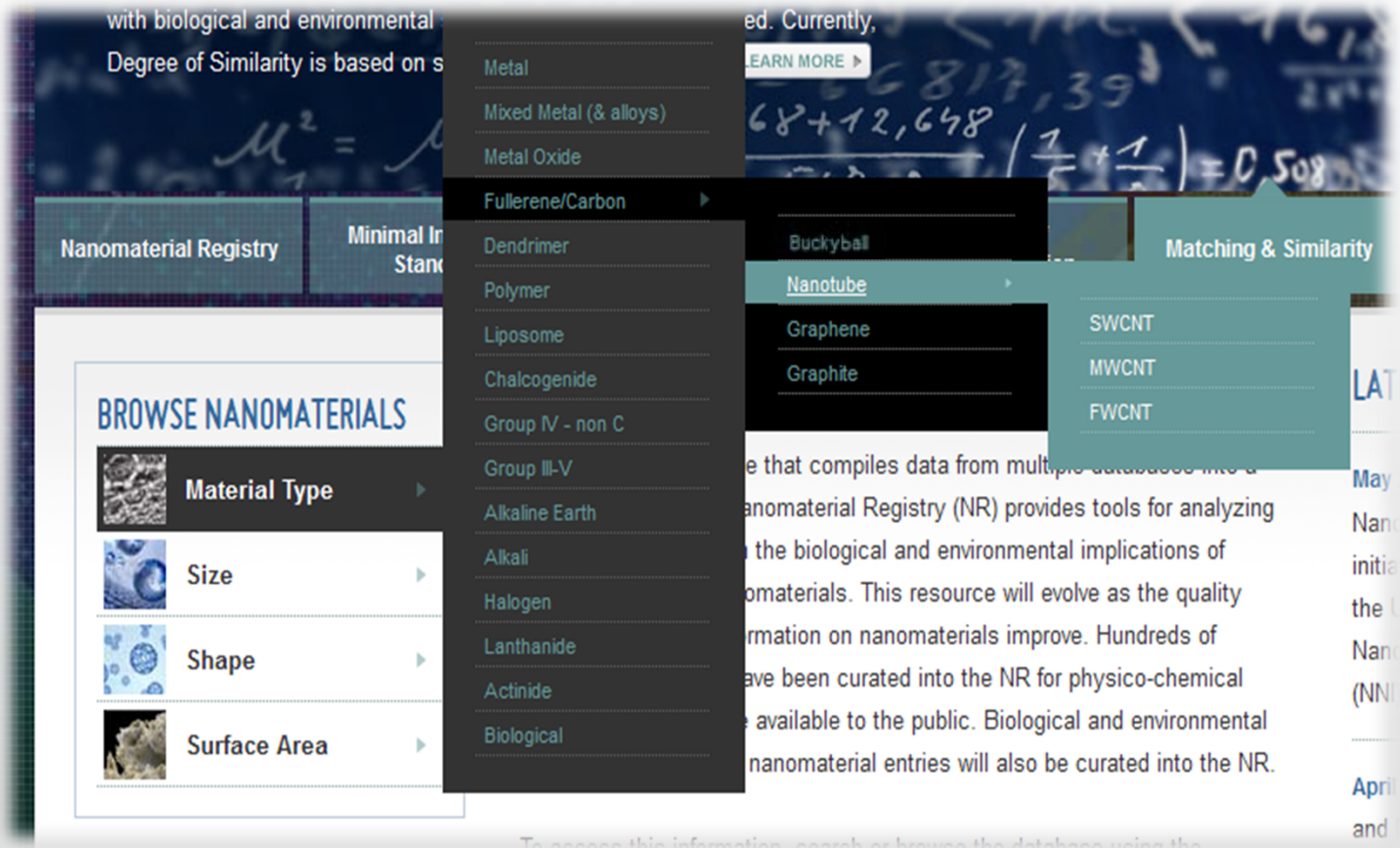
Data for decision making

SHARING THE DATA

Browse

- Locate data using nanomaterial classifications



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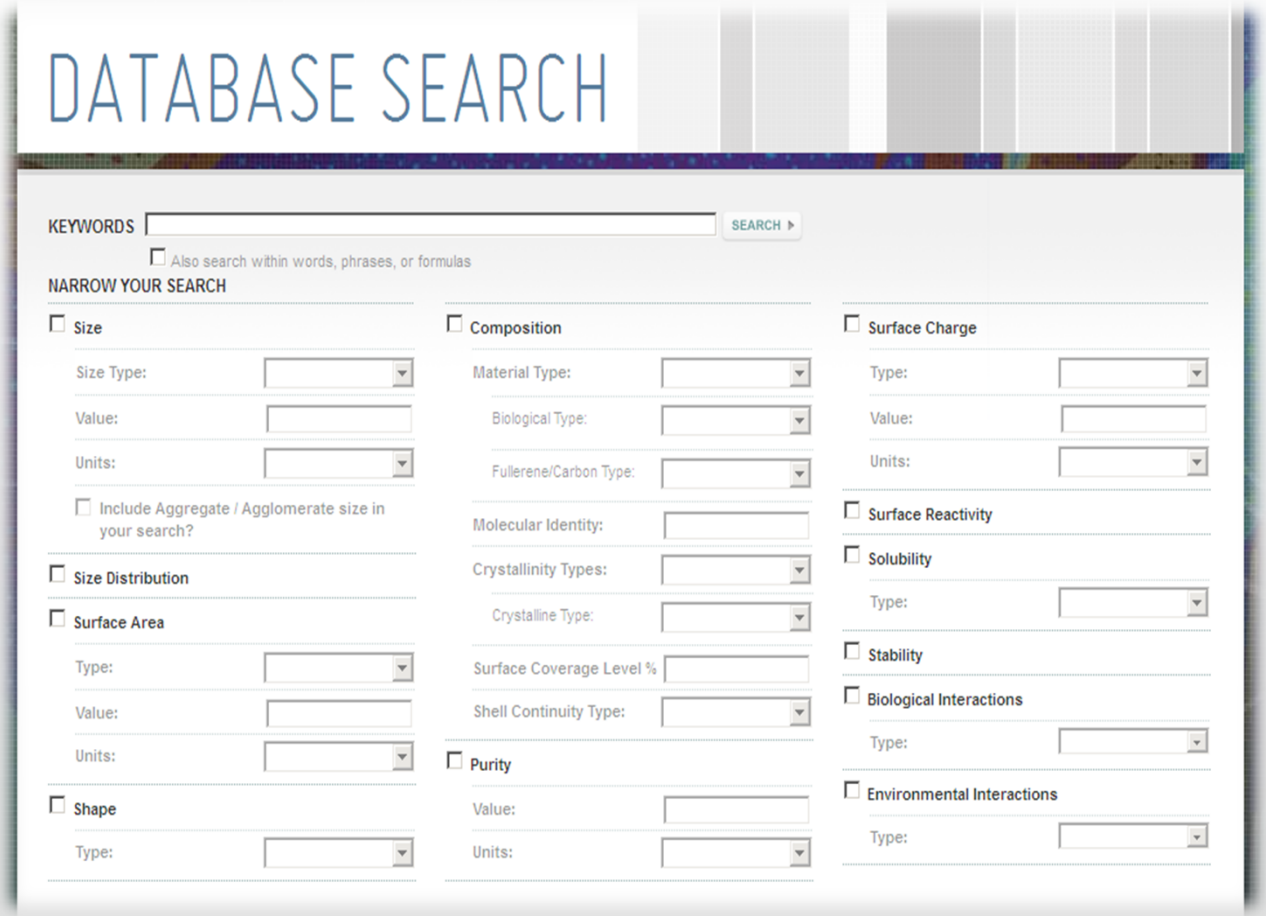
Search

- Find data using keyword(s) and specific characteristic(s)



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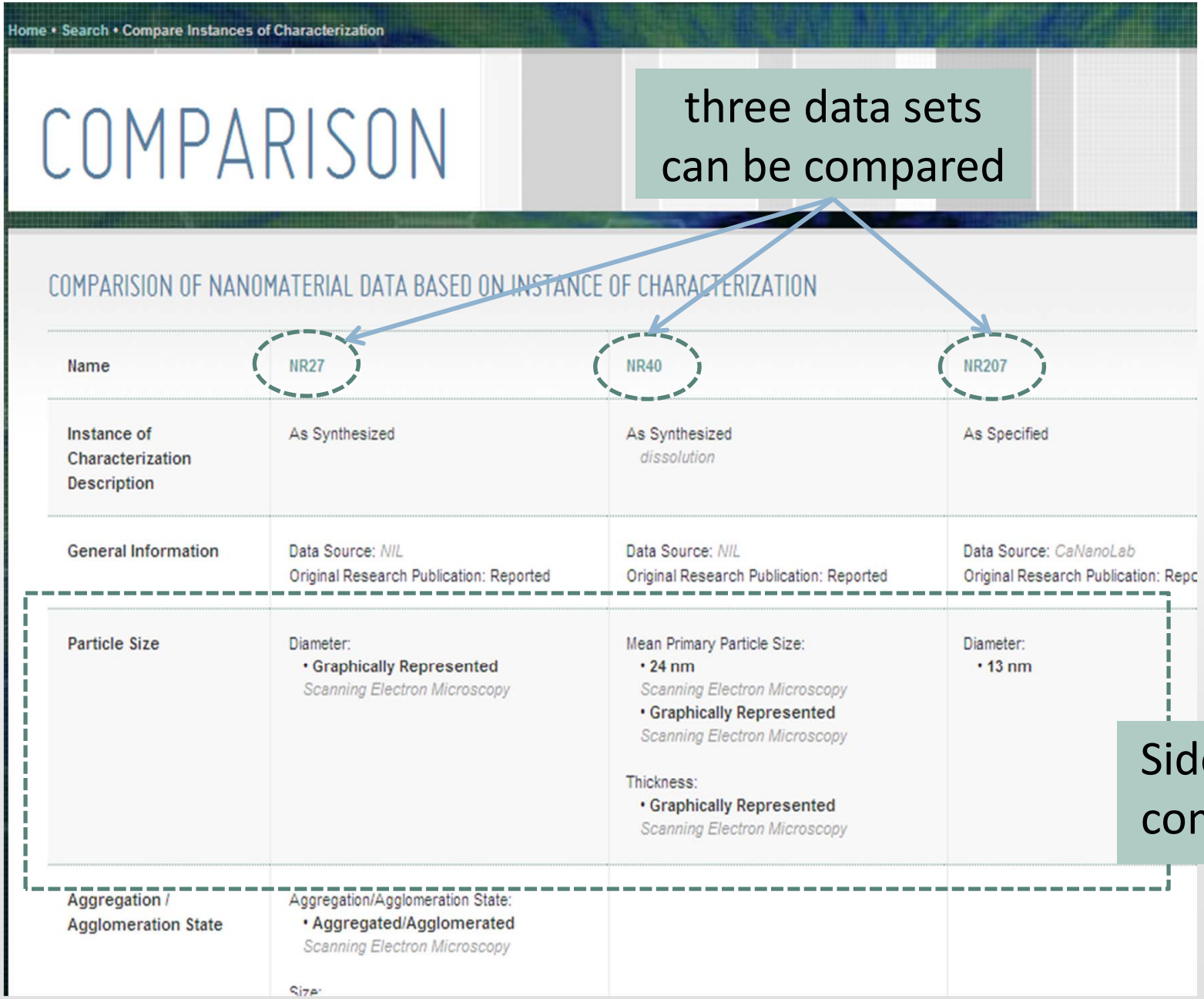

Side by side comparison

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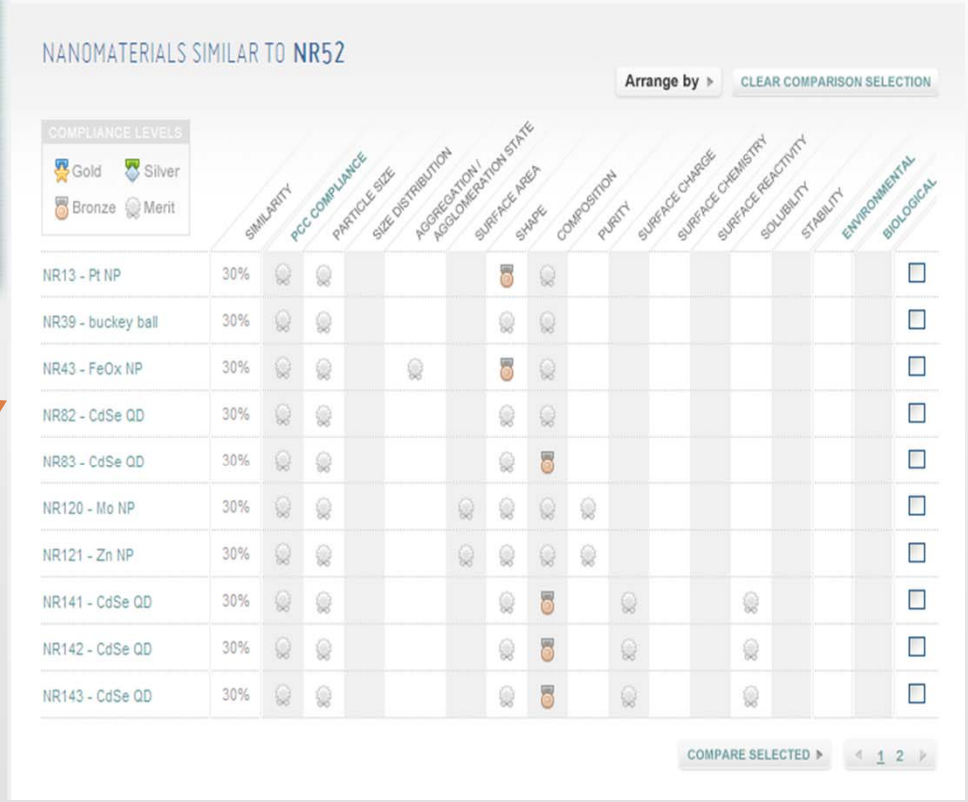
Find Similar Nanomaterials



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Upcoming Features

- Data visualization tools
  - data pattern and trend recognition
- Data export tool
- User accounts/profiles for
  - Saved queries
  - Custom data visualizations
  - Saved data export settings
  - Other custom settings

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Data for decision making

BENEFITS OF THIS APPROACH

Benefits

- Foundational groundwork is in place
  - ✓ An **integrated data** set to interrogate and share
  - ✓ "Efficient" **data curation**
  - ✓ **Flexible** framework for adaptation of new discoveries and expanded scope
  - ✓ Incorporation of **standards**
  - ✓ **Connection** with community

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Data for decision making

OUR VISION: BEYOND DATA CURATION

Utility of the Registry

- The Nanomaterial Registry **VISION**:
  - ✓ **Infer properties** and functions when data are missing for a particular nanomaterial, but available for "similar" nanomaterials
  - ✓ Provide a mechanism to **identify similar nanomaterials** based on properties and endpoints
  - ✓ Identify data gaps and trends

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Data for decision making

COMMUNITY VISION

Partnership

Working directly with researchers is advantageous

- High compliance level data
  - Often more data/meta data is available from the researcher
  - Data to be used to answer broader research questions
- Early data capture
  - Archive data early in it's lifecycle
  - Store data in "non-public" data queue
  - Data can be made public at appropriate time
- A freely available Public tool
  - Data sharing
  - Influencing best practices in nano data informatics

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Thank You!