NANOMATERIALREGISTRY

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RTI International

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NANOMATERIALREGISTRY

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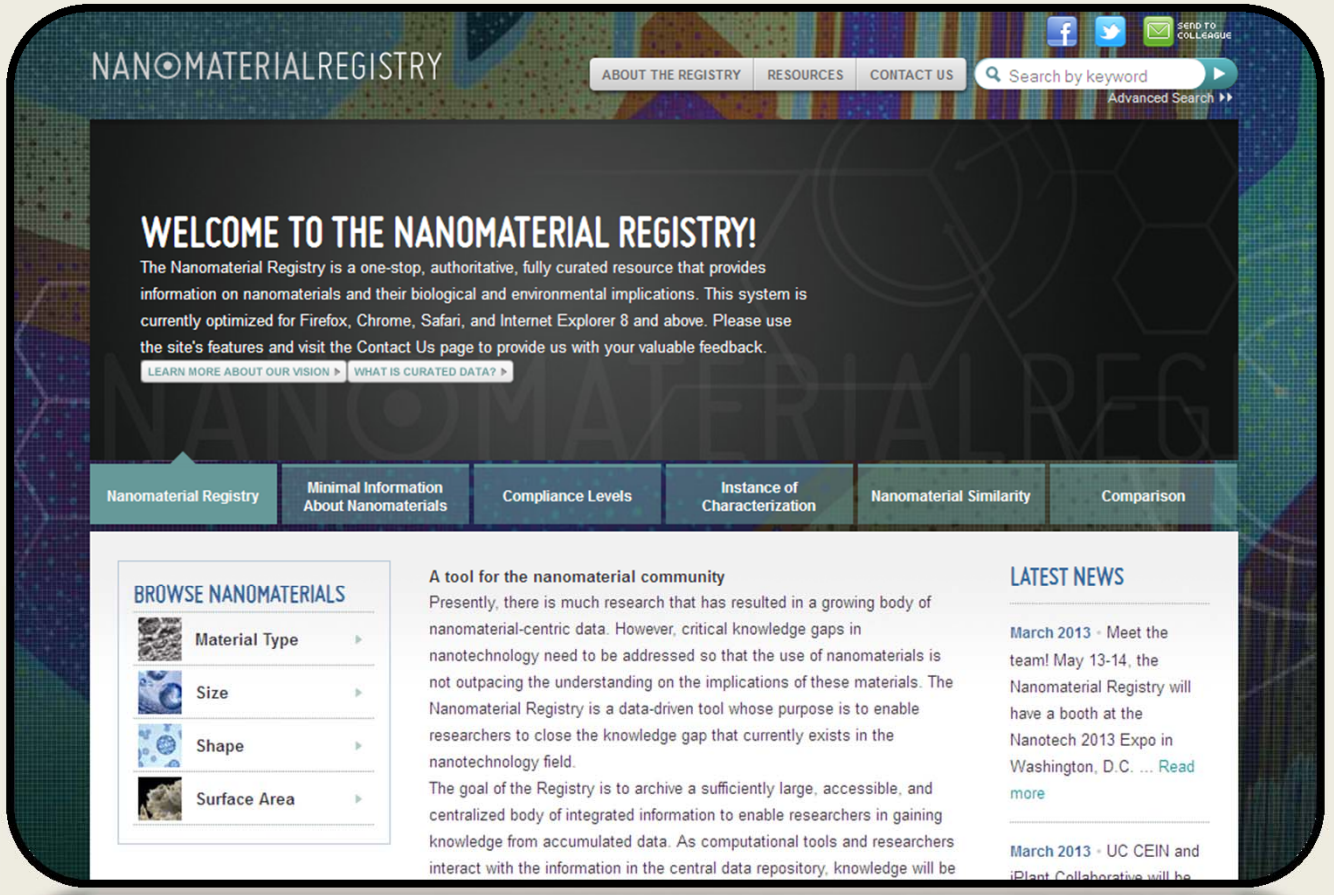
Comprehensively curated, validated data on a scale suitable for decision making



Web Address:

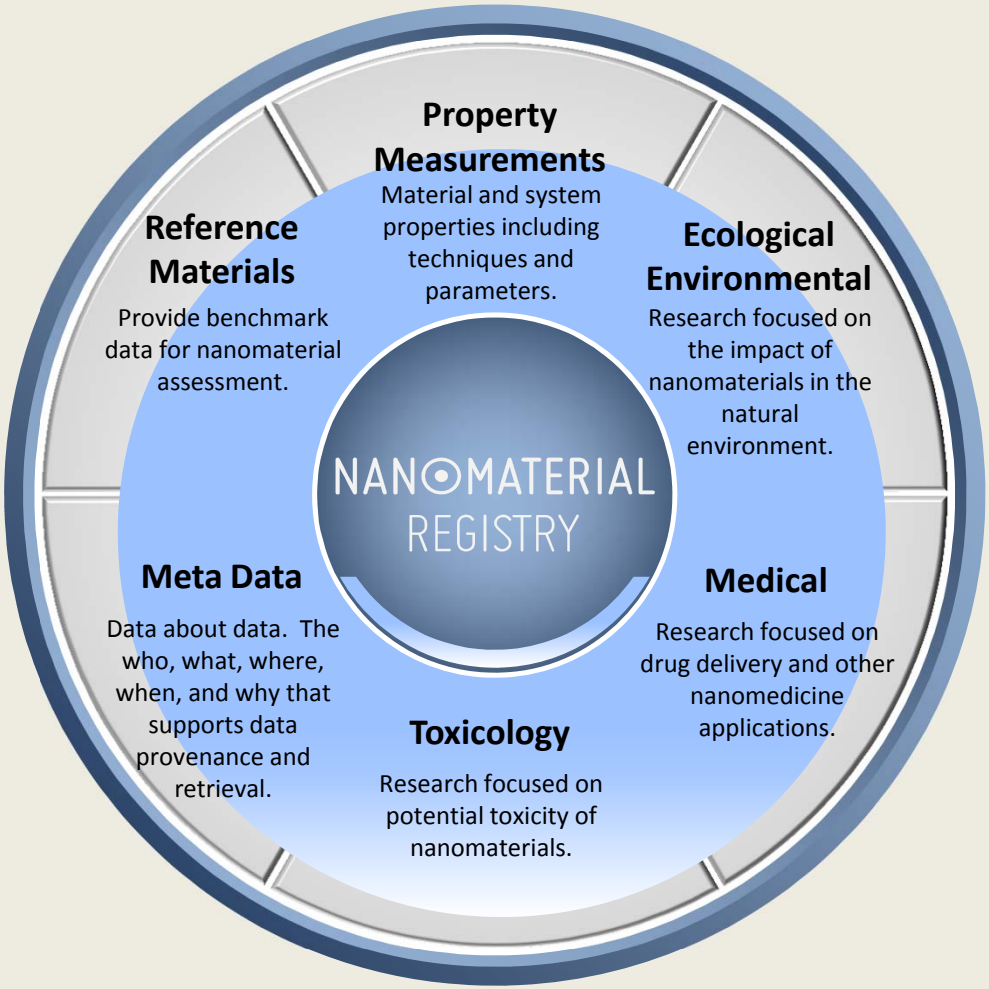
www.nanomaterialregistry.org

Funded by:

NIH National Institutes of Health

NANOMATERIAL INFORMATION

The Scope of the Registry



- **Validated** both programmatically and by a team of scientist and
- **Integrated** through controlled vocabulary and data format
- **Relevant** a growing body of up-to-date data is available to the public

PROPERTY MEASUREMENTS

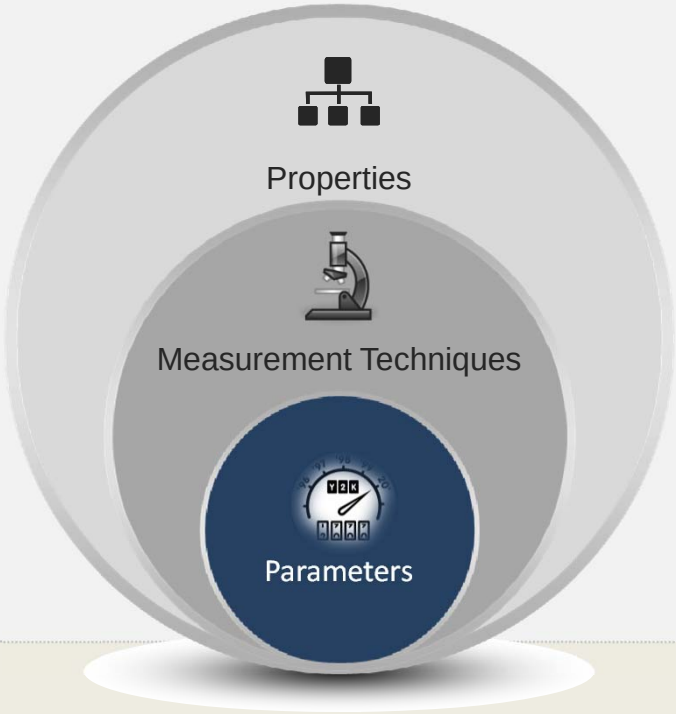
Trends in Data

PROPERTIES

Can be reported as various "measurement types".

Can be measured by different techniques and instruments.

Measurements are impacted by technique/instrument parameters.



- **20+ Measurement types** are curated in the Registry for Particle Size
- Measurements are **reported without technique**
- **Tracking the parameters** validates research data and enables analysis

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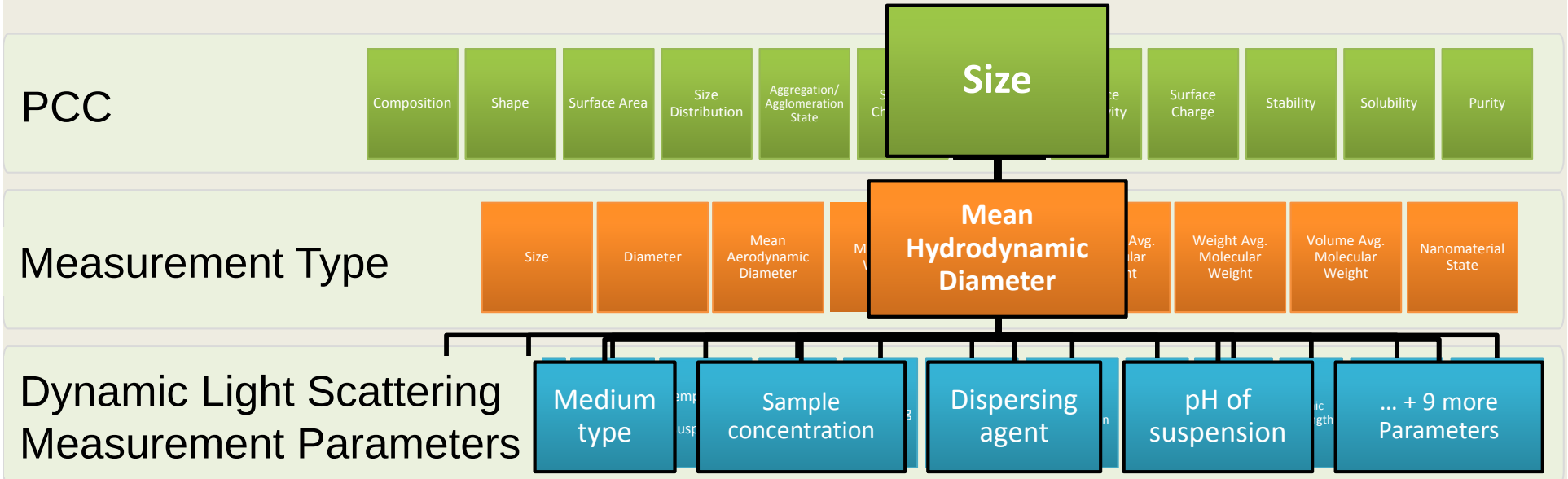
PROPERTY MEASUREMENTS

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



Measurement Best Practice Questions

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

Minimal Information = PCC data + Metadata

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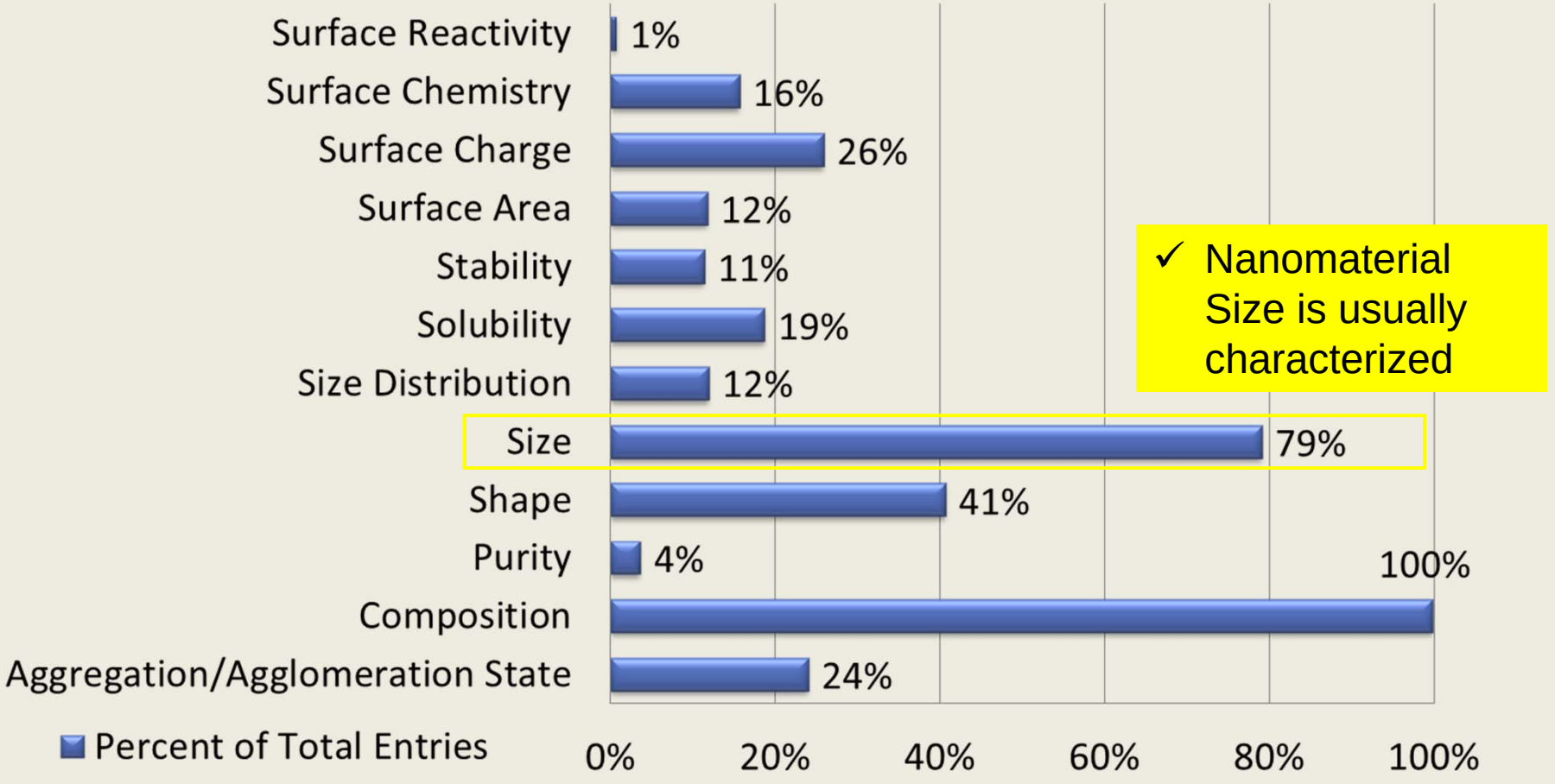
PROPERTY MEASUREMENTS

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

Current Characterization Profile for NR Records



✓ Nanomaterial Size is usually characterized

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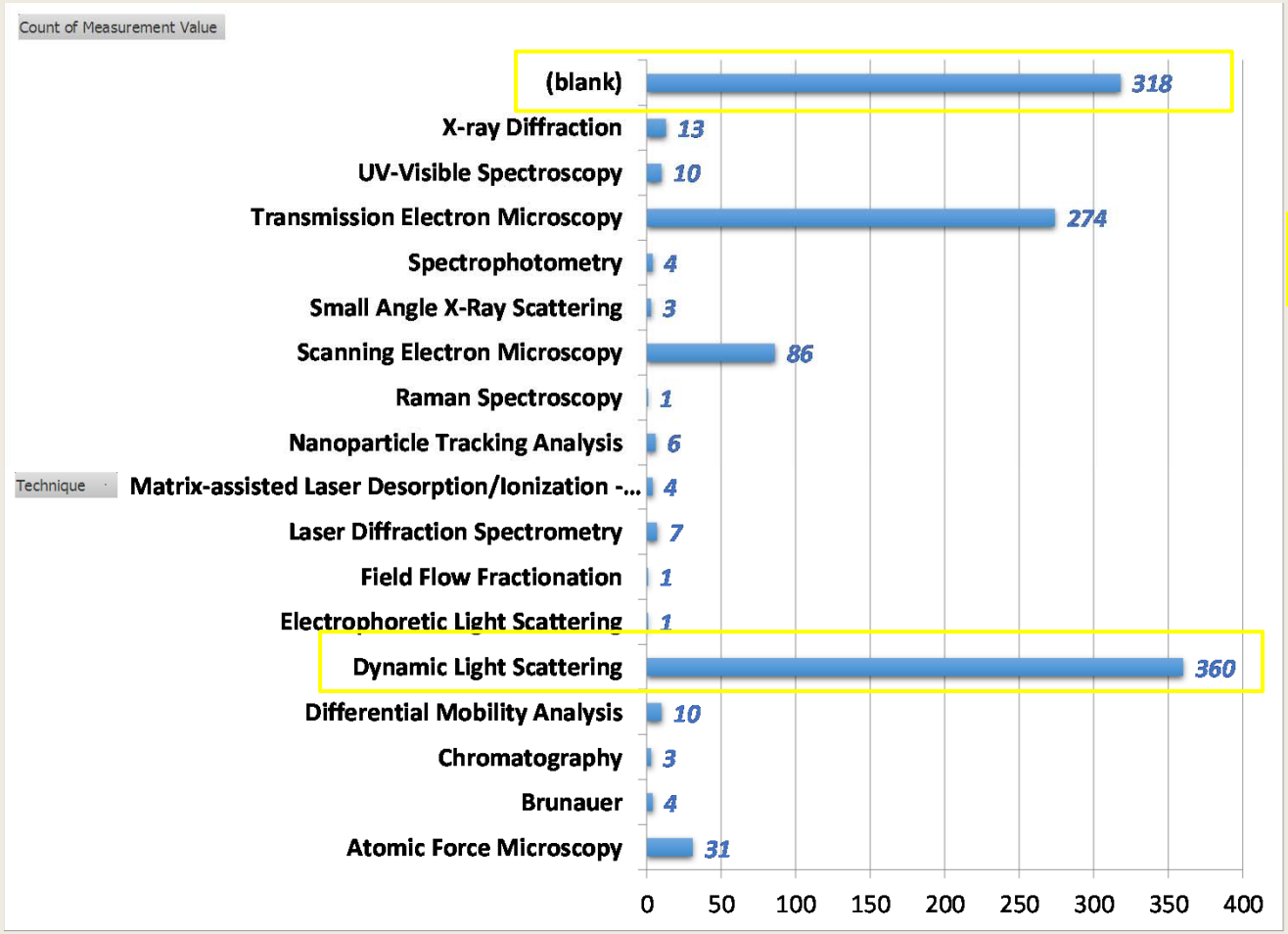
PROPERTY MEASUREMENTS

Particle Size Techniques



- Particle size is frequently reported **without technique** ↘

LOW DATA QUALITY RATING

- **Dynamic light scattering** is the most curated technique

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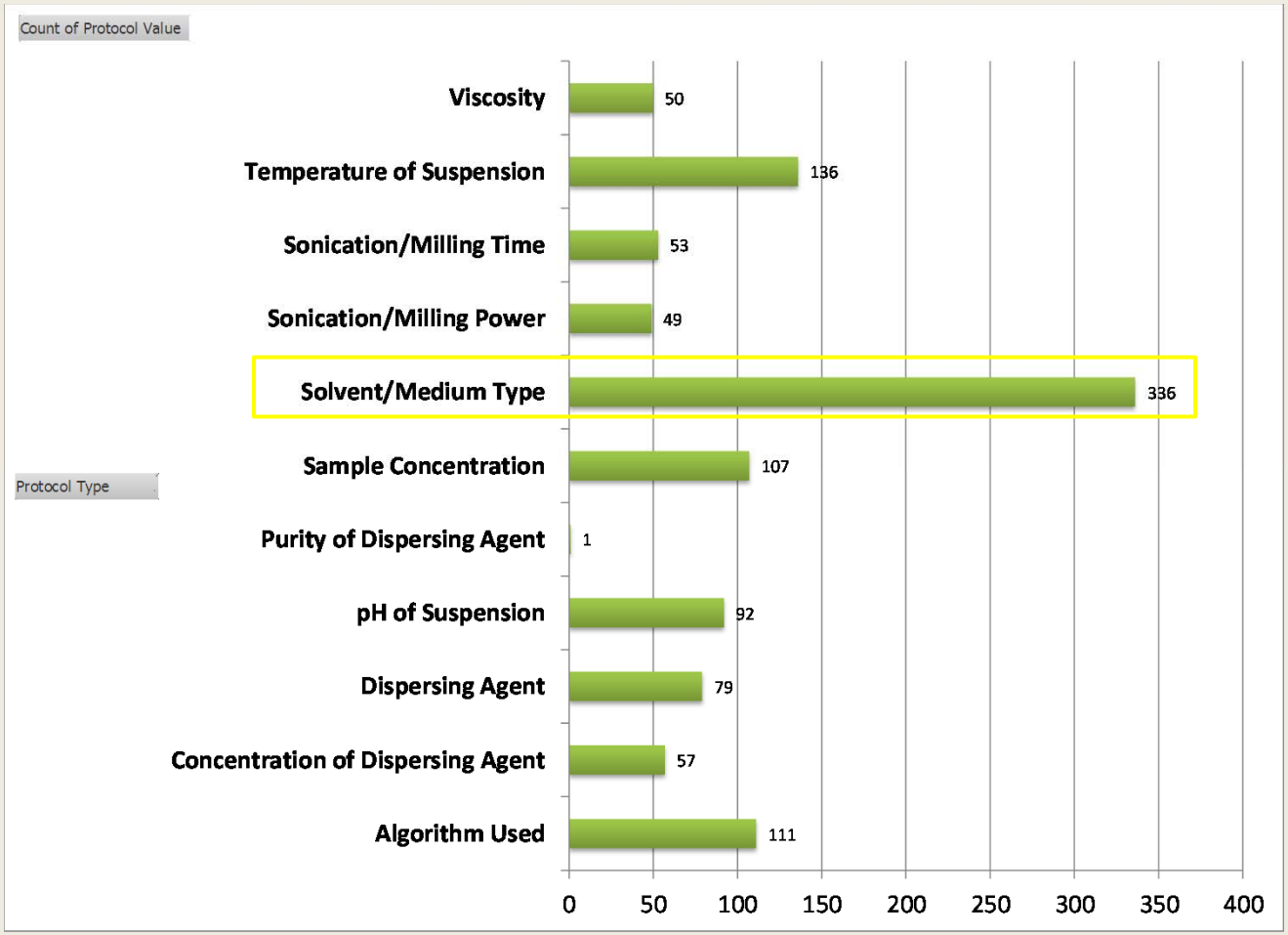
PROPERTY MEASUREMENTS

Parameters for Dynamic Light Scattering



- Other DLS parameters that are collected, but not shown here, include **scattering angle, wave length, and index of refraction**
- **Solvent Type** is the most frequently reported parameter for DLS

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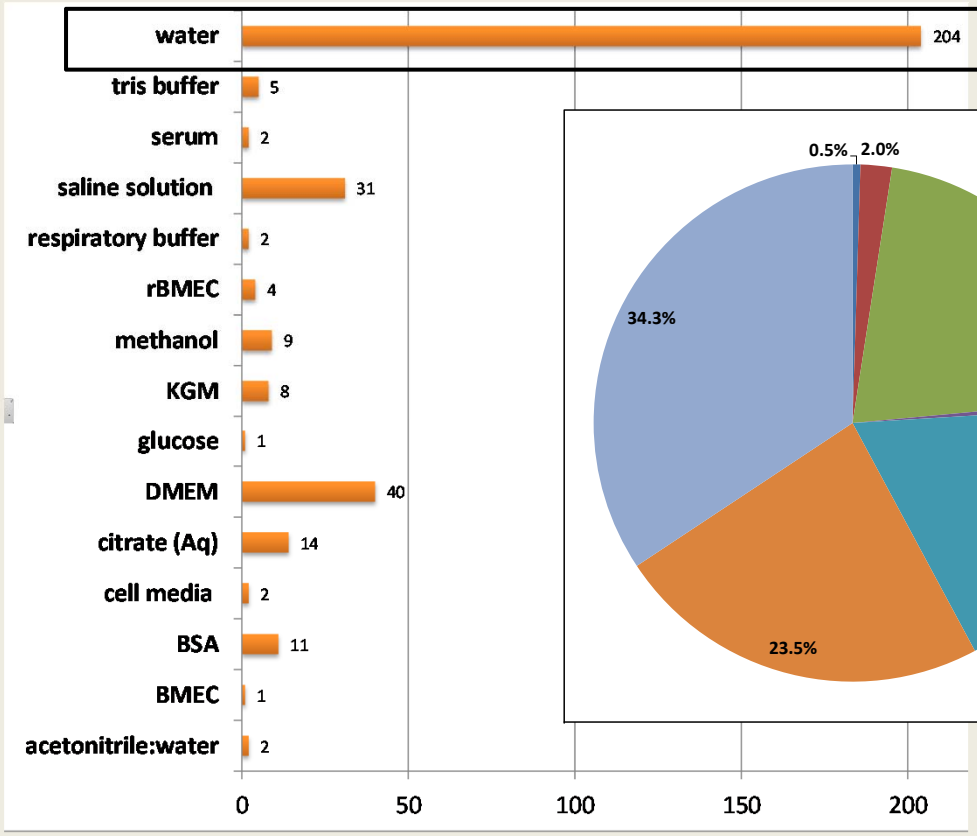
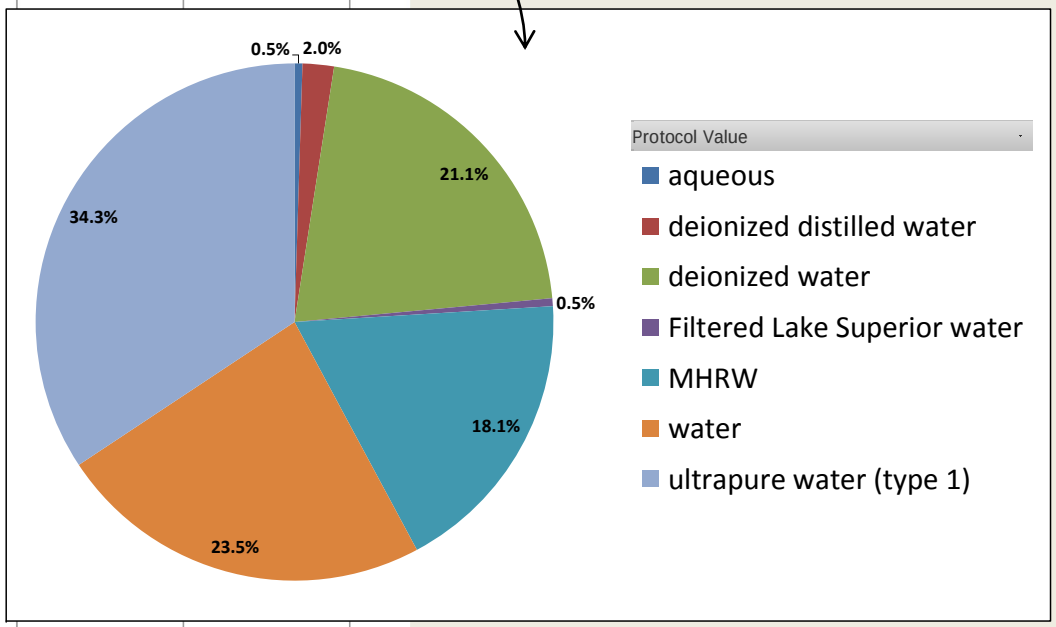
PROPERTY MEASUREMENTS

Parameters for Dynamic Light Scattering



Types of Water that are used



- **Water** is the most commonly used solvent in DLS

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DATA IN THE REGISTRY

Examples of curated records

	In the Registry	Study	Endpoints
Environmental/Ecological	NR1474, 1475	Natural Organic Matter Alters Biofilm Tolerance to Silver Nanoparticles and Dissolved Silver	Cytotoxicity
Medical Applications	NR951, NR966	Dendrimer-Functionalized Iron Oxide Nanoparticles for Specific Targeting and Imaging of Cancer Cells	Viability
Toxicology	NR1010, NR1011	Assessment of the toxicity of silver nanoparticles in vitro: A mitochondrial perspective	Pharmacodynamics
Biological Impact	NR1126, NR1129	Characterization of silver and effects on gene expression using an in-vitro intestinal epithelium co-culture model	Cytotoxicity; gene, protein and enzyme expression, cellular uptake, biotransformation….

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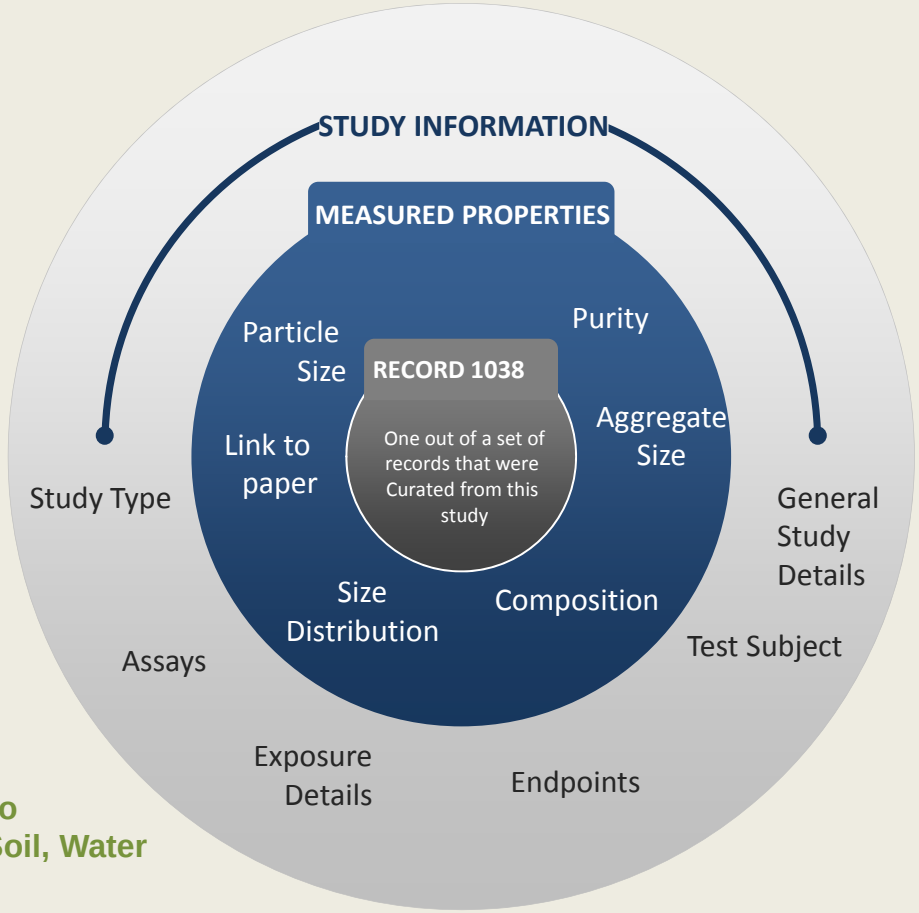
NANOMATERIAL STUDY

Linking Measurements and Impacts



Biological: In Vivo
Environmental: Soil, Water

STUDY TYPE

Long-Term Transformation and Fate of Manufactured Ag Nanoparticles in a Simulated Large Scale Freshwater Emergent Wetland

JOURNAL

Environmental Science & Technology

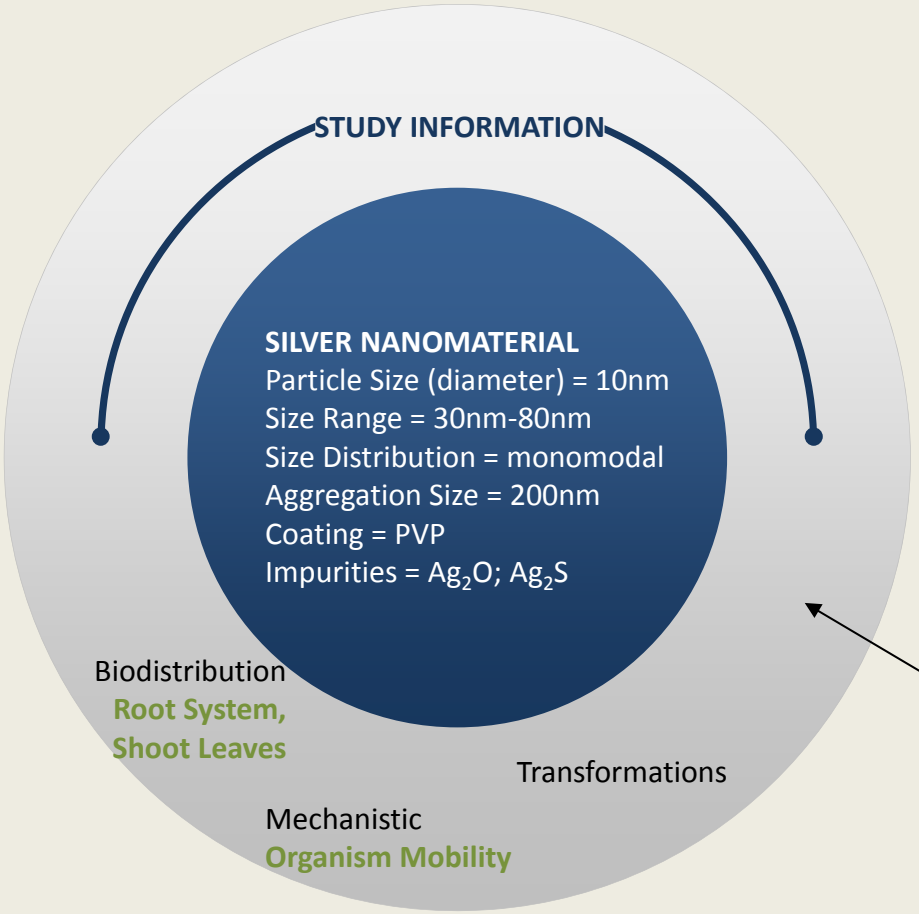
LABORATORY

Center for Environmental Implications about Nanotechnology (CEINT) at Duke University.

SILVER nanomaterial study (data record NR1038)

NANOMATERIAL STUDIES

Linking Measurements and Impacts



STUDY TYPE

- **Biological:** In Vivo
- **Environmental:** Soil, Water

STUDY CONDITIONS

- **Media:** Water, Soil
- **Media Properties 1:** Natural soil, 63% sand 10% clay 26% silt
- **Media Properties 2:** Natural water
- **Subjects:** Mosquitofish; Plants
- **Location:** Simulated Field
- **Exposure Summary:** Acute/Chronic; absorption/dermal inhalation/oral;
- 0.025 mg/mL; 18 months

ASSAYS

- **Laboratory:**
- graphite furnace AA; ICP-MS;
- Acid leaching; Cline method; XAS
- **Field:** YSI probe; sediment coring;
- dialysis

SILVER nanomaterial study (data record NR1038)

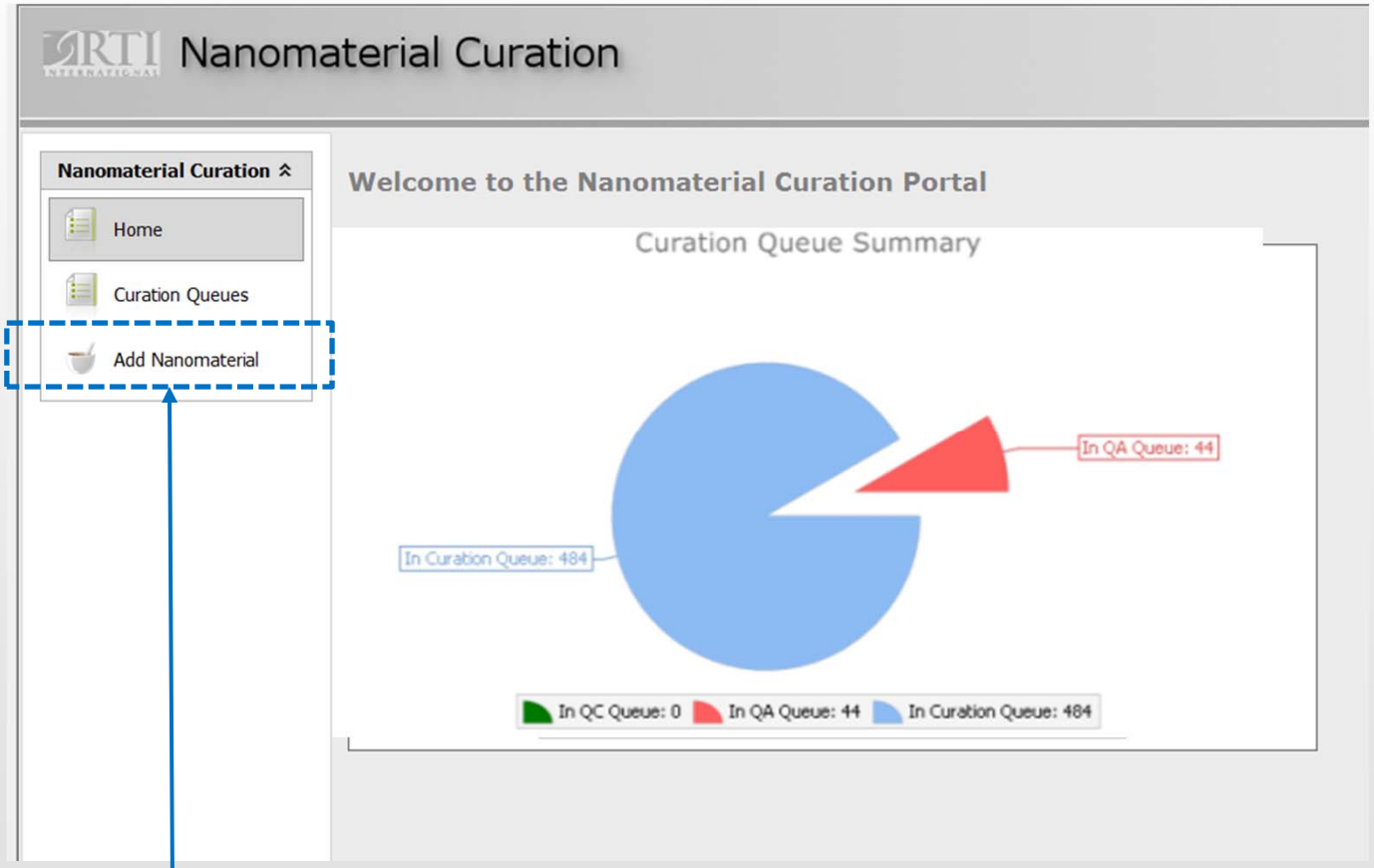
Accelerating the Curation Process

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

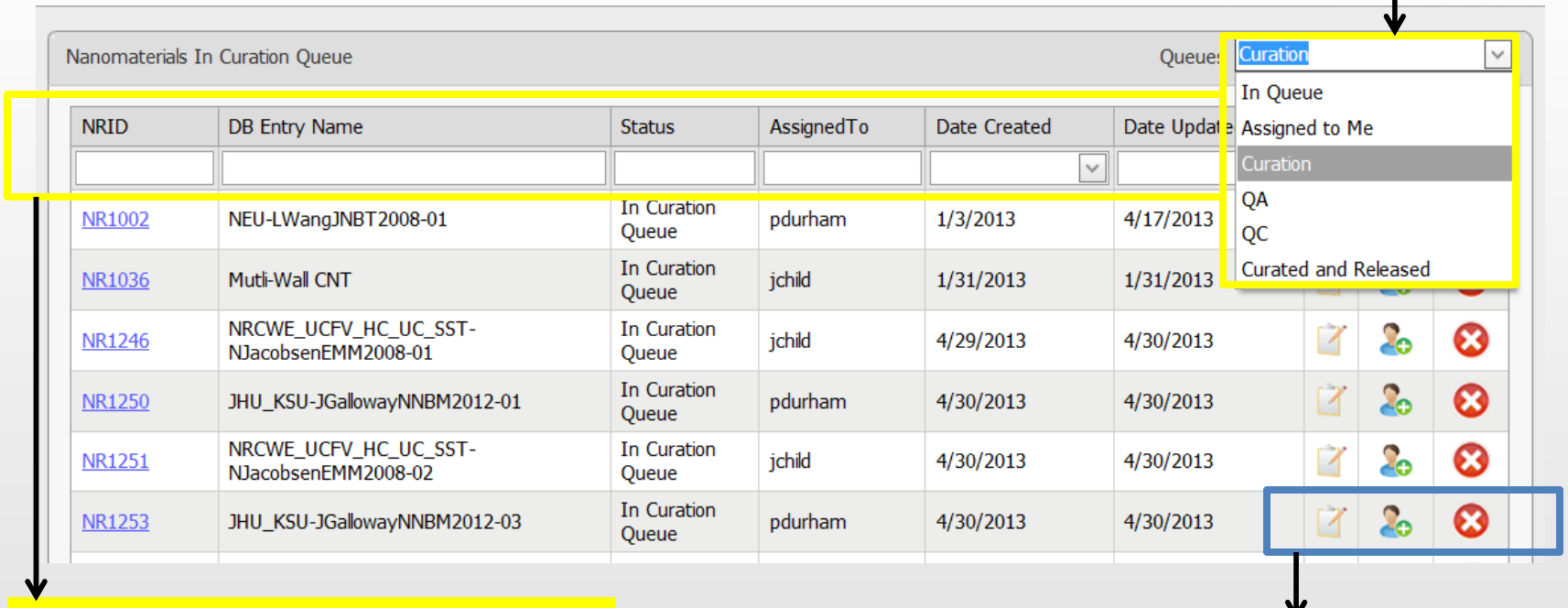
- ✓ check for transcription errors

QUALITY CONTROL

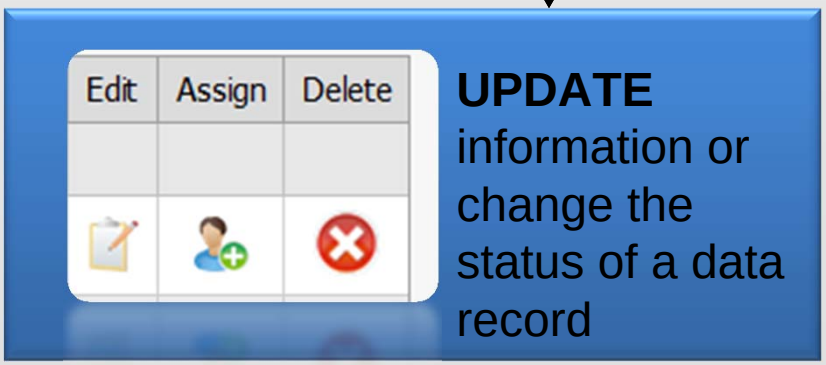
- ✓ correct any errors or inconsistencies in the scientific interpretation

Systematic Data Archiving:
DATA CURATION TOOL

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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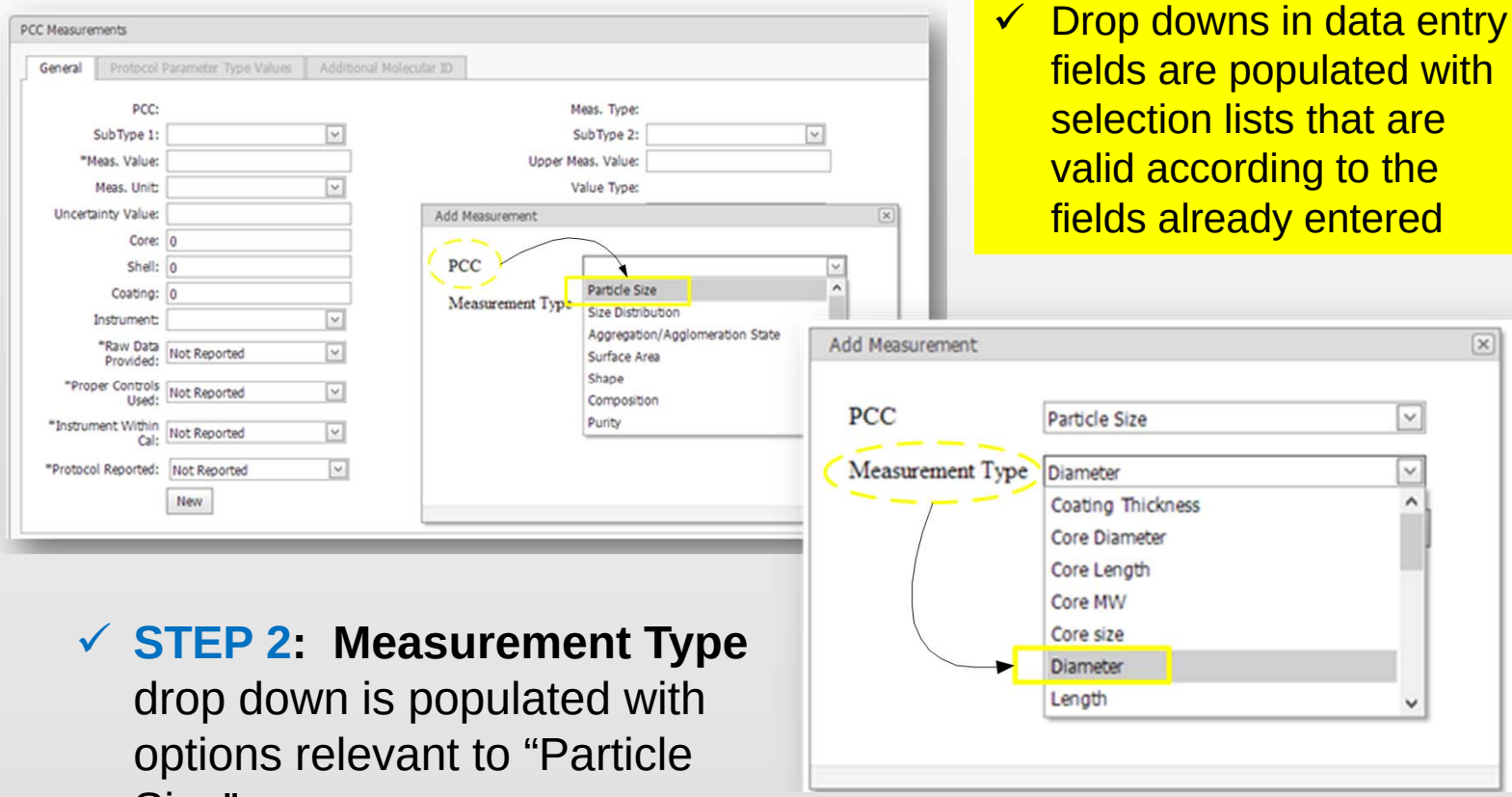
Systematic Data Archiving:
DATA CURATION TOOL

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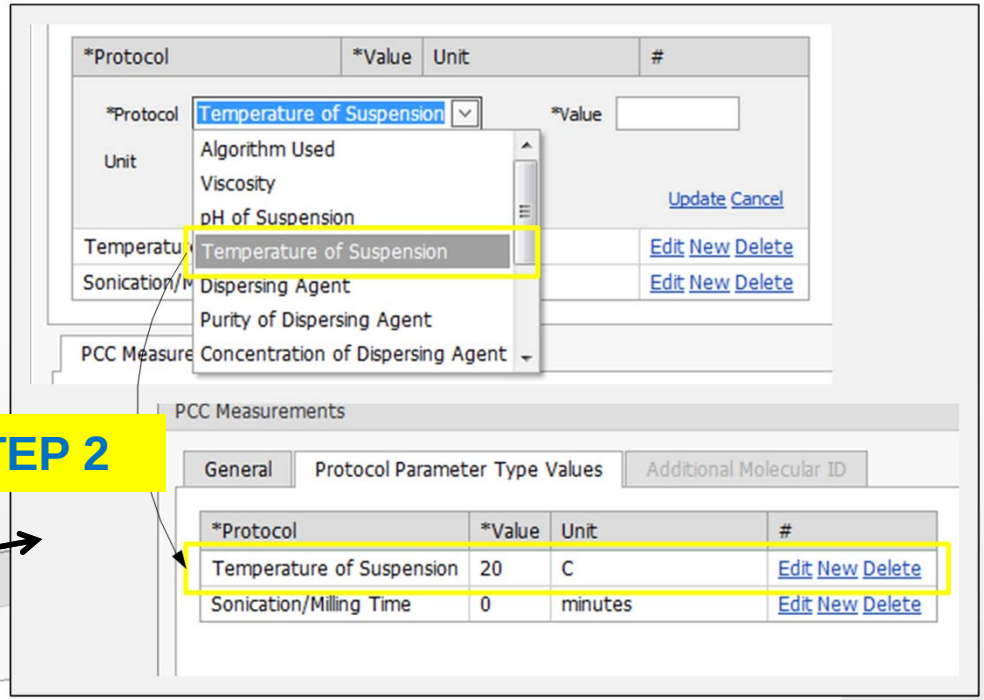
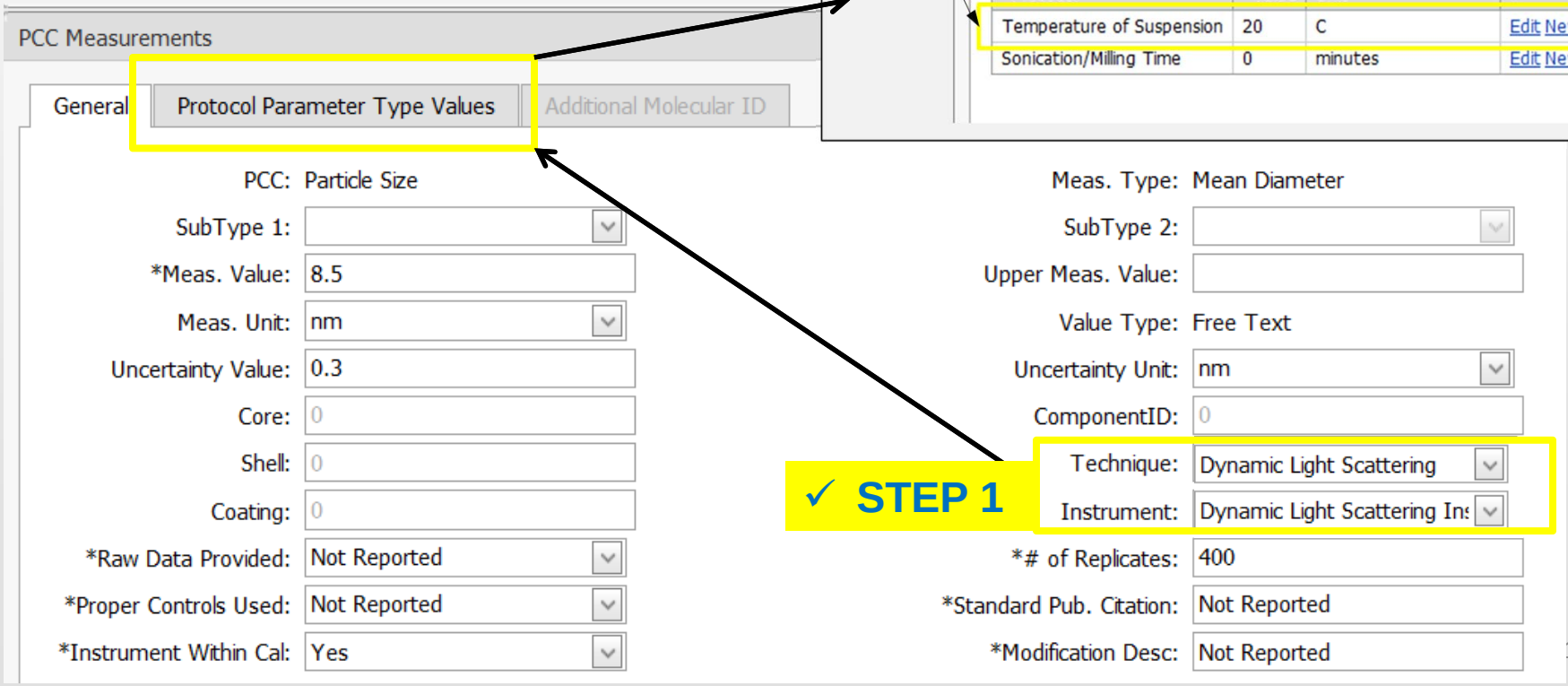
Systematic Data Archiving: *DATA CURATION TOOL*

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**

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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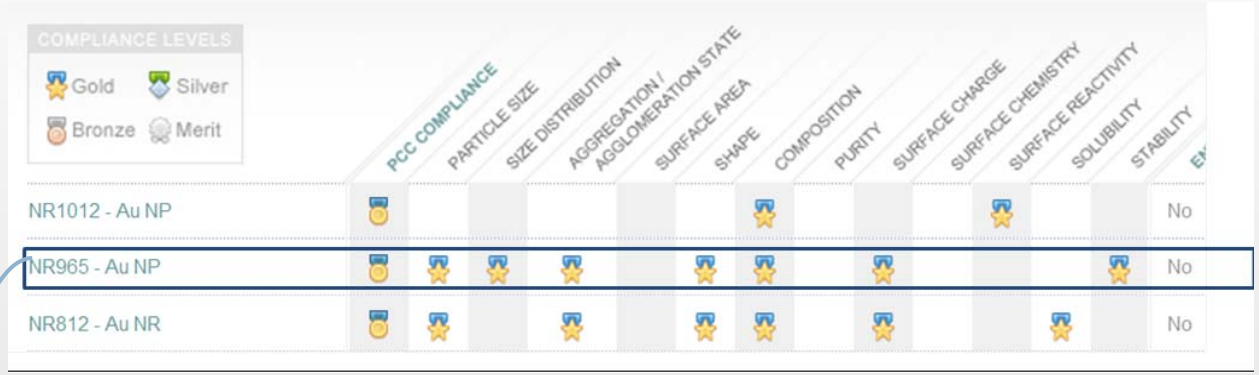
Evaluating the Information

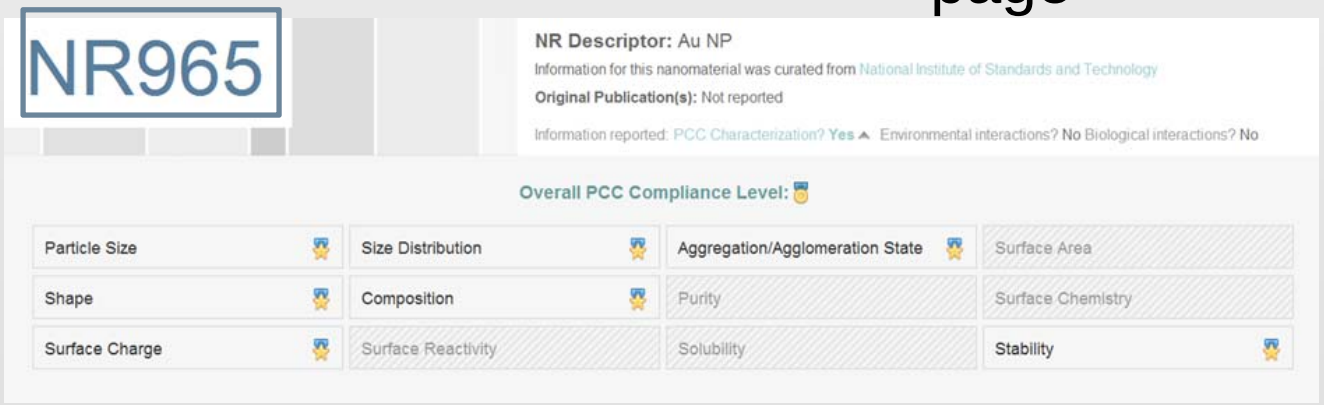
Compliance Level on the Registry

COMPLIANCE LEVEL for individual characterizations are displayed



✓ On the SEARCH RESULTS page

✓ On the DETAILS PAGE

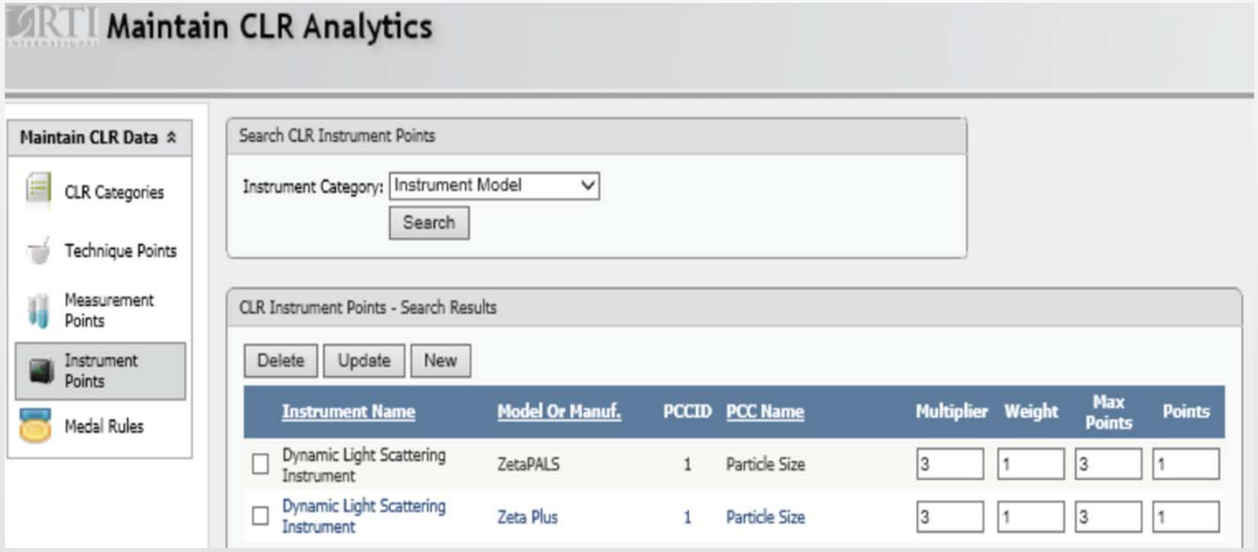


Evaluating the Information

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***.



algorithms can be tested on actual data sets

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THANK YOU!

www.nanomaterialregistry.org

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