Discussion on Curation
Nano WG – June 6, 2013

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Website, Outreach, & Curation Task Leader

RTI International

NANOMATERIALREGISTRY

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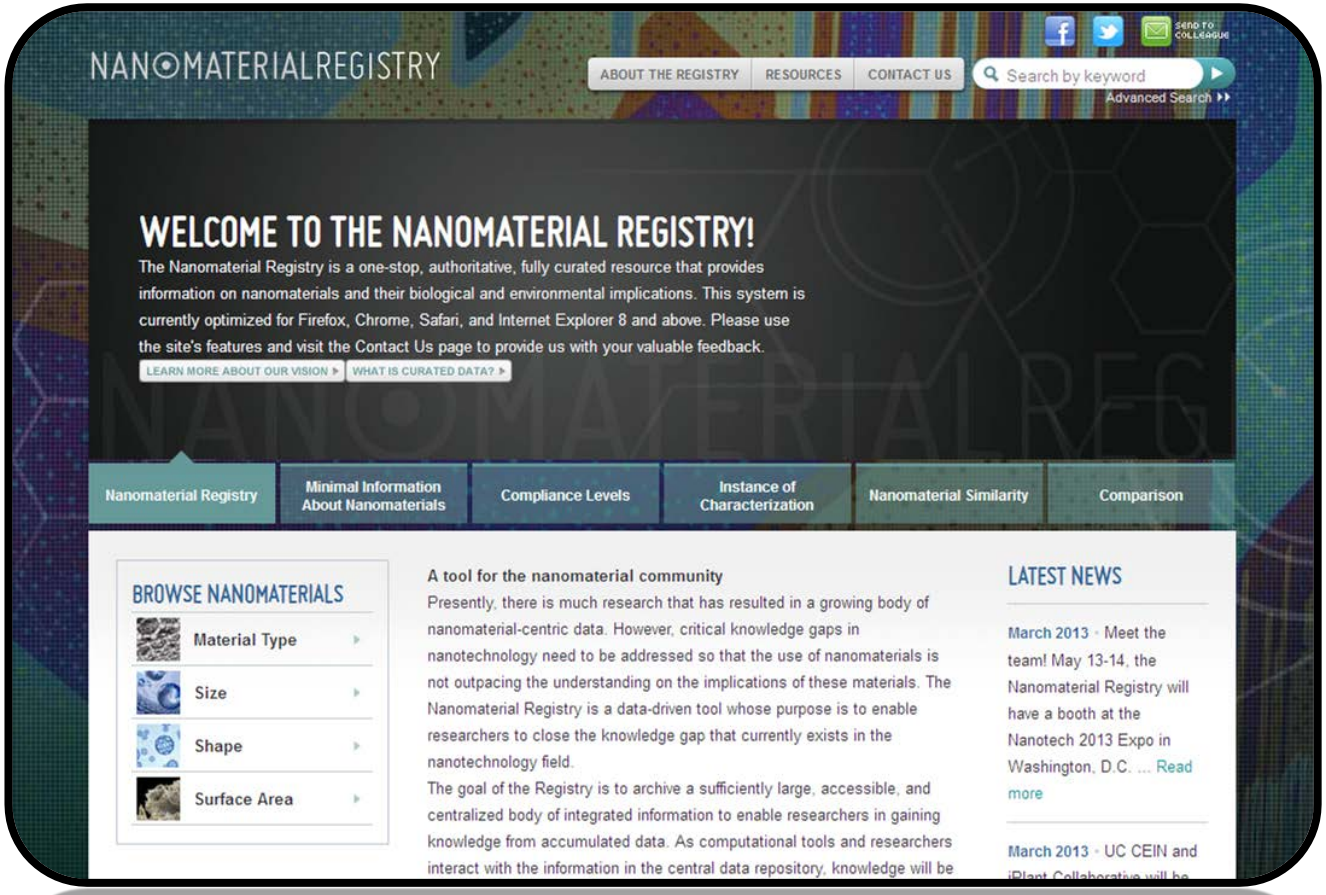
Comprehensively curated, validated data on a scale suitable for decision making



Web Address:

www.nanomaterialregistry.org

Funded by:

NIH National Institutes of Health

Registry User Goals

Short Term:

- Easily visualize what been done in the community
  - Instrumentation
  - Assays
  - Chemistries

Long Term:

- Use curated data to predict the behavior of new nanomaterials

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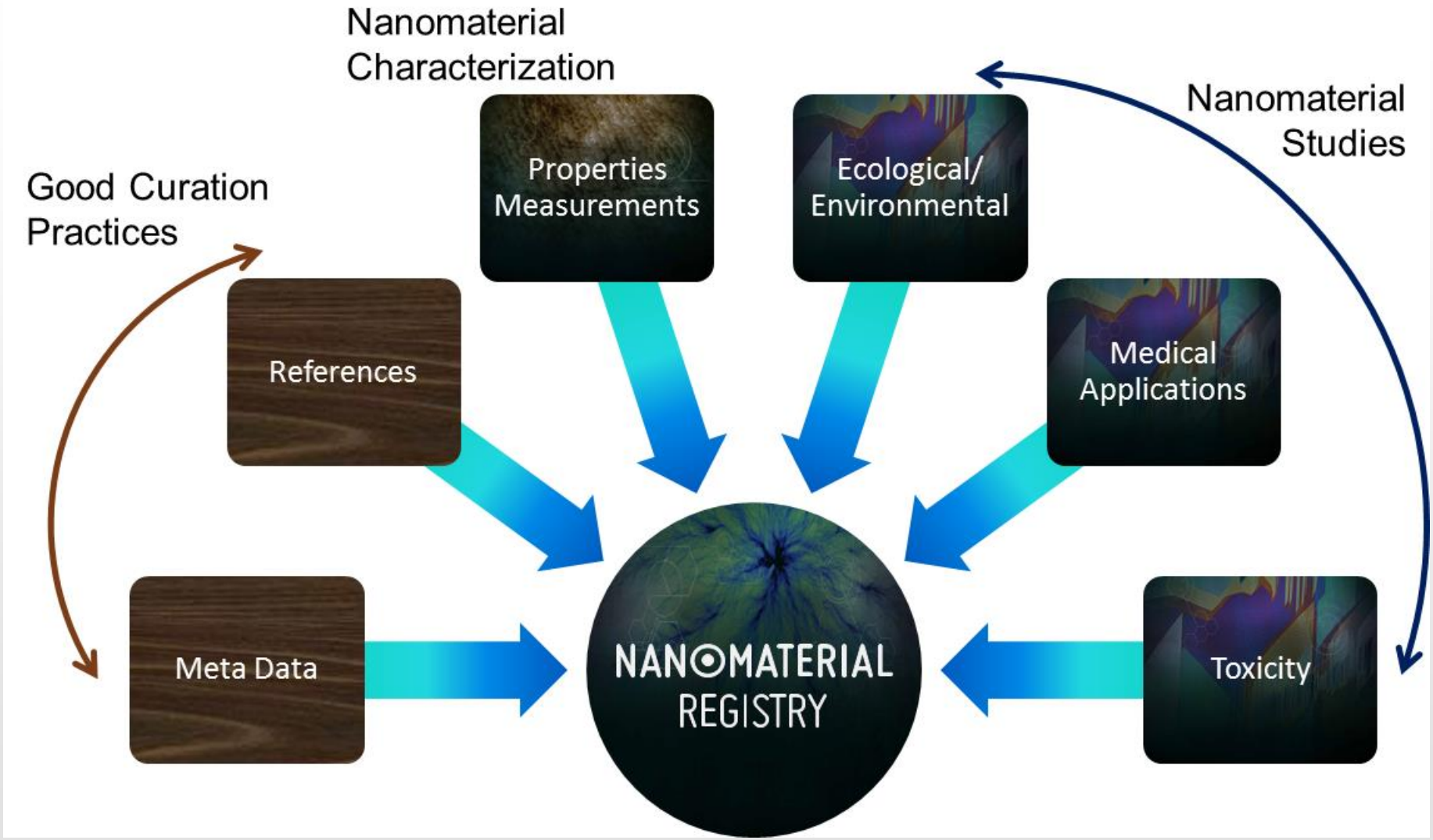
Current Data Scope 1



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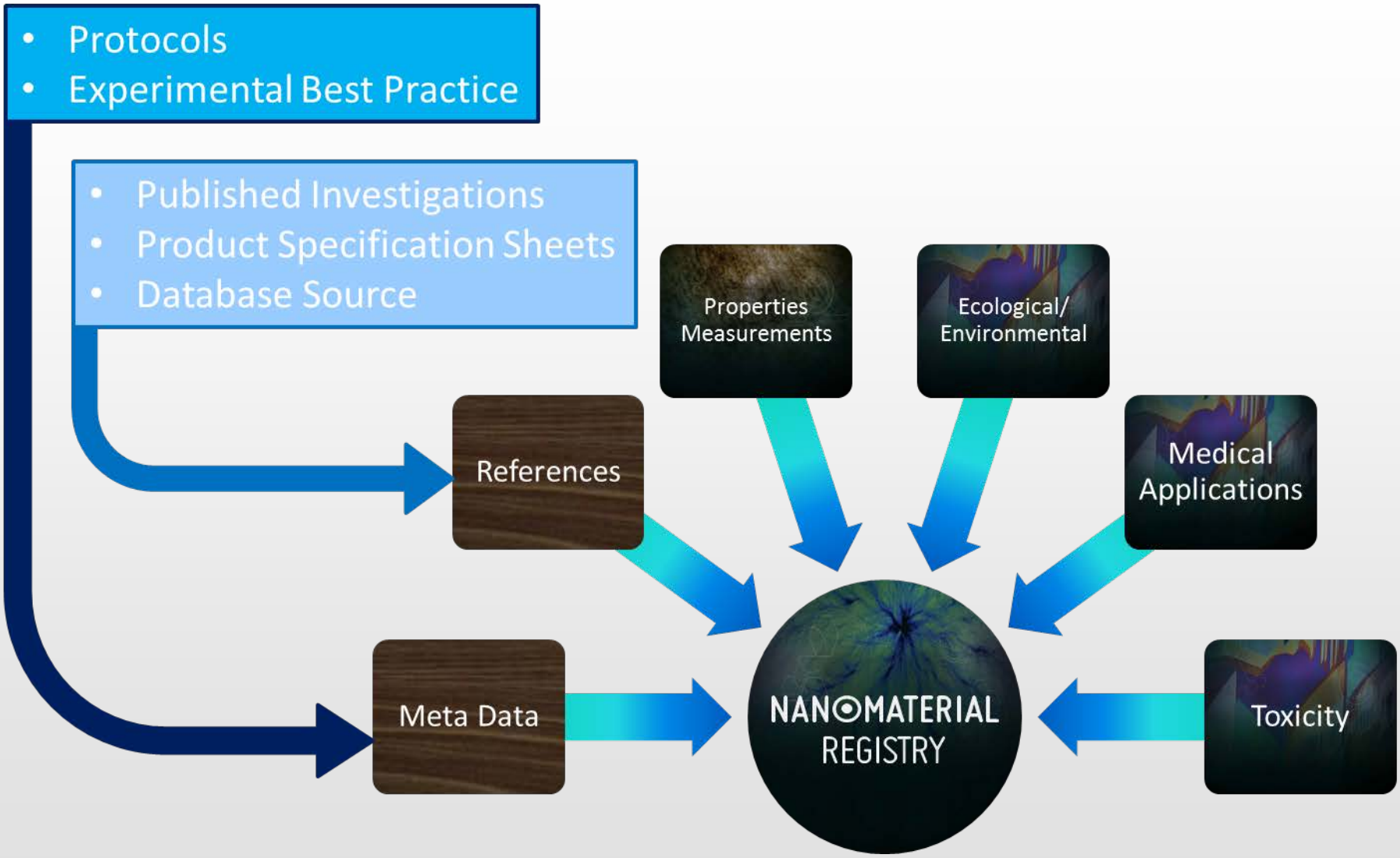
Current Data Scope 2



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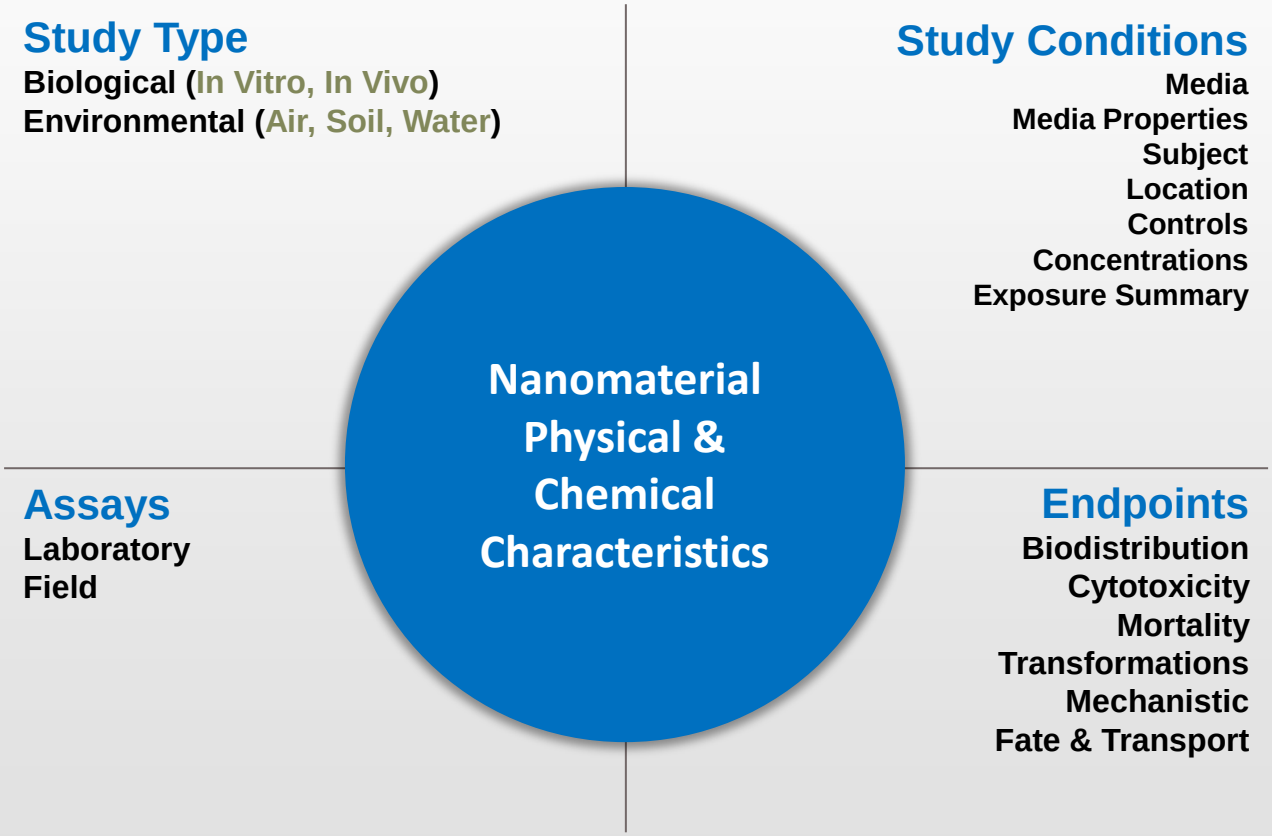
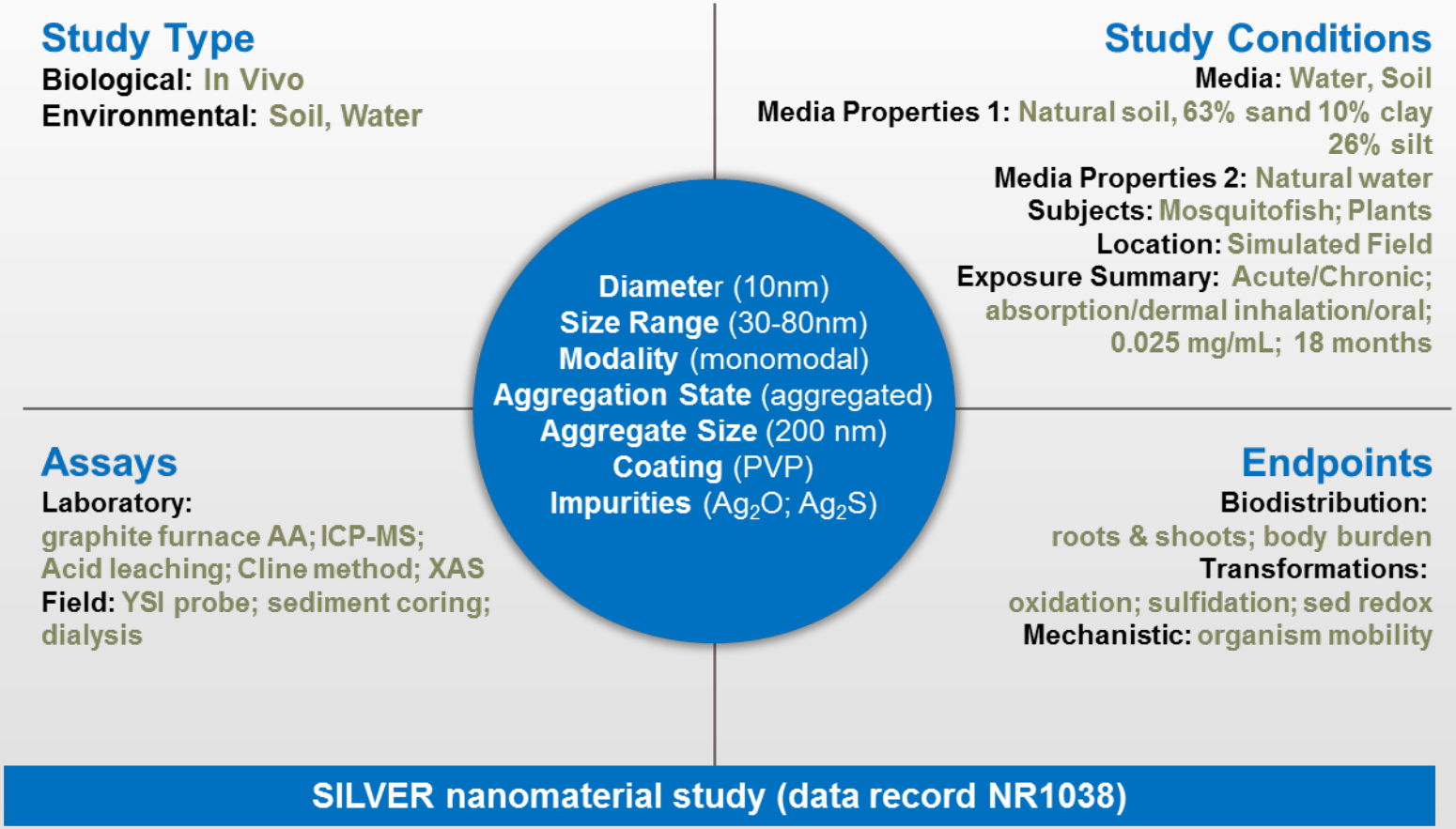
Linking PCCs with Impacts

Capturing Biological and Environmental Impacts



Linking Data Example

Analysis of the connections between properties and environmental and biological impacts of nanomaterials



Data Source: CEINT
https://www.nanomaterialregistry.org/NanomaterialDetails2.aspx?pid=1038

Minimal Information about Nanomaterials

Physico-Chemical Characteristics

MIAN PCC

MIAN for Physico-Chemical Characteristics

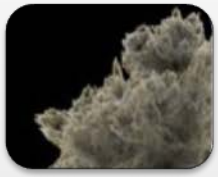
Composition

Size

Size Distribution

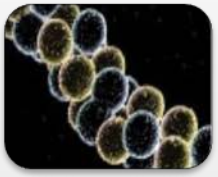
Shape

Aggregation/
Agglomeration State



Surface Area

Surface Charge



Surface Chemistry

Surface Reactivity

Purity

Solubility

Stability

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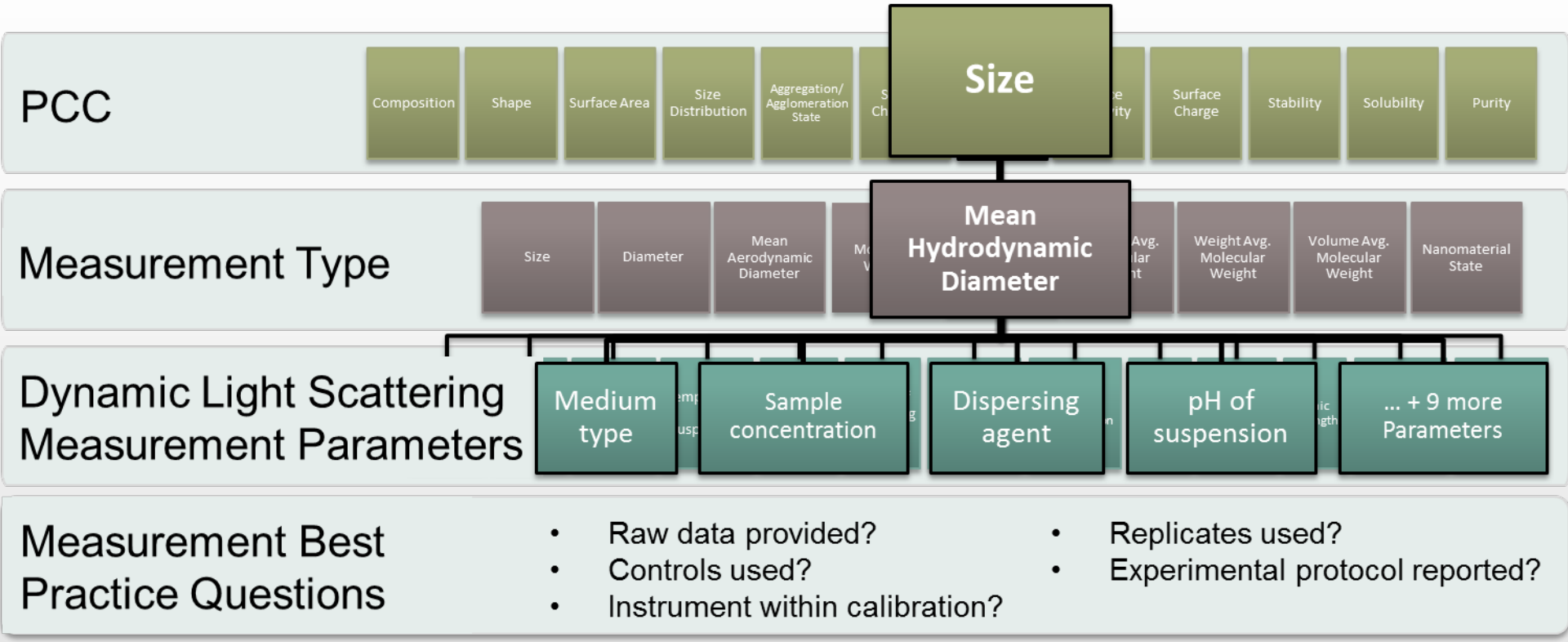
Metadata in the MIAN



Minimal Information = PCC data + Metadata

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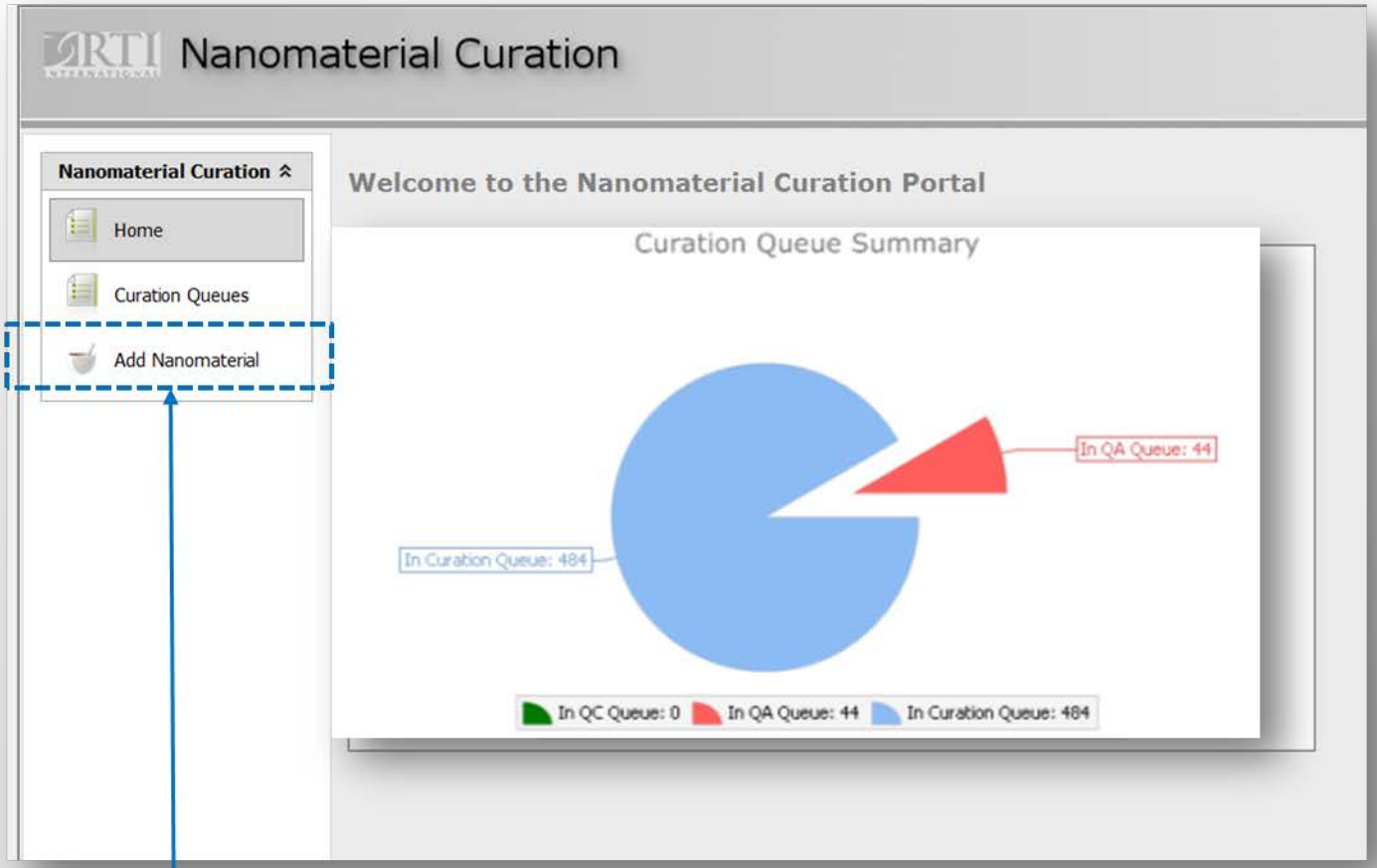
Accelerating the Curation Process

Minimizing Error Propagation

CURATION TOOL

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

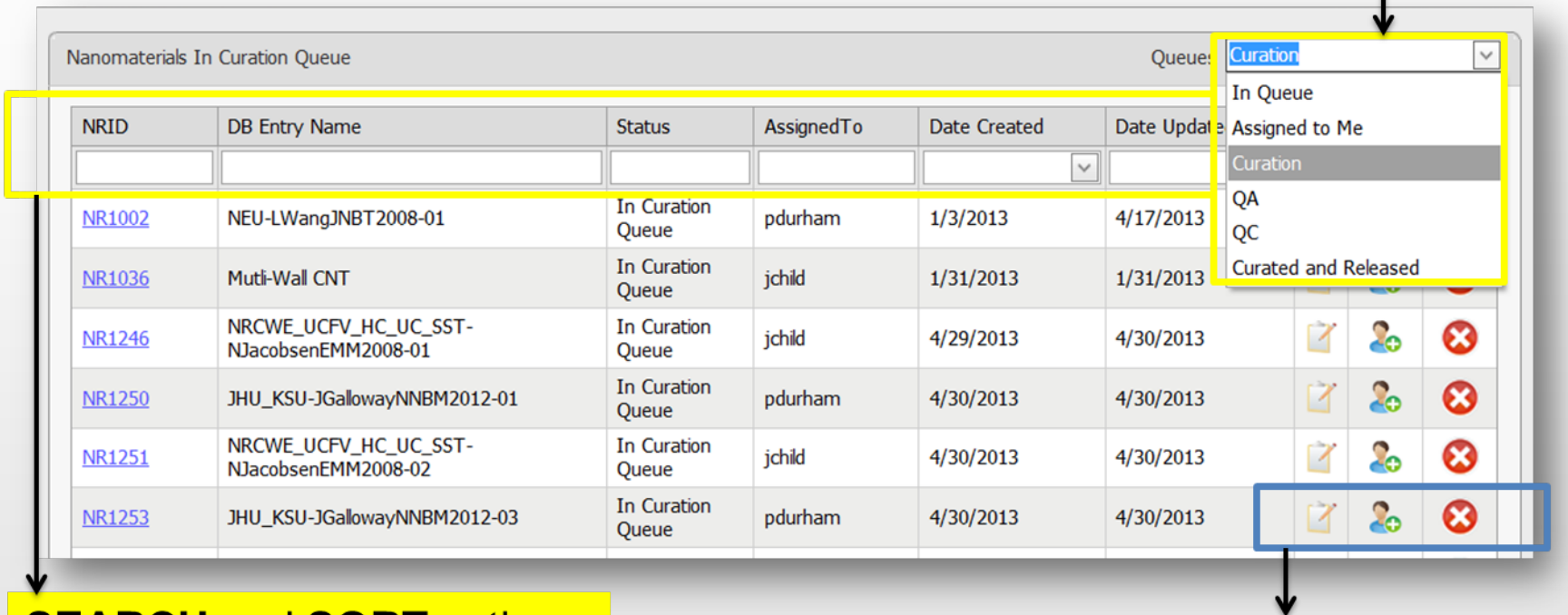
QUALITY CONTROL

- ✓ correct any errors or inconsistencies in the scientific interpretation

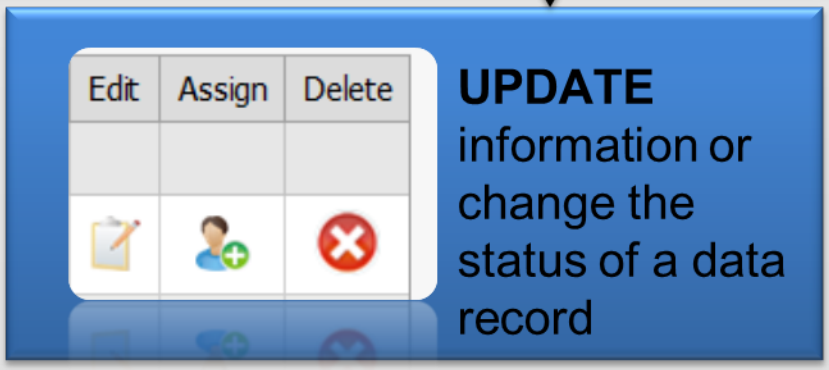
Systematic Data Archiving:

DATA CURATION TOOL 1

Data records are promoted through **QUEUES**



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



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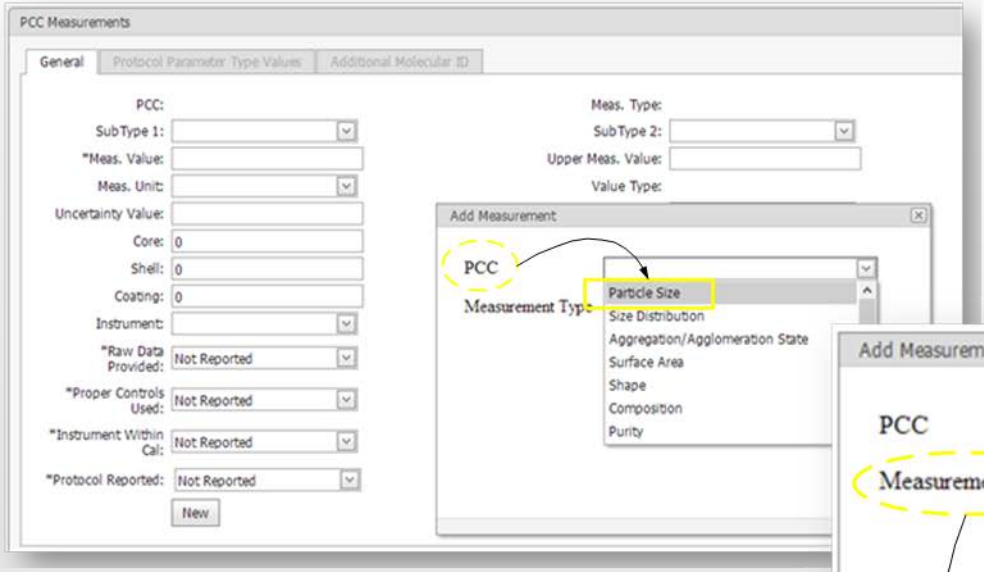
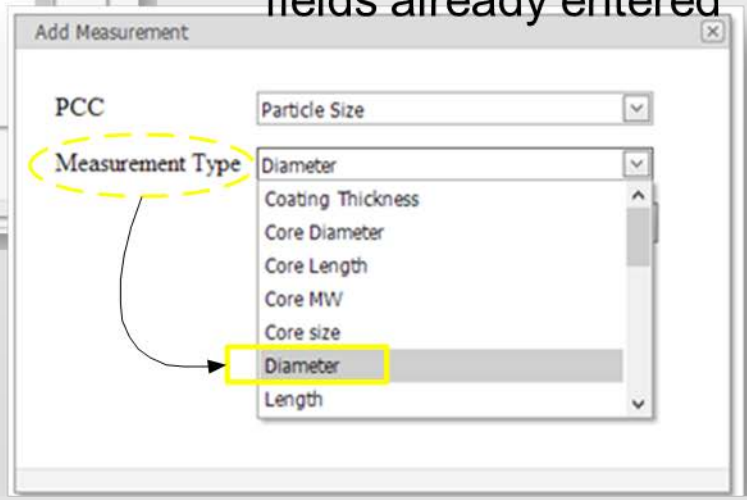
Systematic Data Archiving:
DATA CURATION TOOL 2

✓ **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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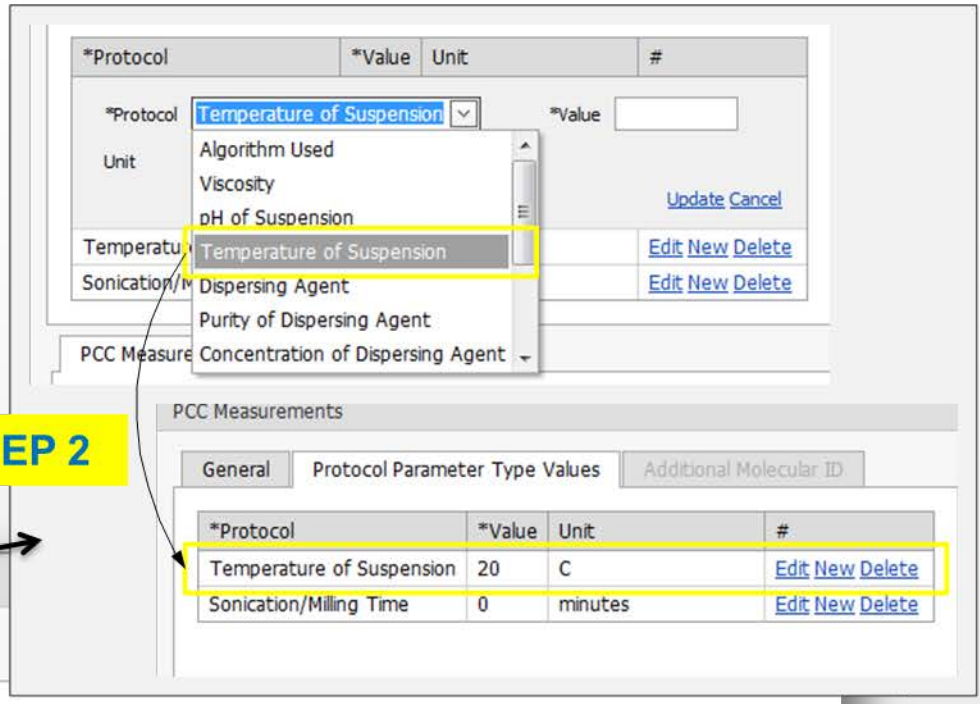
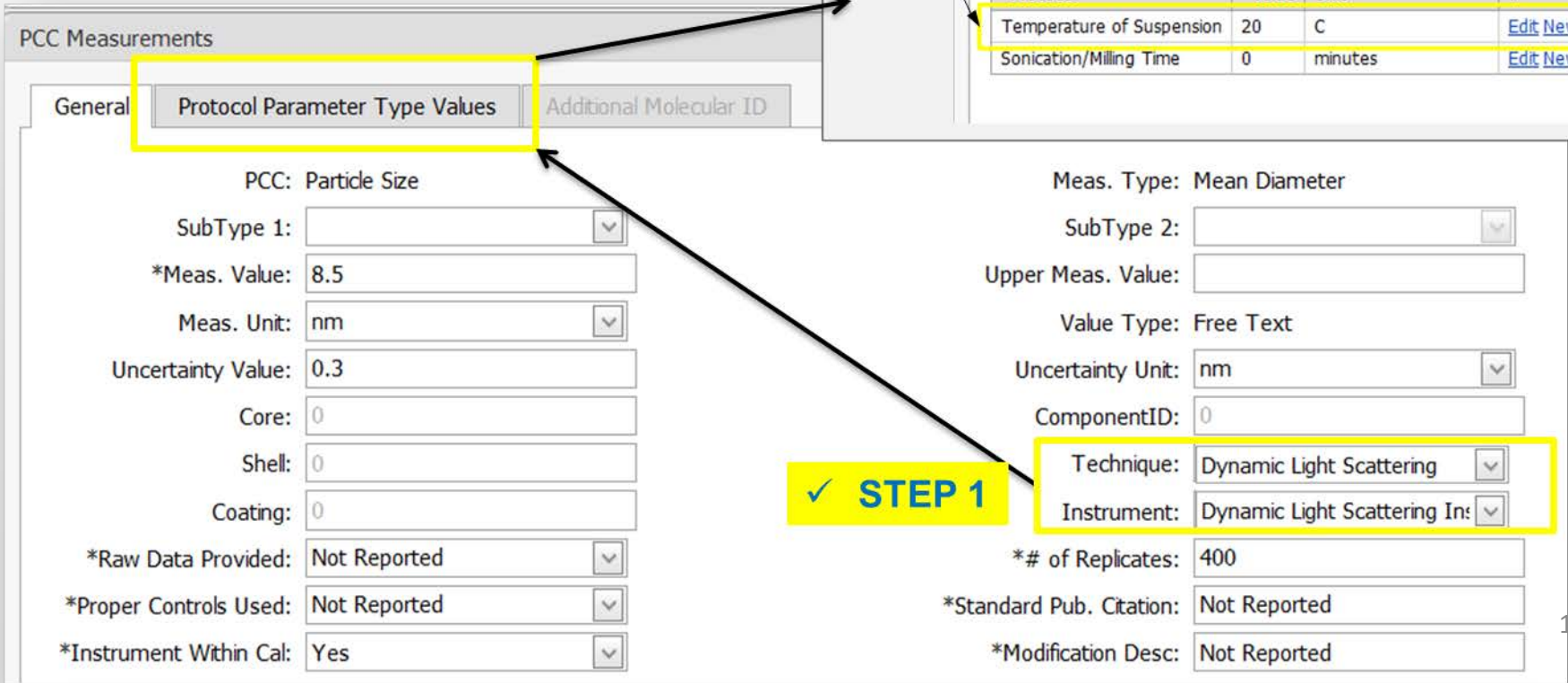
Systematic Data Archiving: *DATA CURATION TOOL 3*

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

Evaluating the Information

Compliance Level 1

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 2

- **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 3

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

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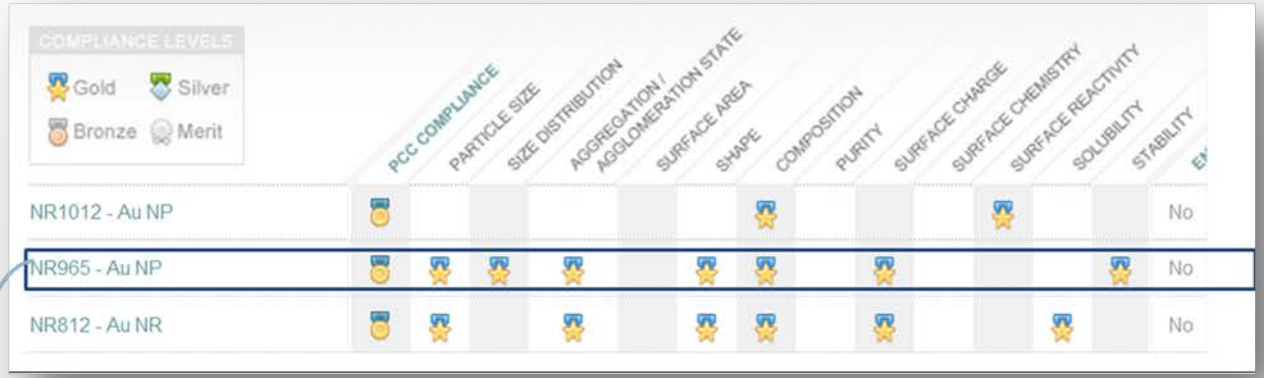
Evaluating the Information

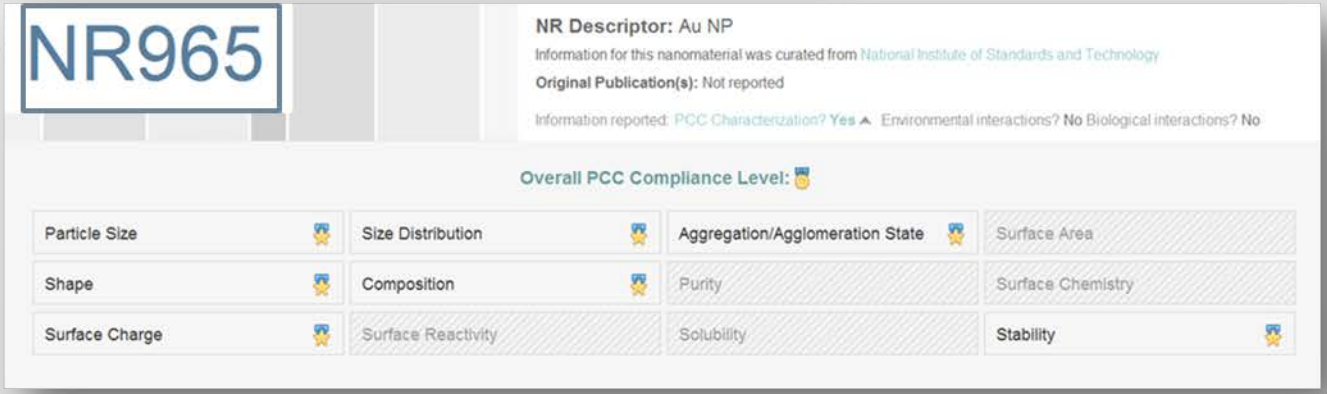
Compliance Level on the Registry

COMPLIANCE LEVEL for individual characterizations are displayed



✓ On the SEARCH RESULTS page

✓ On the DETAILS PAGE



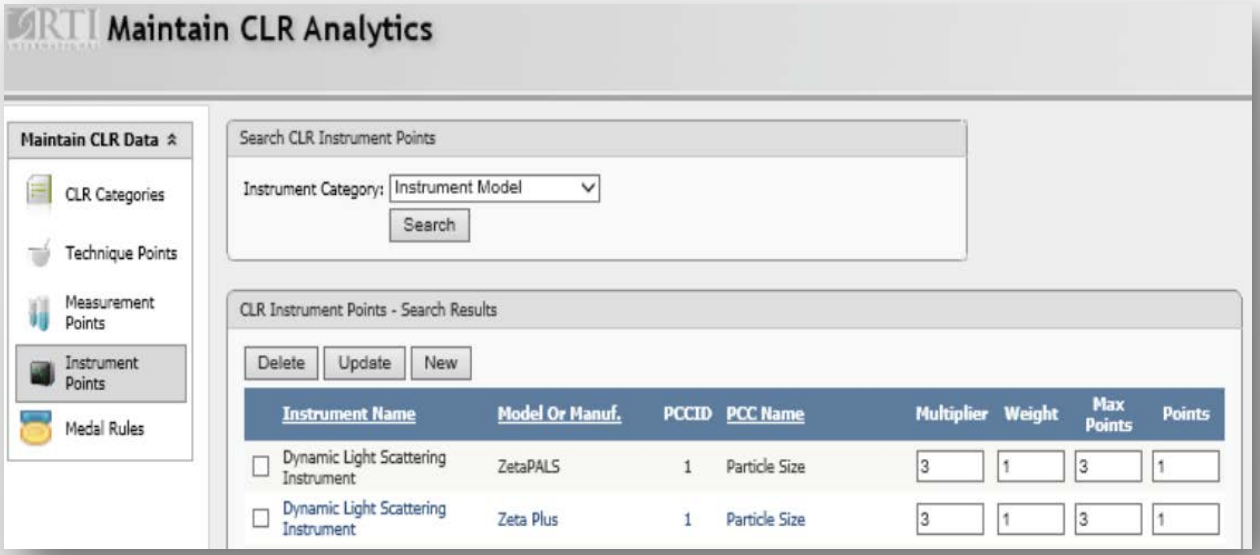
Evaluating the Information

Compliance Level - work is ongoing

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

Implementation of new algorithms can be tested on actual data sets

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



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