

NANOMATERIALREGISTRY

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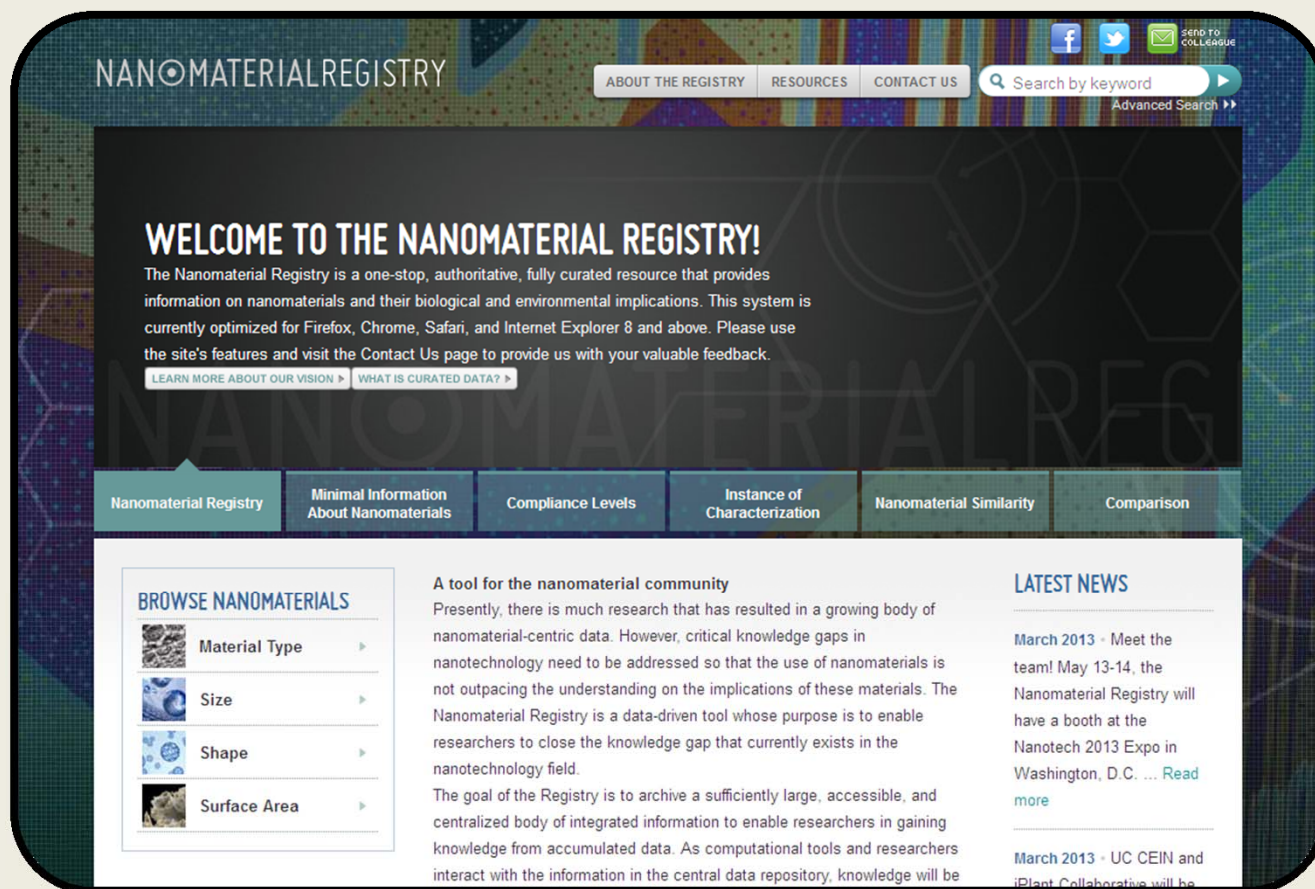
RTI International

June 7, 2013

NANOMATERIALREGISTRY



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



Web Address:

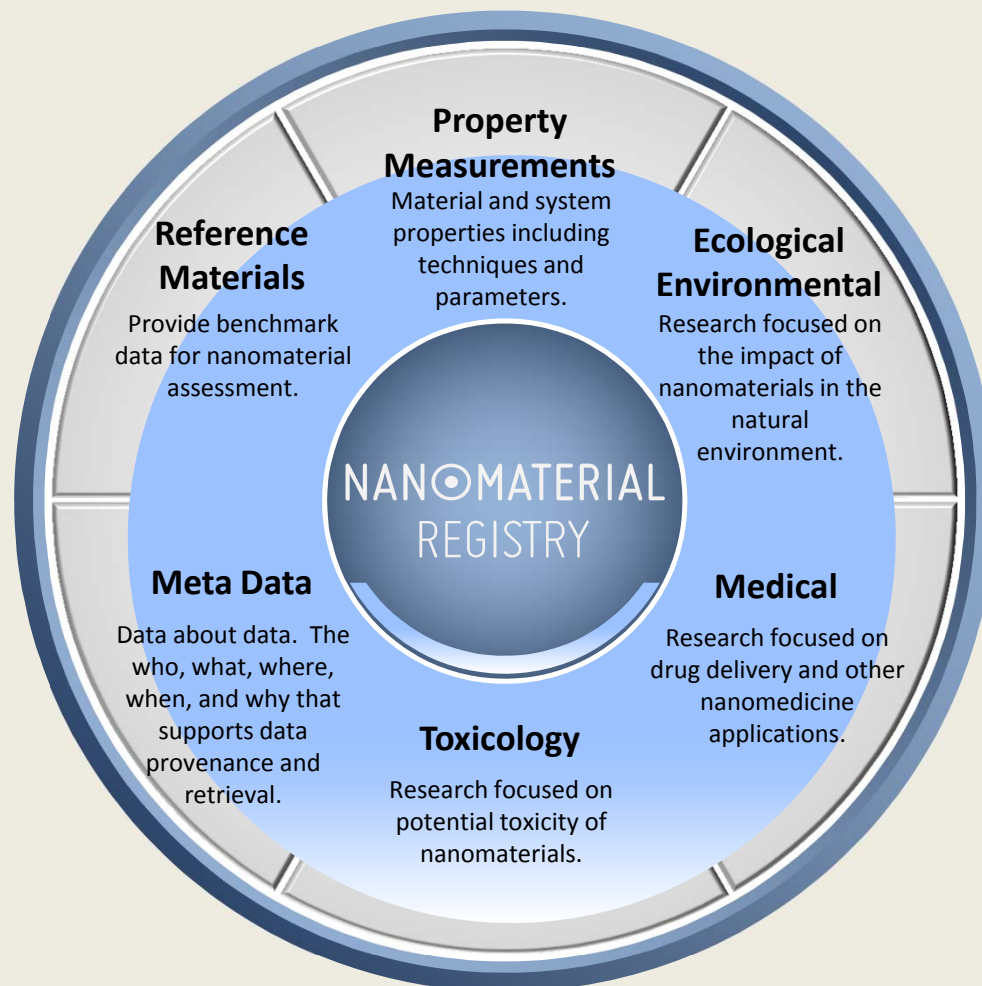
www.nanomaterialregistry.org

Funded by:



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

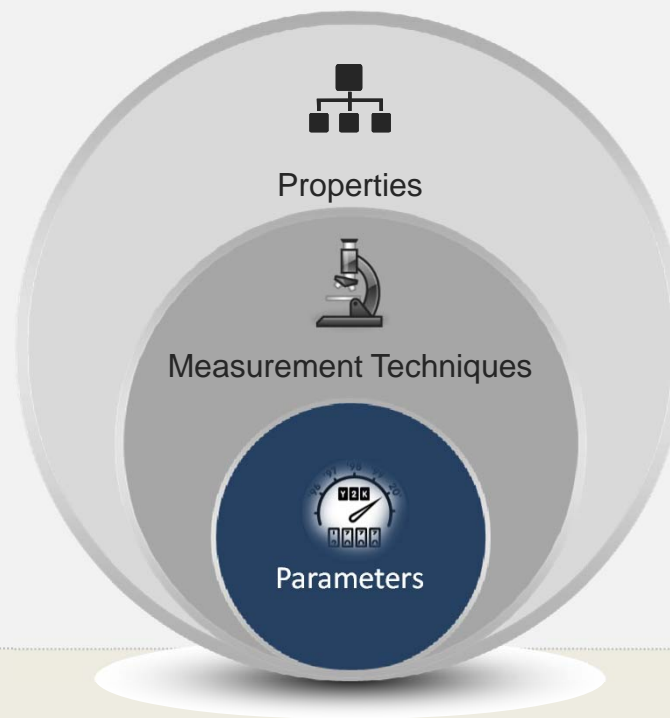
Trends in Data

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

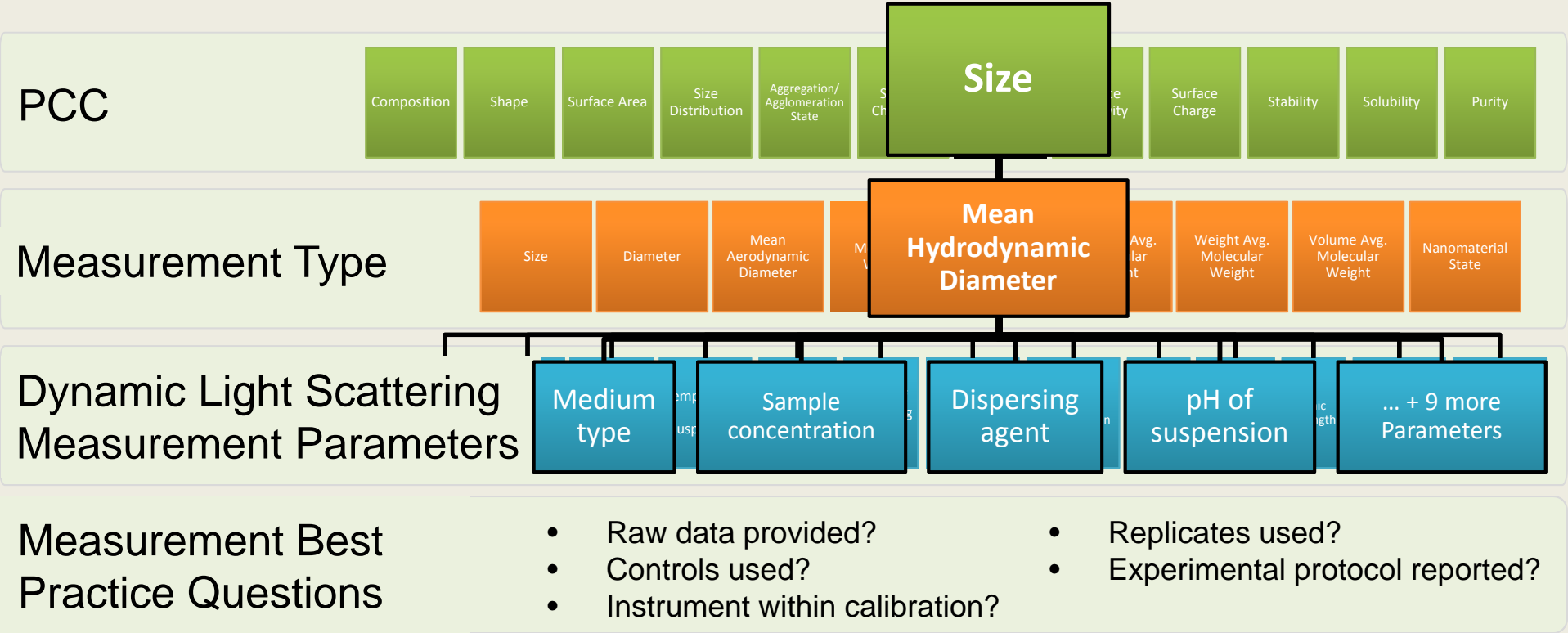
▶ Measurements are **reported without technique**

▶ **Tracking the parameters** validates research data and enables analysis

PROPERTY MEASUREMENTS



Minimal Information About Nanomaterials for Physico-Chemical Characteristics

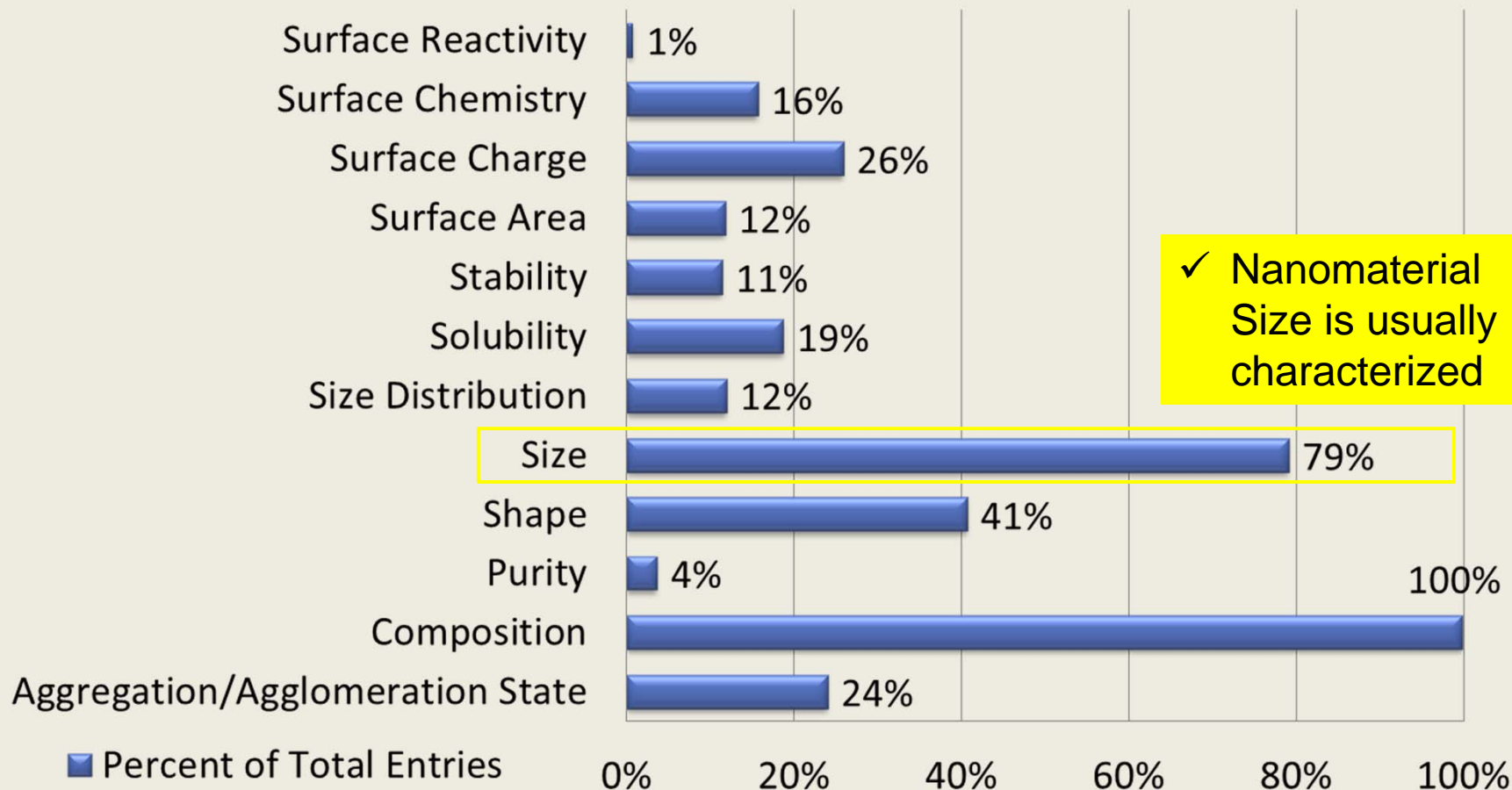


Minimal Information = PCC data + Metadata

PROPERTY MEASUREMENTS

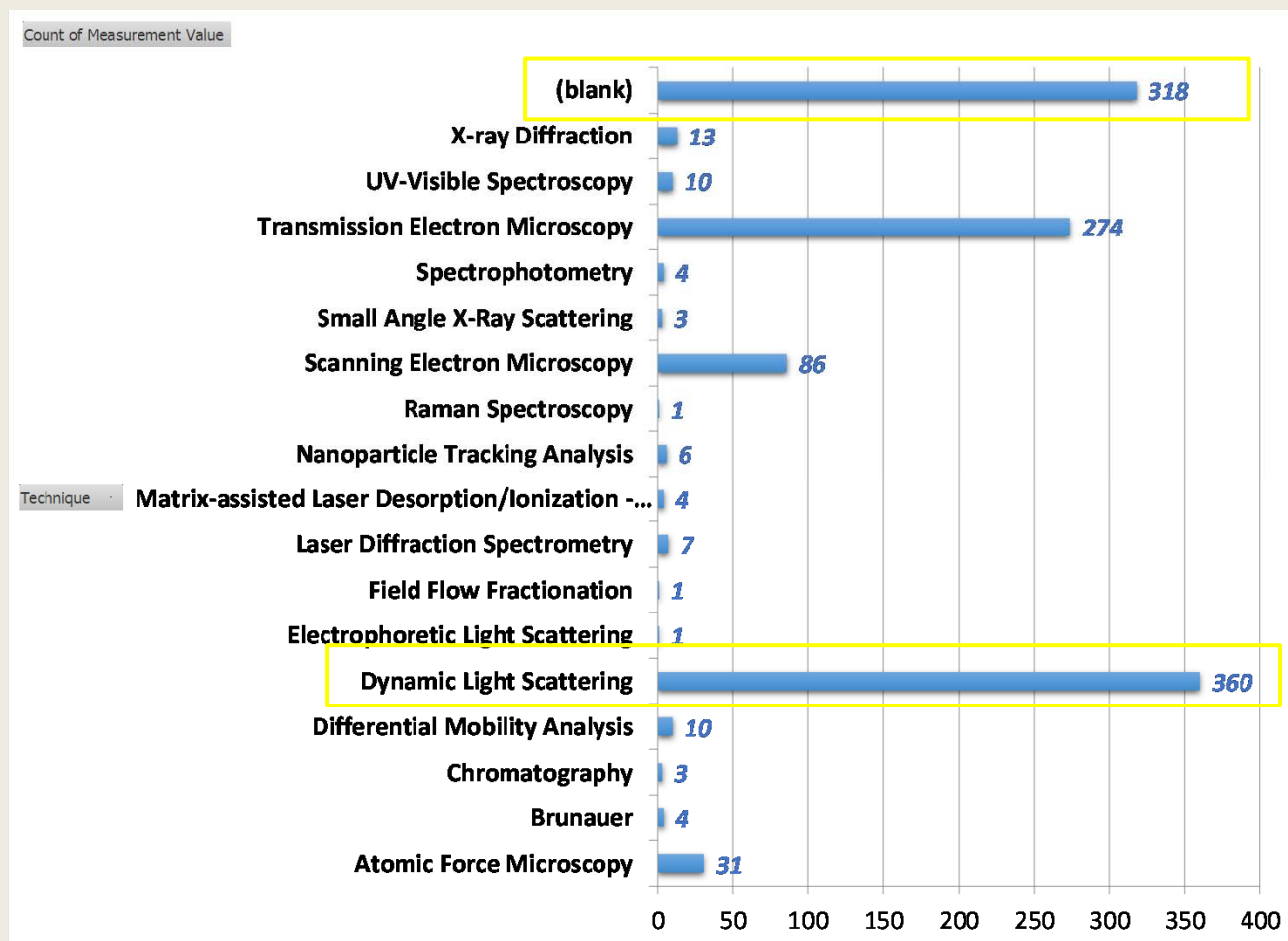
Minimal Information About Nanomaterials for Physico-Chemical Characteristics

Current Characterization Profile for NR Records



PROPERTY MEASUREMENTS

Particle Size Techniques



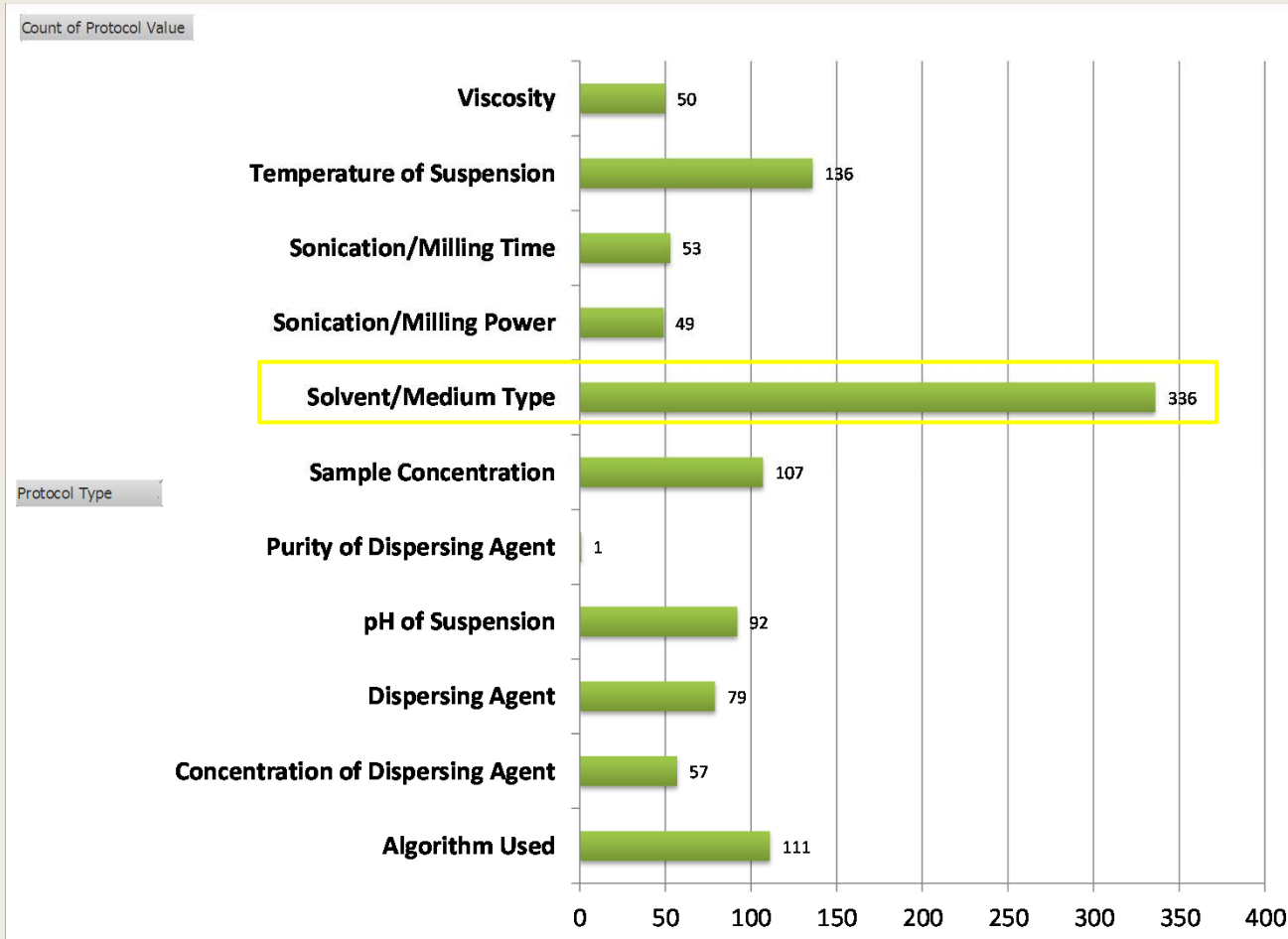
▶ Particle size is frequently reported **without technique**

⊕ **LOW DATA QUALITY RATING**

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

PROPERTY MEASUREMENTS

Parameters for Dynamic Light Scattering

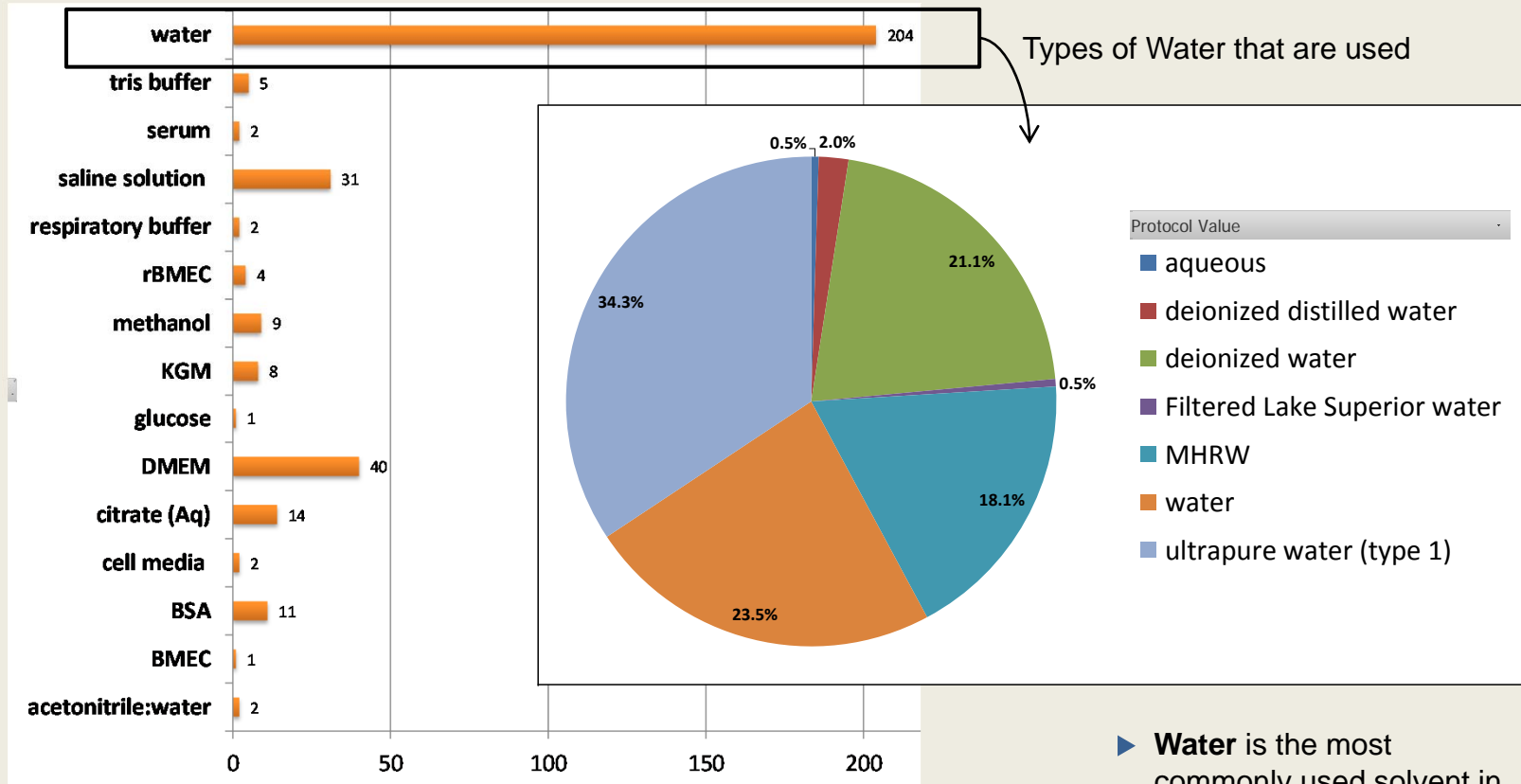


► Other DLS parameters that are collected, but not shown here, include **scattering angle, wave length, and index of refraction**

► **Solvent Type** is the most frequently reported parameter for DLS

PROPERTY MEASUREMENTS

Parameters for Dynamic Light Scattering



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

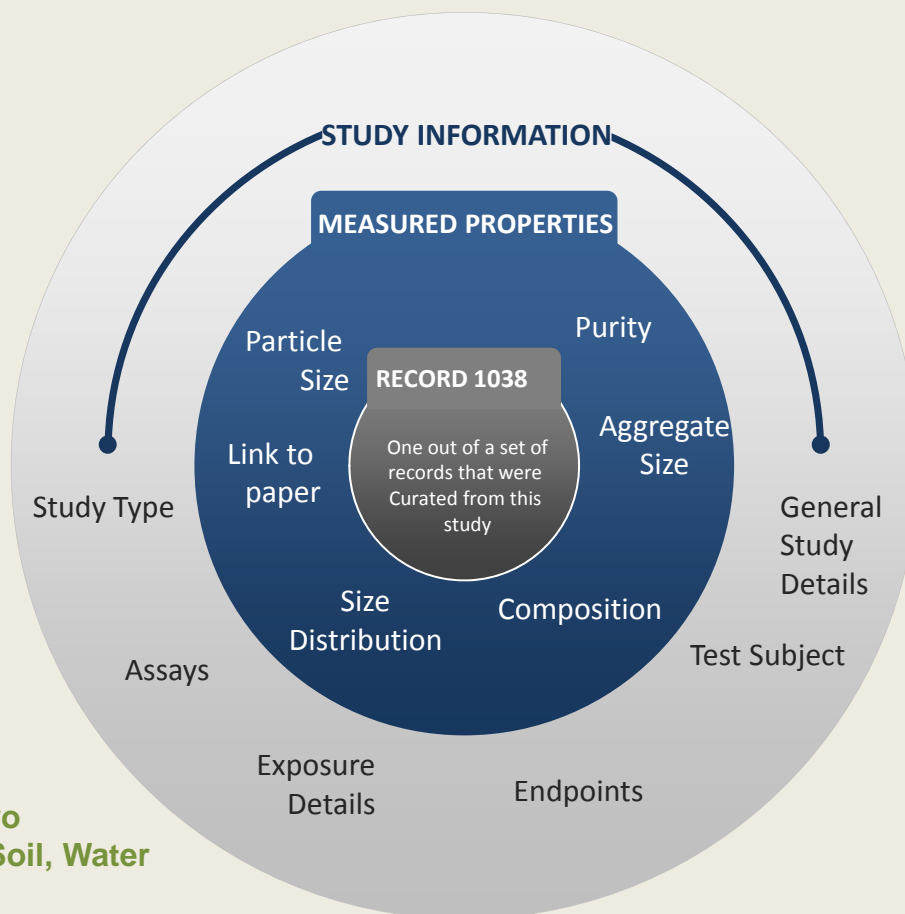
DATA IN THE REGISTRY

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....

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

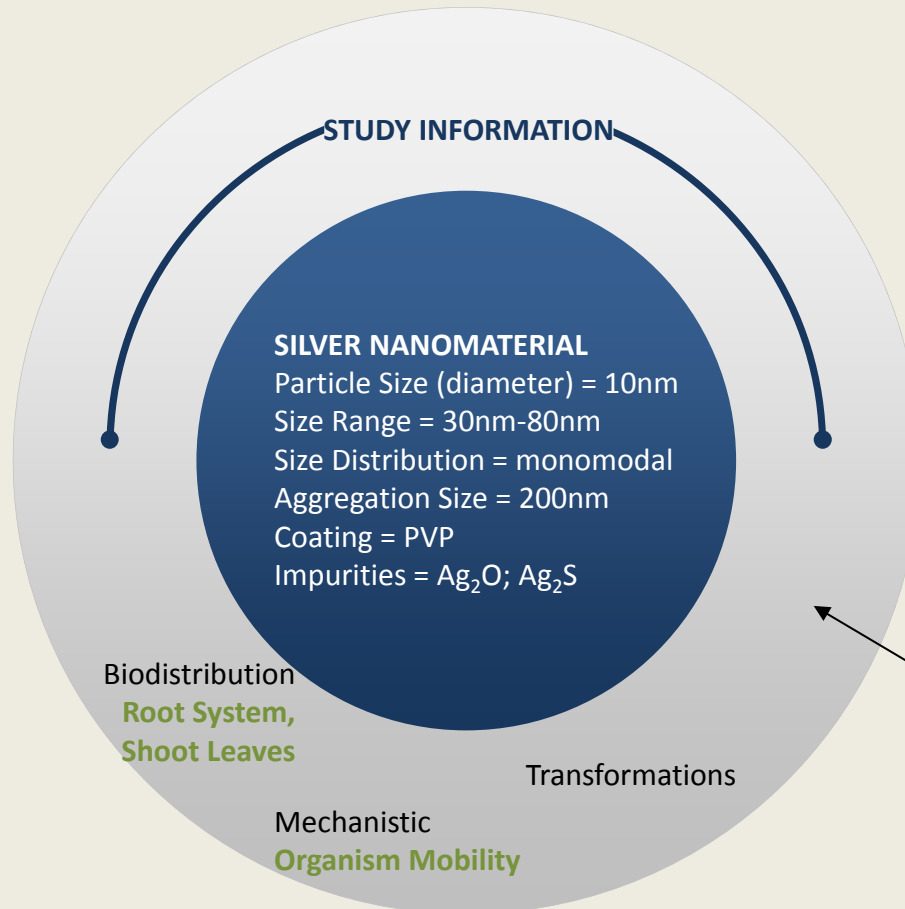
LABORATORY

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

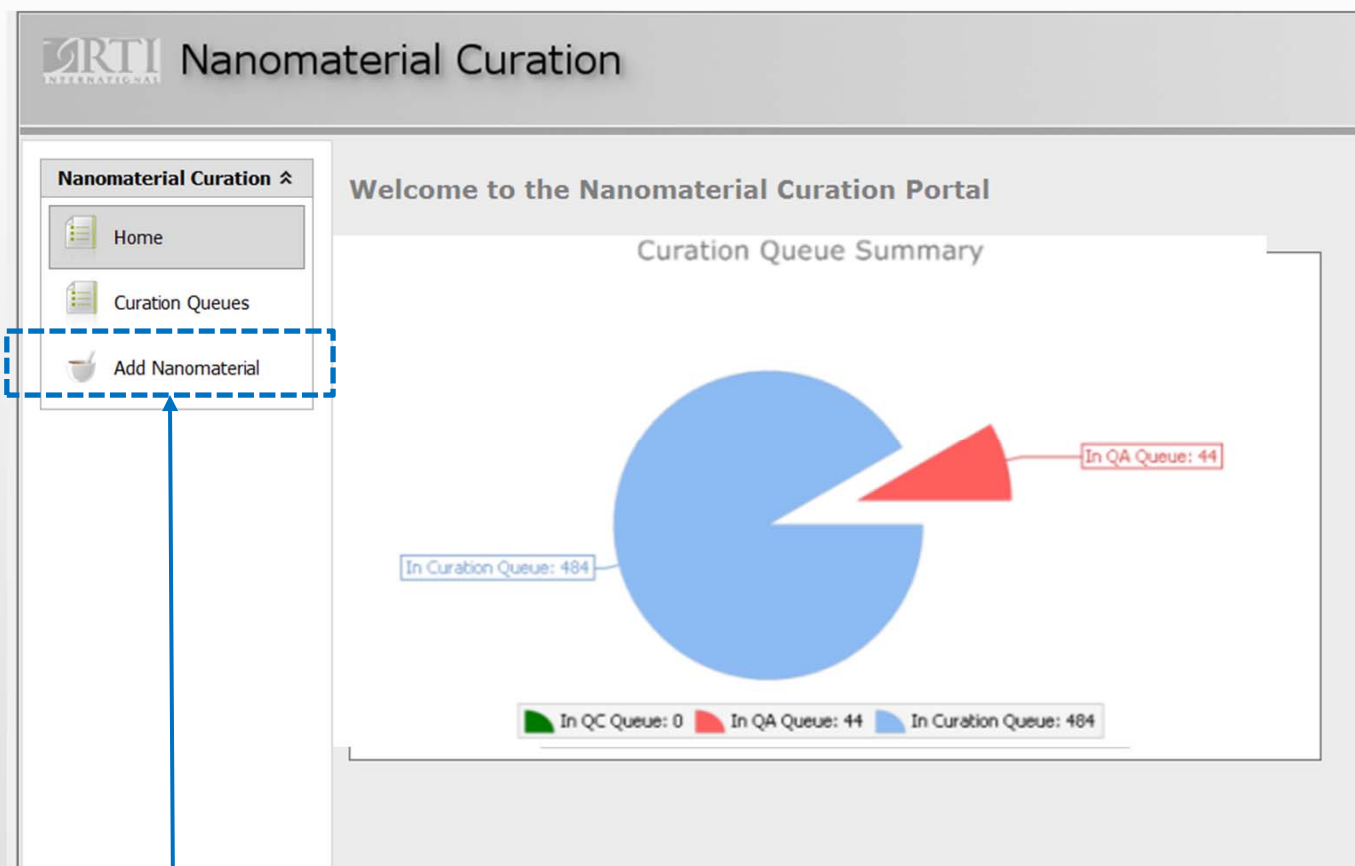
SILVER nanomaterial study (data record NR1038)

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**

Nanomaterials In Curation Queue

NRID	DB Entry Name	Status	AssignedTo	Date Created	Date Update			
NR1002	NEU-LWangJNBT2008-01	In Curation Queue	pdurham	1/3/2013	4/17/2013			
NR1036	Muti-Wall CNT	In Curation Queue	jchild	1/31/2013	1/31/2013			
NR1246	NRCWE_UCFV_HC_UC_SST-NJacobsenEMM2008-01	In Curation Queue	jchild	4/29/2013	4/30/2013			
NR1250	JHU_KSU-JGallowayNNBM2012-01	In Curation Queue	pdurham	4/30/2013	4/30/2013			
NR1251	NRCWE_UCFV_HC_UC_SST-NJacobsenEMM2008-02	In Curation Queue	jchild	4/30/2013	4/30/2013			
NR1253	JHU_KSU-JGallowayNNBM2012-03	In Curation Queue	pdurham	4/30/2013	4/30/2013			

Queue: Curation

- In Queue
- Assigned to Me
- Curation
- QA
- QC
- Curated and Released

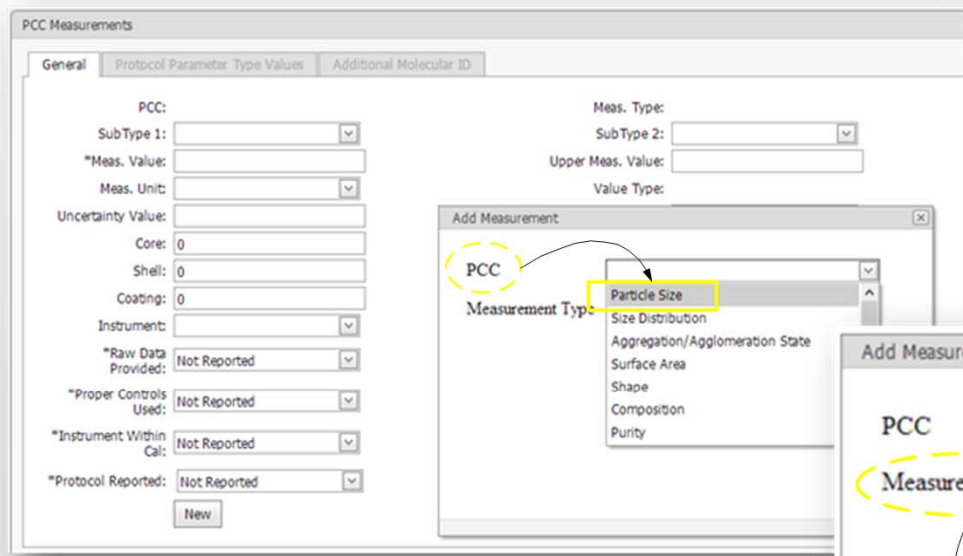
SEARCH and **SORT** options for data in queues

Edit	Assign	Delete

UPDATE information or change the status of a data record

Systematic Data Archiving: *DATA CURATION TOOL*

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

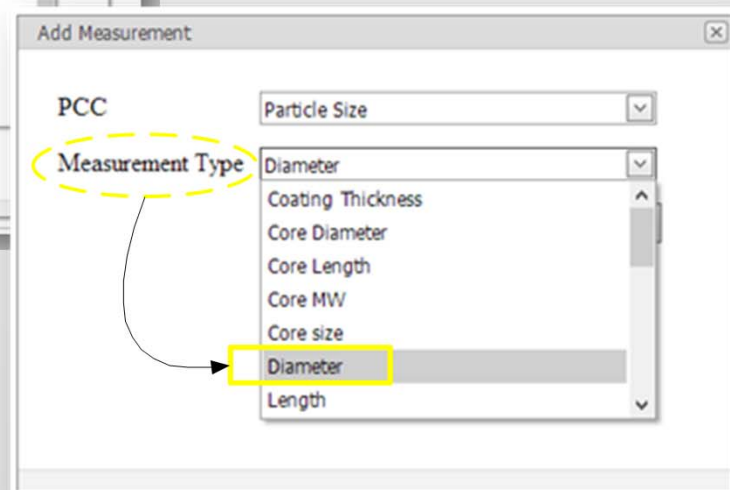


The screenshot shows the 'PCC Measurements' form with the 'Add Measurement' dialog box open. The 'PCC' dropdown in the dialog is highlighted with a yellow circle, and the 'Particle Size' option is highlighted with a yellow box. The main form has fields for PCC, SubType 1, Meas. Value, Meas. Unit, Uncertainty Value, Core, Shell, Coating, Instrument, Raw Data Provided, Proper Controls Used, Instrument Within Cal, and Protocol Reported.

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”



The screenshot shows the 'Add Measurement' dialog box with the 'Measurement Type' dropdown menu open. The 'Measurement Type' label is circled in yellow, and the 'Diameter' option is highlighted with a yellow box. The dropdown menu lists options: Diameter, Coating Thickness, Core Diameter, Core Length, Core MW, Core size, Diameter, and Length.

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”

The screenshot displays the 'PCC Measurements' interface. The 'Protocol Parameter Type Values' tab is selected and highlighted with a yellow box. A dropdown menu is open for the 'Temperature of Suspension' protocol, showing a list of options including 'Algorithm Used', 'Viscosity', 'pH of Suspension', 'Temperature of Suspension', 'Dispersing Agent', 'Purity of Dispersing Agent', and 'Concentration of Dispersing Agent'. The 'Temperature of Suspension' option is highlighted with a yellow box. Below the dropdown, a table lists the selected protocol parameters:

*Protocol	*Value	Unit	#
Temperature of Suspension	20	C	Edit New Delete
Sonication/Milling Time	0	minutes	Edit New Delete

Below the table, the 'General' tab is selected, showing the following fields:

PCC: Particle Size

SubType 1:

*Meas. Value: 8.5

Meas. Unit: nm

Uncertainty Value: 0.3

Core: 0

Shell: 0

Coating: 0

*Raw Data Provided: Not Reported

*Proper Controls Used: Not Reported

*Instrument Within Cal: Yes

Meas. Type: Mean Diameter

SubType 2:

Upper Meas. Value:

Value Type: Free Text

Uncertainty Unit: nm

ComponentID: 0

Technique: Dynamic Light Scattering

Instrument: Dynamic Light Scattering In:

*# of Replicates: 400

*Standard Pub. Citation: Not Reported

*Modification Desc: Not Reported





✓ **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)

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

Evaluating the Information

Compliance Level

	 MERIT	 BRONZE	 SILVER	 GOLD
Particle Size 37.5 nm				
Reported as Mean Hydrodynamic Diameter				
Technique Dynamic Light Scattering				
Instrument Malvern Zeta Sizer Nano ZS				
Measurement parameters 11 out of 12 reported				
Protocol ASTM E2490-09				

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

Evaluating the Information

Compliance Level on the Registry

COMPLIANCE LEVEL for individual characterizations are displayed

	PCC COMPLIANCE	PARTICLE SIZE	SIZE DISTRIBUTION	AGGREGATION/ AGGLOMERATION STATE	SURFACE AREA	SHAPE	COMPOSITION	PURITY	SURFACE CHARGE	SURFACE CHEMISTRY	SOLUBILITY	STABILITY	EX
NR1012 - Au NP	🏆								🏆				No
NR965 - Au NP	🏆	🏆	🏆	🏆	🏆	🏆	🏆	🏆	🏆	🏆	🏆	🏆	No
NR812 - Au NR	🏆	🏆		🏆		🏆	🏆	🏆		🏆			No

✓ On the SEARCH RESULTS page

✓ On the DETAILS PAGE

NR965

NR Descriptor: Au NP
 Information for this nanomaterial was curated from [National Institute of Standards and Technology](#)
 Original Publication(s): Not reported
 Information reported: PCC Characterization? Yes ▲ Environmental interactions? No Biological interactions? No

Overall PCC Compliance Level: 🏆

Particle Size	🏆	Size Distribution	🏆	Aggregation/Agglomeration State	🏆	Surface Area	
Shape	🏆	Composition	🏆	Purity		Surface Chemistry	
Surface Charge	🏆	Surface Reactivity		Solubility		Stability	🏆

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.**

The screenshot shows the 'Maintain CLR Analytics' interface. On the left is a sidebar with navigation options: 'Maintain CLR Data', 'CLR Categories', 'Technique Points', 'Measurement Points', 'Instrument Points', and 'Medal Rules'. The main area contains a search box for 'Search CLR Instrument Points' with a dropdown for 'Instrument Category' set to 'Instrument Model' and a 'Search' button. Below the search box is a table titled 'CLR Instrument Points - Search Results' with buttons for 'Delete', 'Update', and 'New'. The table has columns for 'Instrument Name', 'Model Or Manuf.', 'PCCID', 'PCC Name', 'Multiplier', 'Weight', 'Max Points', and 'Points'. Two rows are visible, both for 'Dynamic Light Scattering Instrument'.

Instrument Name	Model Or Manuf.	PCCID	PCC Name	Multiplier	Weight	Max Points	Points
<input type="checkbox"/> Dynamic Light Scattering Instrument	ZetaPALS	1	Particle Size	<input type="text" value="3"/>	<input type="text" value="1"/>	<input type="text" value="3"/>	<input type="text" value="1"/>
<input type="checkbox"/> Dynamic Light Scattering Instrument	Zeta Plus	1	Particle Size	<input type="text" value="3"/>	<input type="text" value="1"/>	<input type="text" value="3"/>	<input type="text" value="1"/>

algorithms can be tested on actual data sets

NANOMATERIALREGISTRY

THANK YOU!

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