NANOMATERIALREGISTRY

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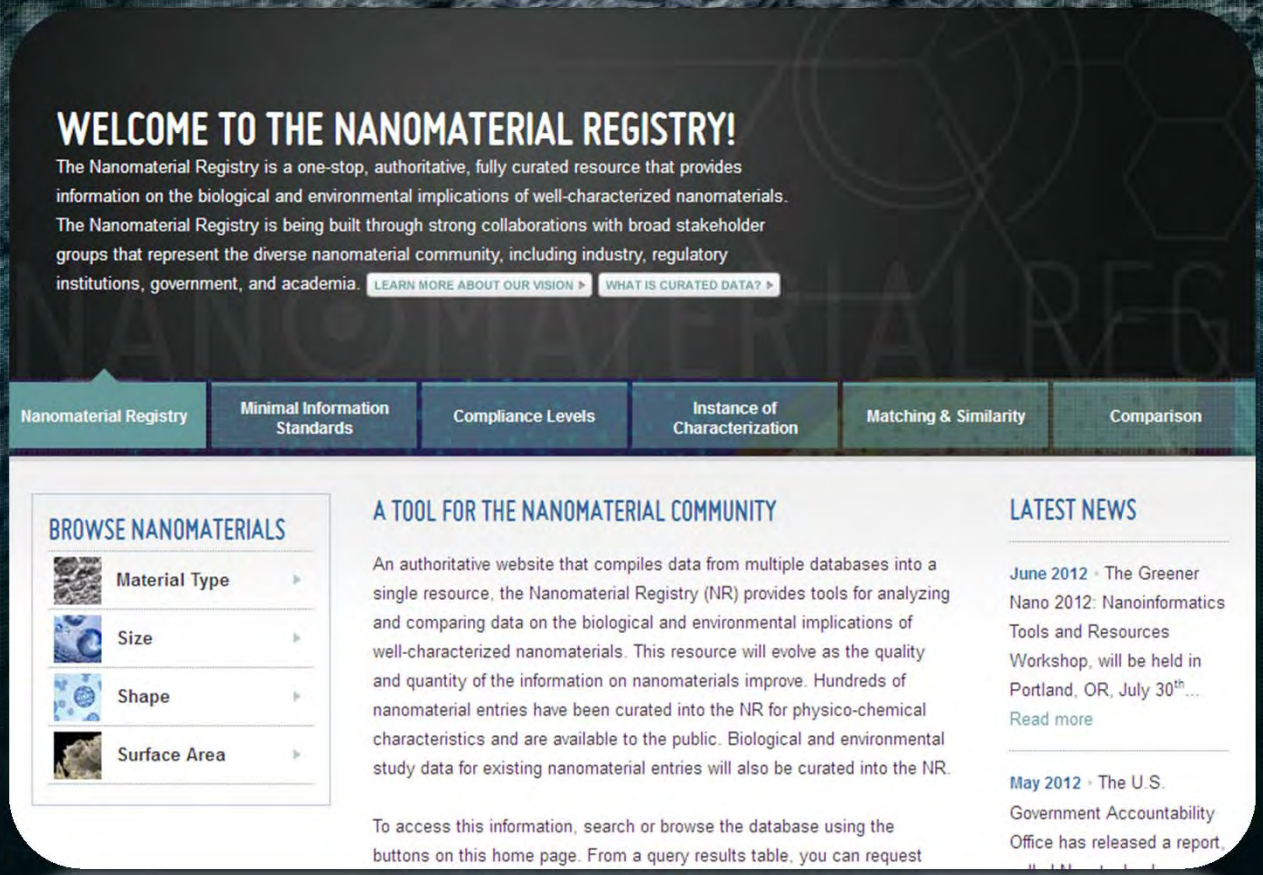
RTI International

NANOMATERIALREGISTRY

A tool for the storing, sharing, and analysis of data from the nanomaterial community



Funded by:

NIEHS

NIBIB

National Cancer Institute

Web Address:

www.nanomaterialregistry.org

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Registry as a Tool

End Users:

- Nanomaterial researchers who generate or analyze data
- SME's who make research decisions/guide research
- Groups that want to share data globally

- DATA ACCESS – What research is being done, finding data with specific PCC or endpoints
- DATA ANALYSIS – extracting data sets across resources, modeling
- REVIEWING DATA STANDARDS – What are protocols and best practices, what should be reported
- DIRECTING RESEARCH – Where are gaps in existing research, what are the data rich areas

NANOMATERIALREGISTRY

Authoritative Data

- Organize and archive data using systematic curation tools and methods
  - Controlled vocabulary
  - Using a minimal information about nanomaterials (MIAN)
  - Data model
  - Curation tool
- To impart the highest degree of authoritativeness to the data
  - QA & QC reviewers
  - Product Life
- Curation = Data validation and quality

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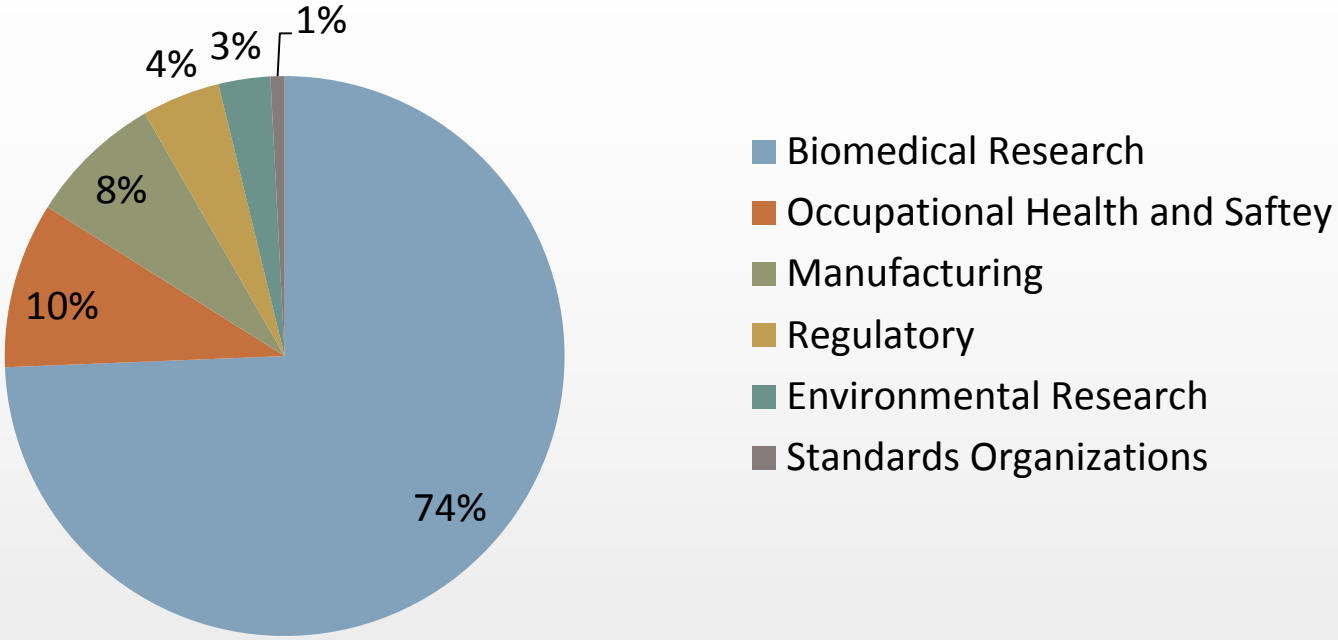
Data Records



Stakeholder Group	Data Records
Biomedical Research	1018
Occupational Health and Saftey	131
Manufacturing	106
Regulatory	62
Environmental Research	41
Standards Organizations	11

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Minimal Information about Nanomaterials

For Physico-Chemical Characteristics

MIAN PCC

MIAN for Physico-Chemical Characteristics

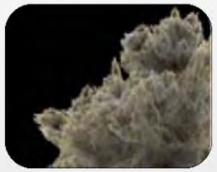
Composition

Size

Size Distribution

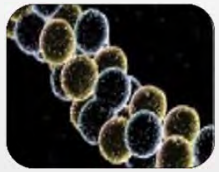
Shape

Aggregation/ Agglomeration State



Surface Area

Surface Charge



Surface Chemistry

Surface Reactivity

Purity

Solubility

Stability

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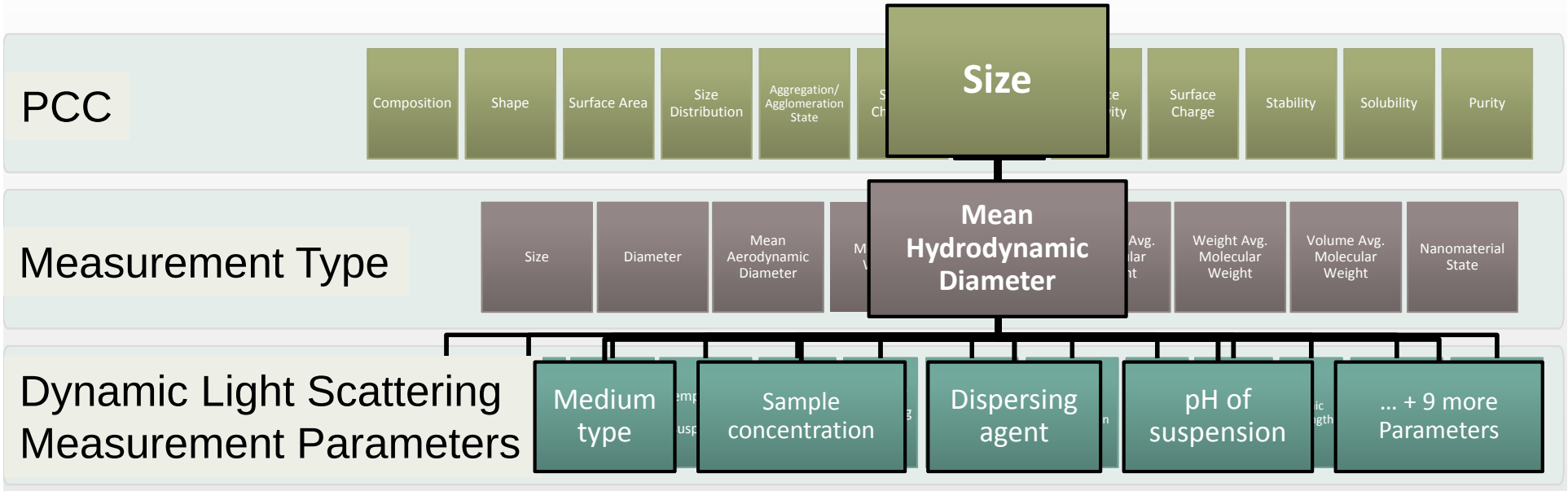
Metadata in the MIAN



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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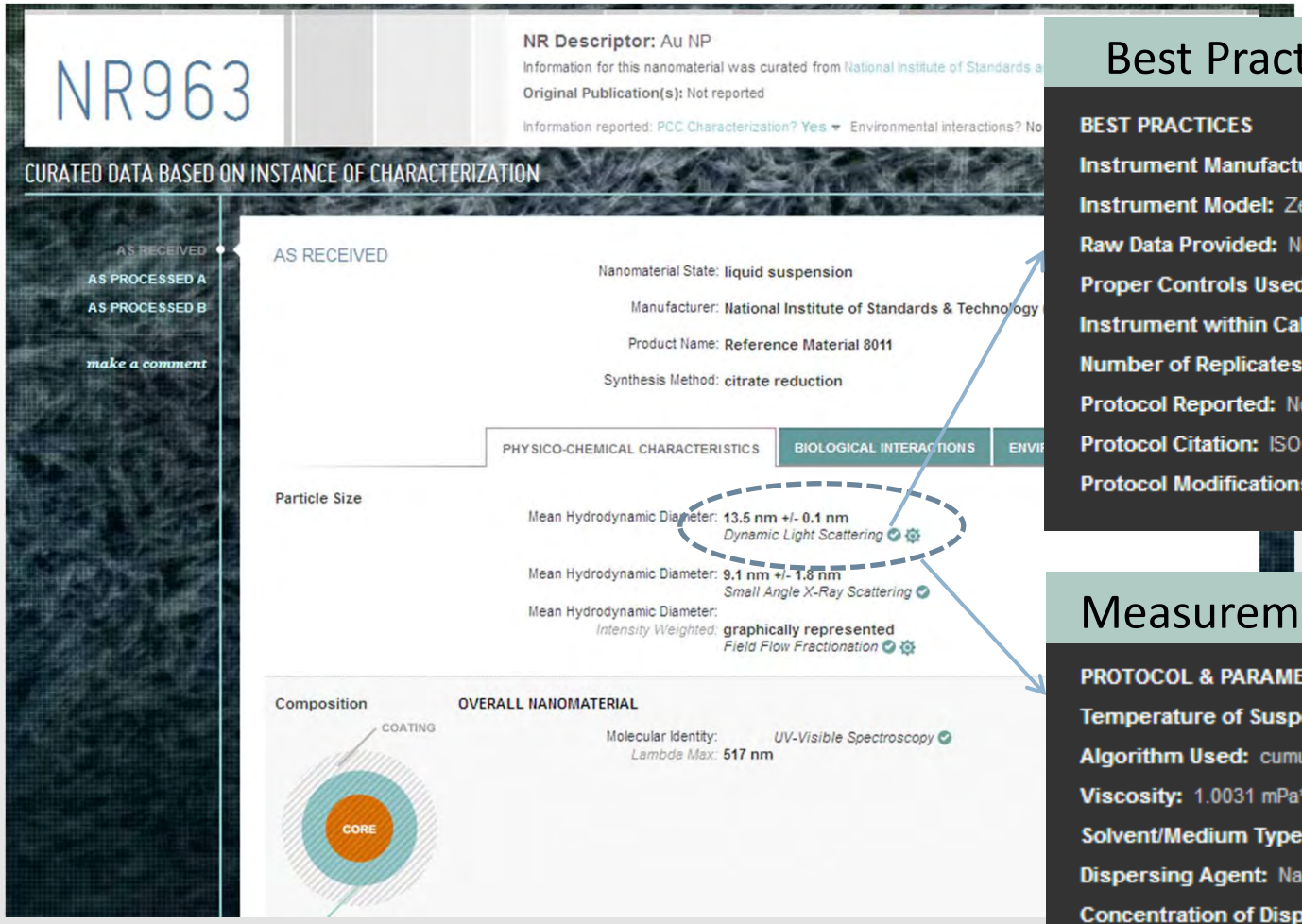
Metadata in the MIAN



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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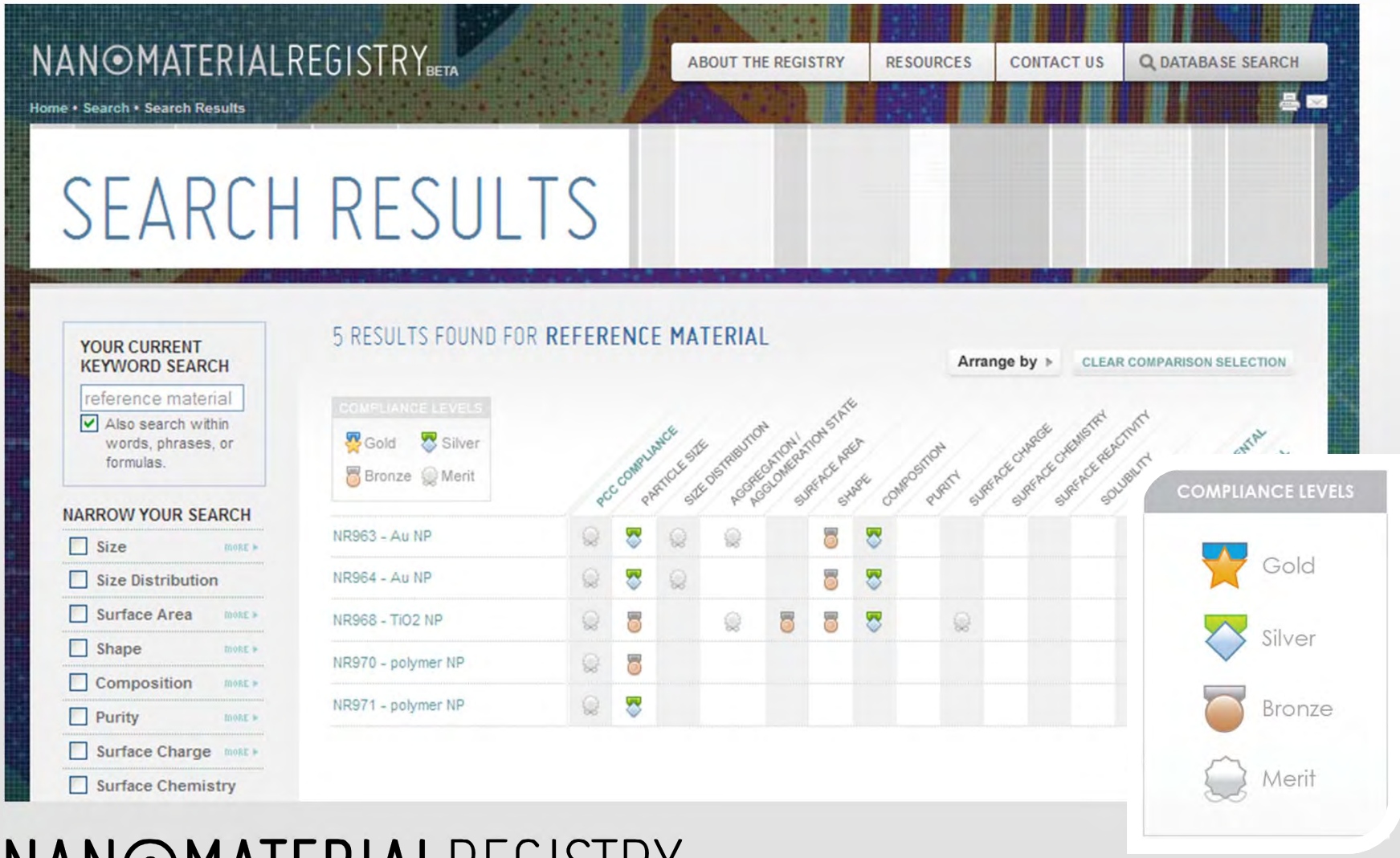
Compliance Ratings



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Compliance Example for PCC of Size

Curated Data:	**Size= 37.5 nm**	**Size= 37.5 nm** **Mean Hydrodynamic Diameter**	**Size= 37.5 nm** **Mean Hydrodynamic Diameter** **Dynamic Light Scattering** **Malvern Zeta Sizer Nano ZS**	**Size= 37.5 nm** **Mean Hydrodynamic Diameter** **Dynamic Light Scattering** **Malvern ZetaSizer Nano ZS** ✓ **11 of 12 measurement parameters reported** **Protocol: ASTM E2490 - 09**
Compliance Score:	**16.5%**	**38.5%**	**60.4%**	**78.0%**
Compliance Level:	**Merit**	**Bronze**	**Silver**	**Gold**

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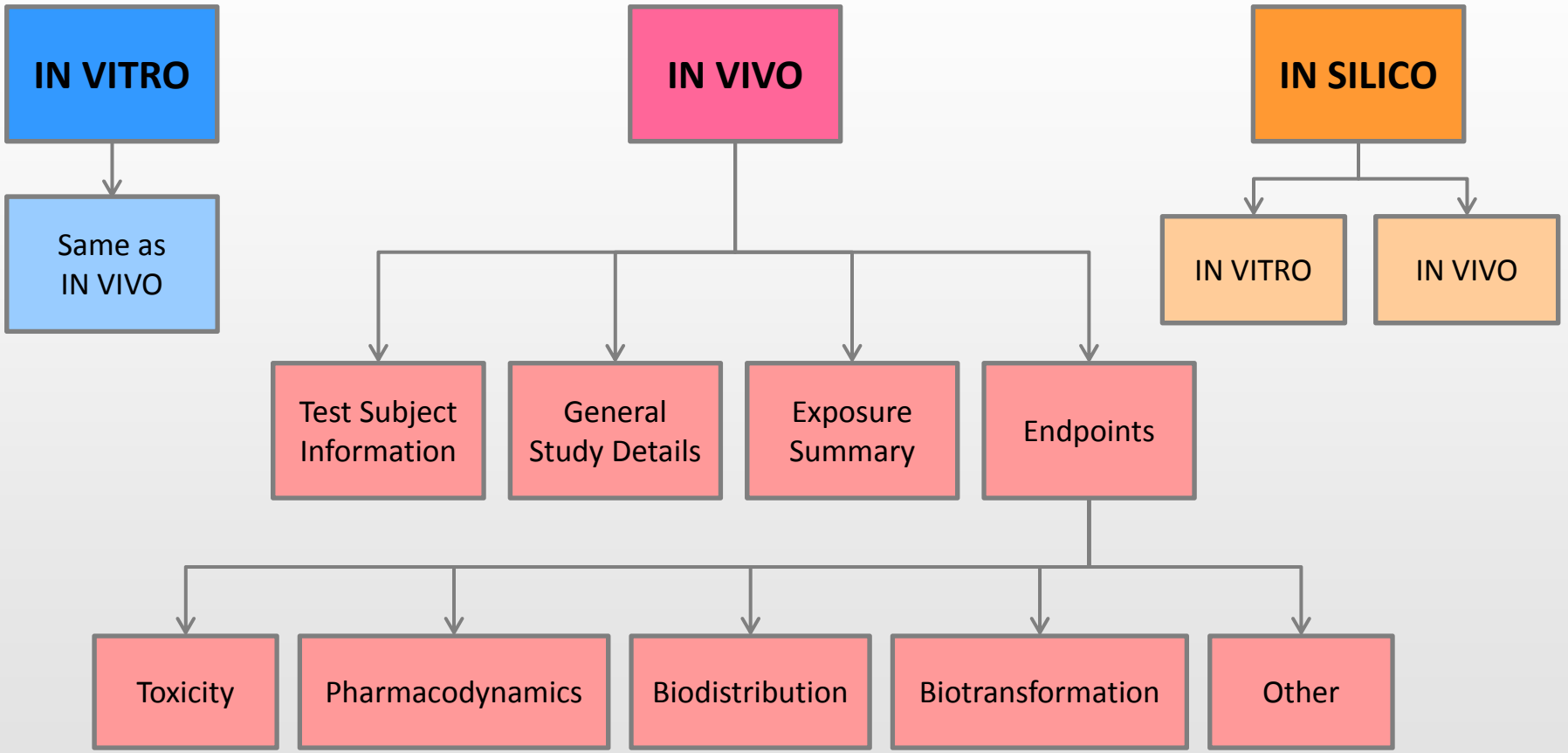
Data Domain: Biological Studies



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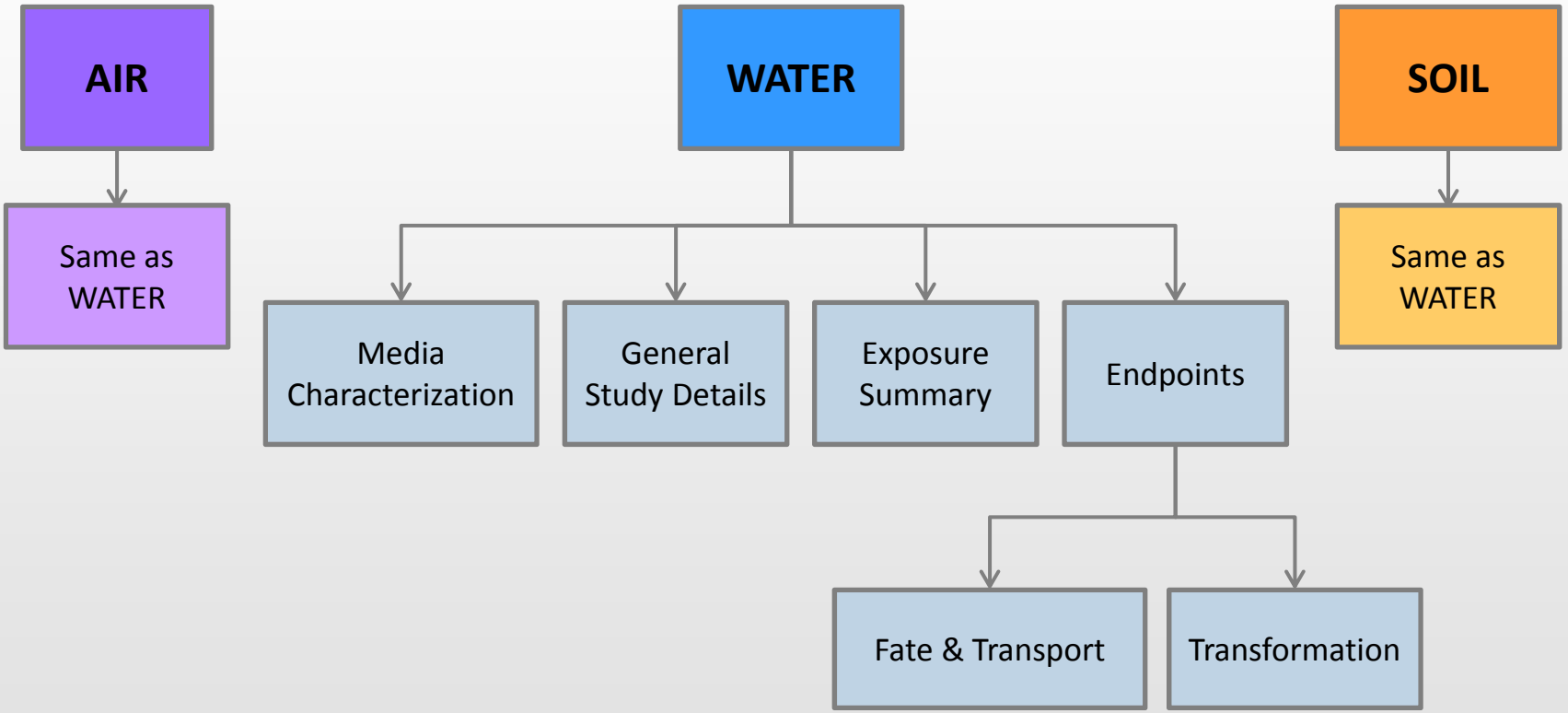
Data Domain: Environmental Studies



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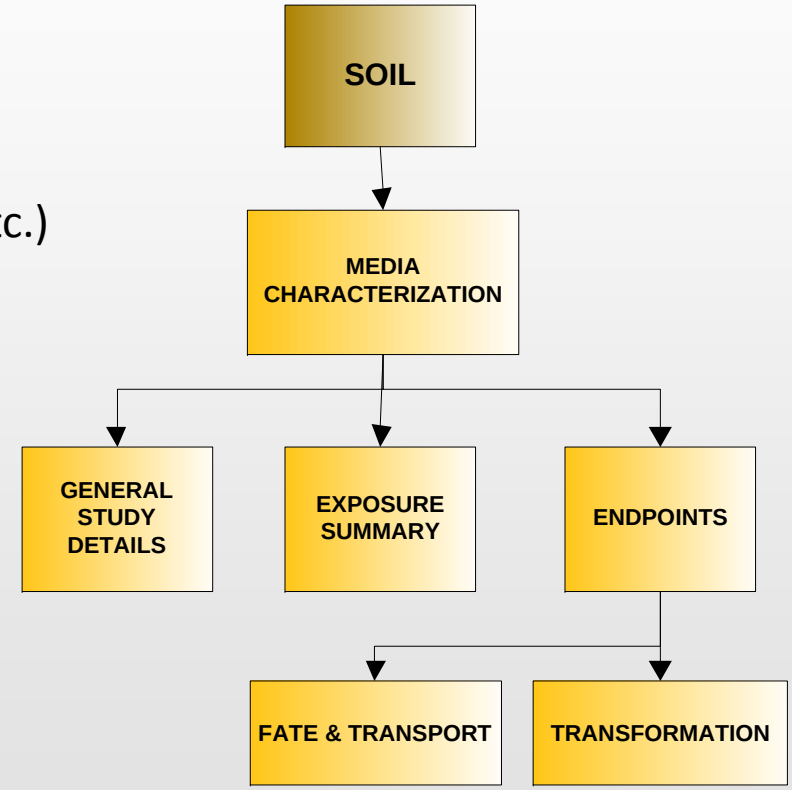
Example: Soil Fate & Transport

- Information Captured:
  - Media Characterization
    - Soil Type
    - Soil Details (moisture, pH, void volume, etc.)
    - Total Weight or Volume
  - General Study Details
    - Test Location
    - Controls? Standard Protocol Used?
    - Assay Used
  - Exposure Characterization
    - Nanomaterial Exposure Concentration
  - Study Results
    - Fate & Transport Level
    - Transformation

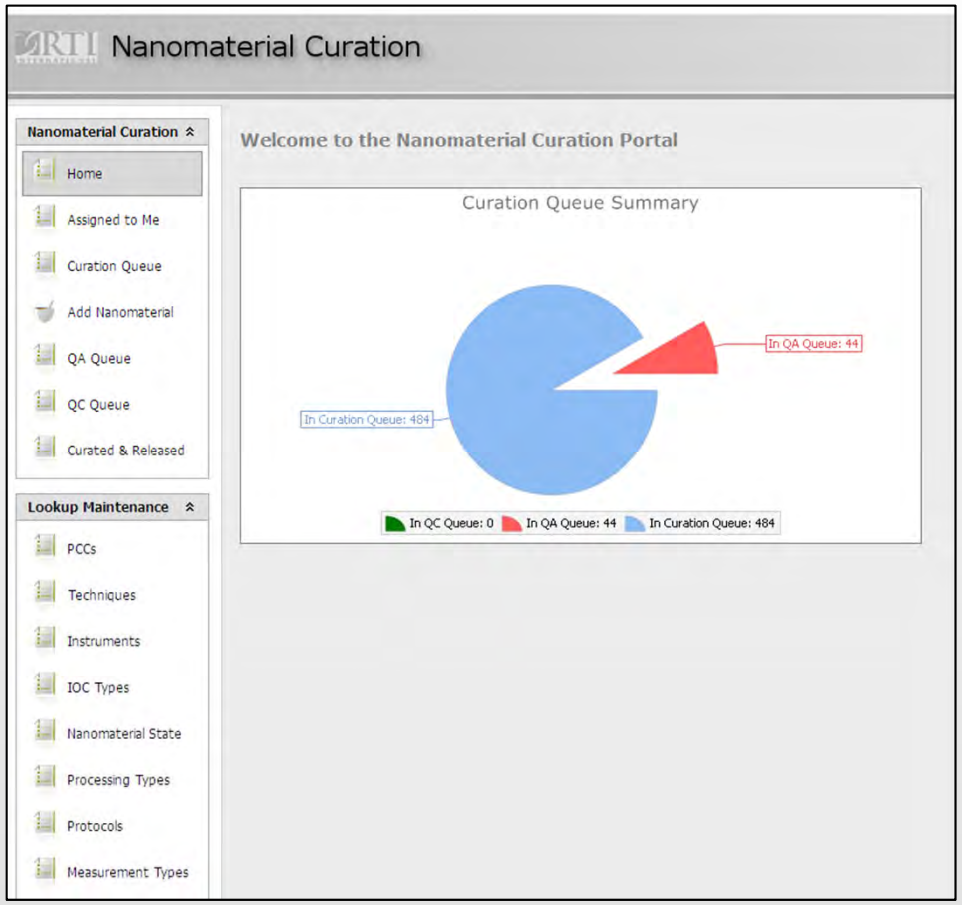


Accelerating the Curation Process

Minimizing Error Propagation

CURATION TOOL

Curation Tool



- Errors are mitigated
  - Dropdowns available for many fields
  - Preview option to view data as displayed on website
- Notifications on queues
- Access control
- Workflow management
  - Curation → Quality Assurance → Quality Control

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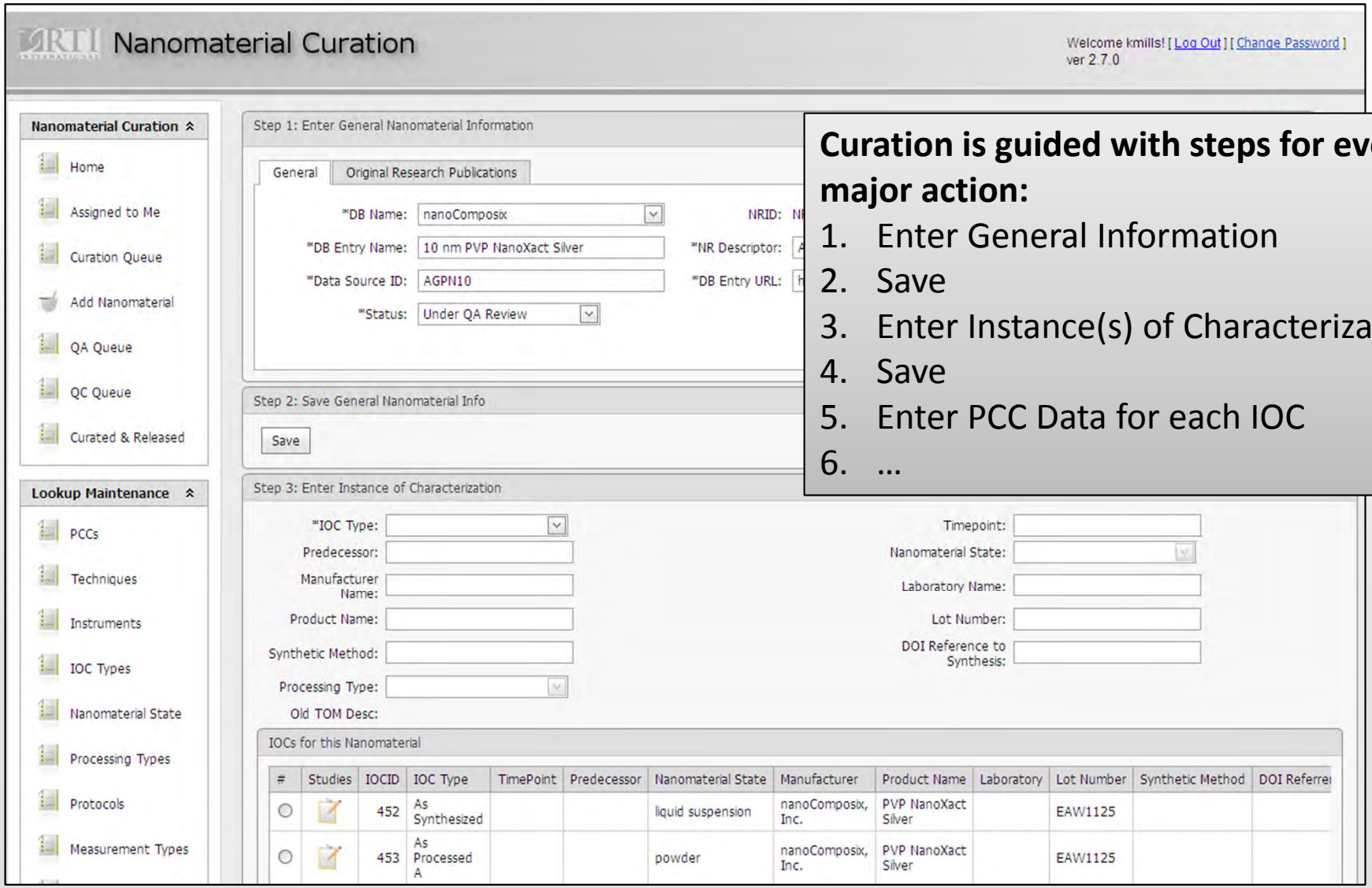
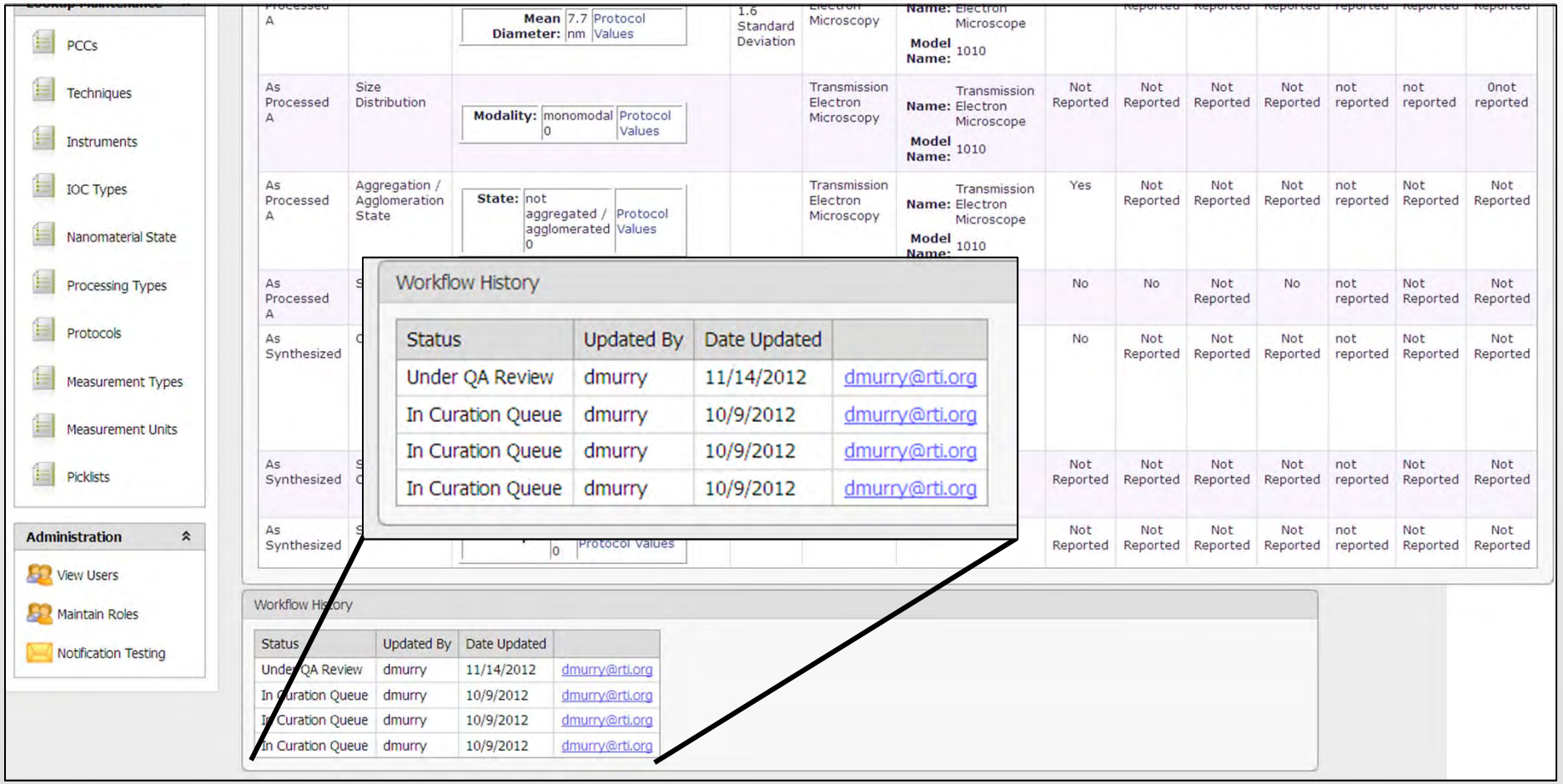
Curation of an Entry



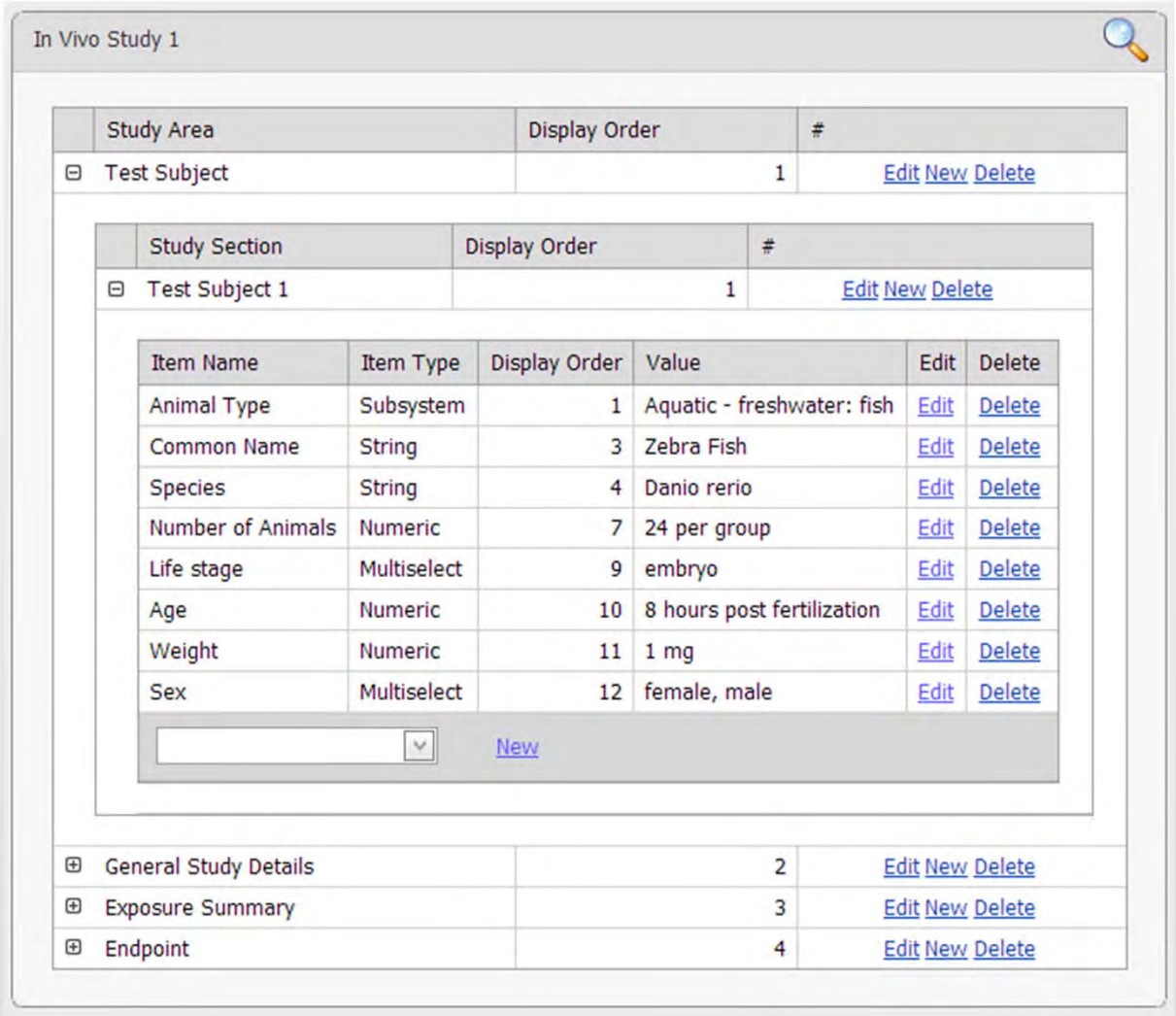
Curation is guided with steps for every major action:

1. Enter General Information
2. Save
3. Enter Instance(s) of Characterization
4. Save
5. Enter PCC Data for each IOC
6. …

Curation Tool: Tracking the Workflow



Bio/Env Curation



In Vivo Study 1

	Study Area	Display Order	#
⊟	Test Subject	1	Edit New Delete

	Study Section	Display Order	#
⊟	Test Subject 1	1	Edit New Delete

Item Name	Item Type	Display Order	Value	Edit	Delete
Animal Type	Subsystem	1	Aquatic - freshwater: fish	Edit	Delete
Common Name	String	3	Zebra Fish	Edit	Delete
Species	String	4	Danio rerio	Edit	Delete
Number of Animals	Numeric	7	24 per group	Edit	Delete
Life stage	Multiselect	9	embryo	Edit	Delete
Age	Numeric	10	8 hours post fertilization	Edit	Delete
Weight	Numeric	11	1 mg	Edit	Delete
Sex	Multiselect	12	female, male	Edit	Delete

New

⊞	General Study Details	2	Edit New Delete
⊞	Exposure Summary	3	Edit New Delete
⊞	Endpoint	4	Edit New Delete

- In vivo template for curation (showing NBI data)

Browse

Search

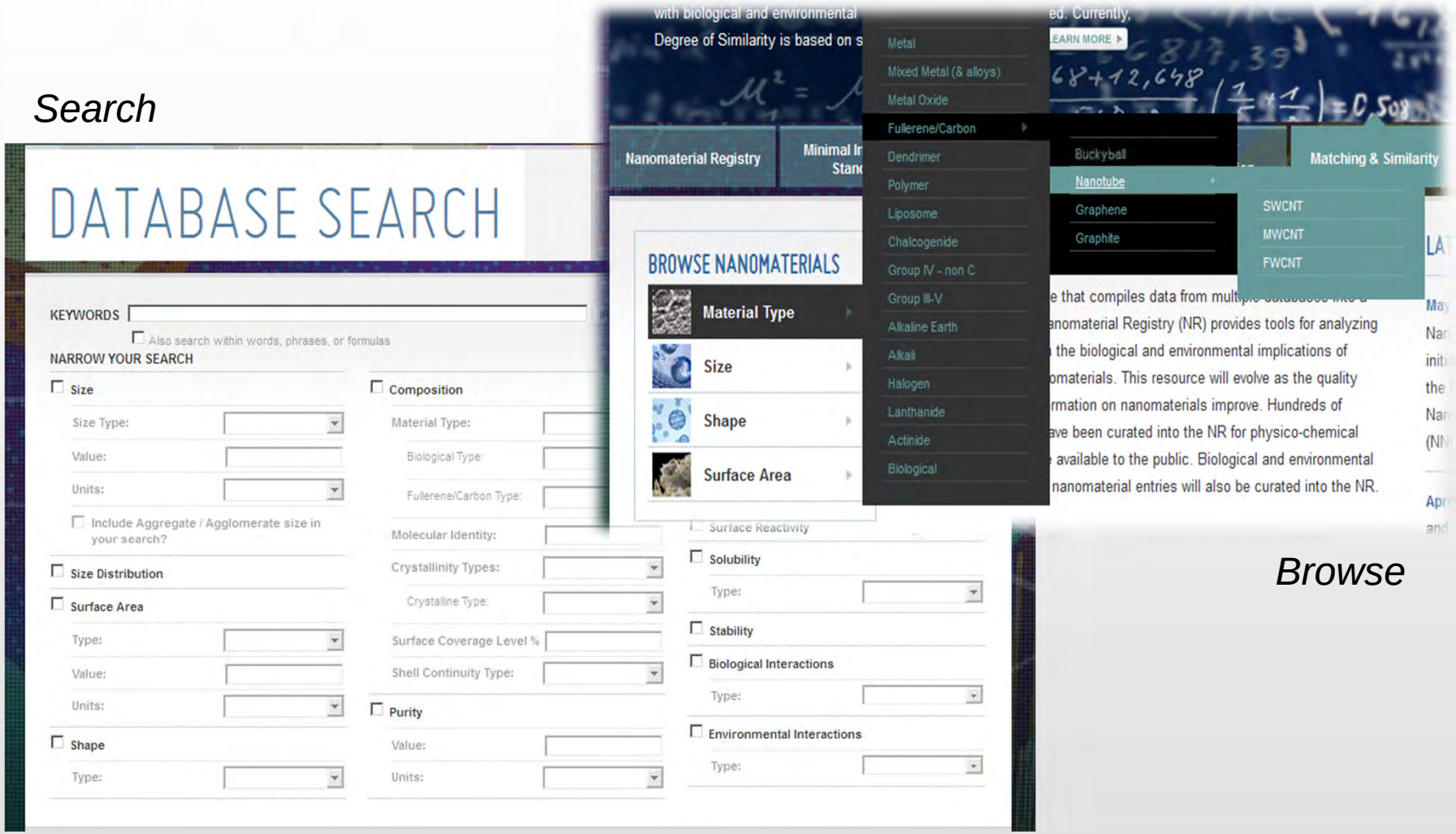
Compare

Find Similar Nanomaterials

WEBSITE FEATURES

Applied MIAN

Search



Browse

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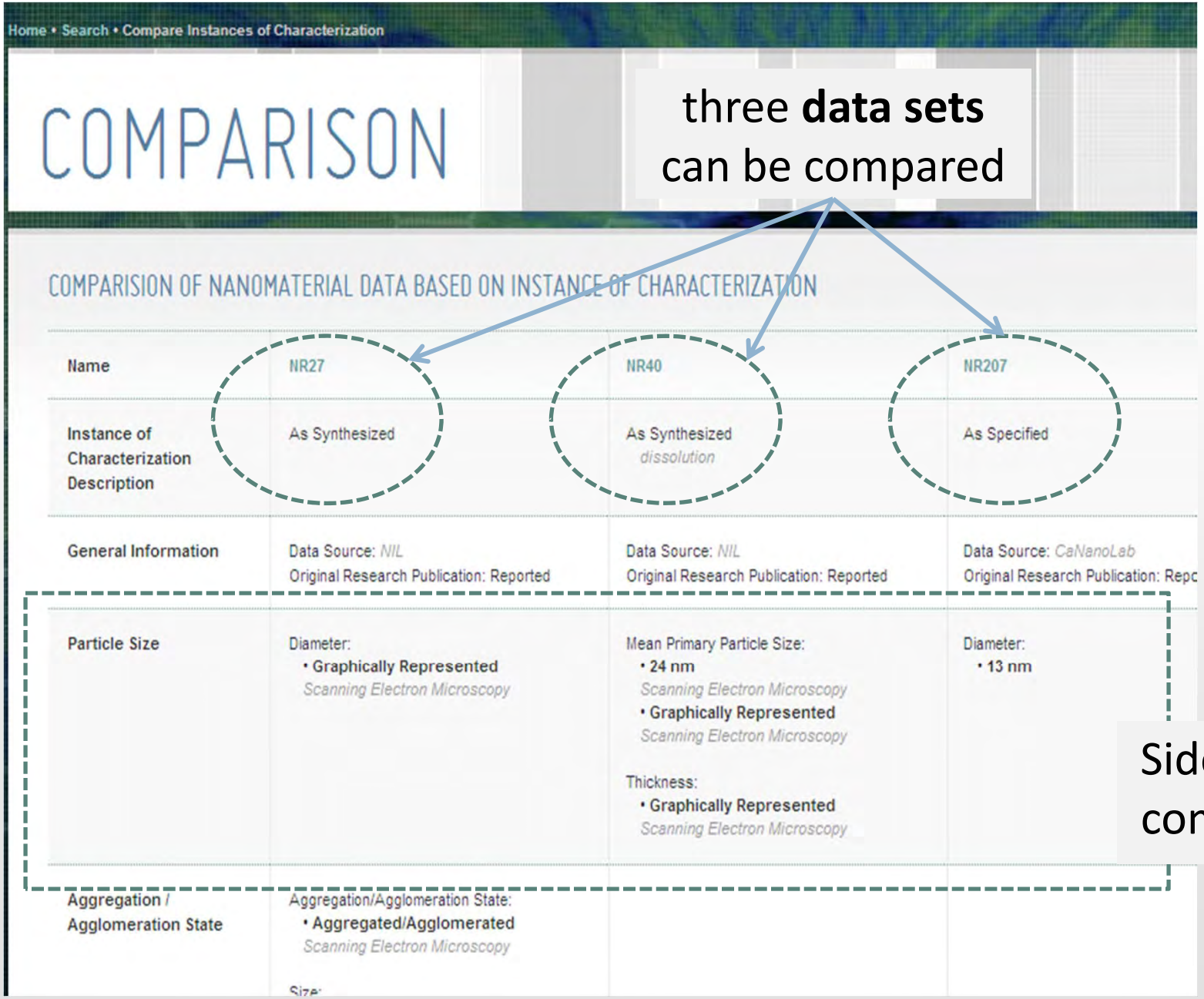

Side by side comparison

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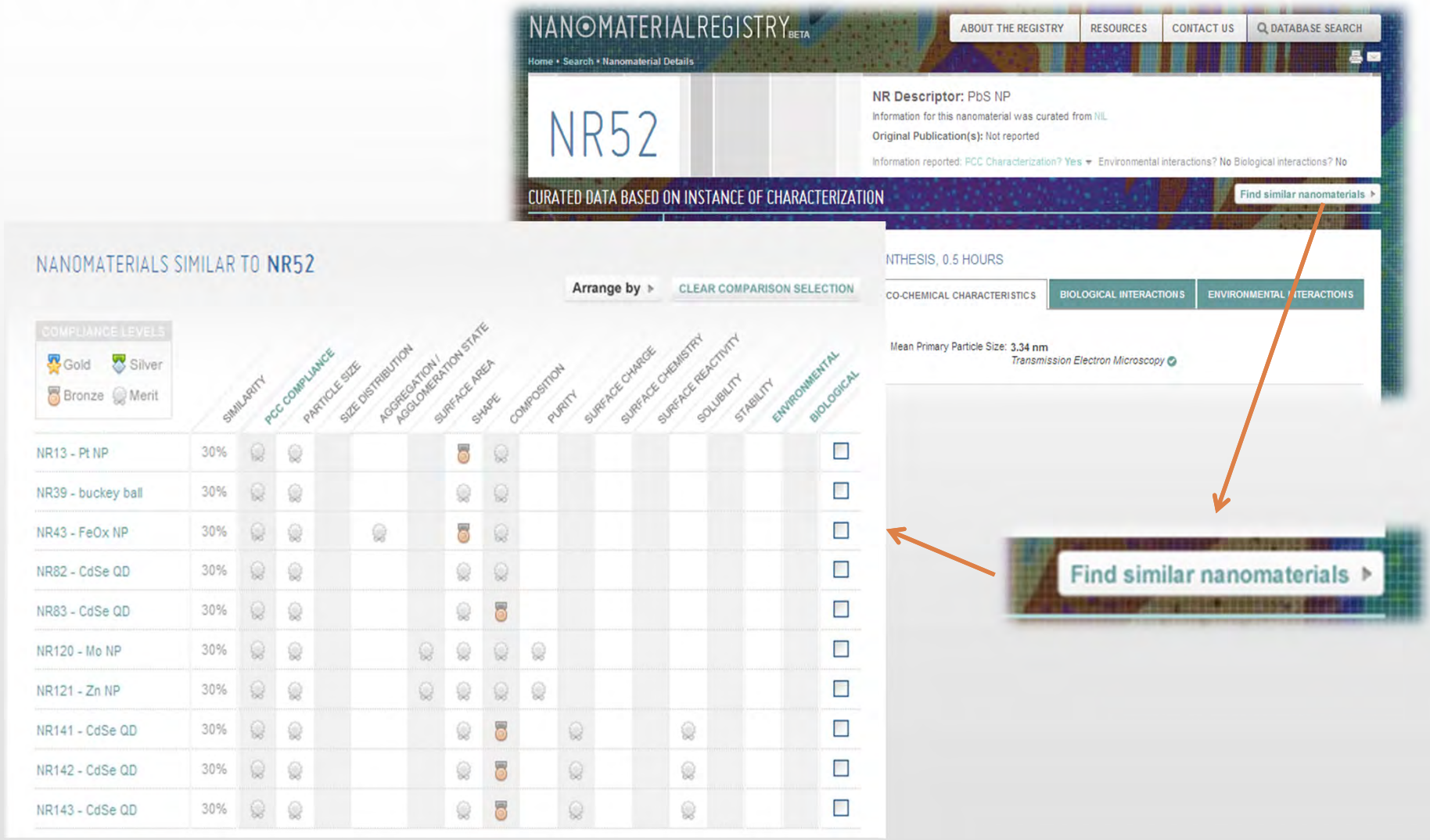
Find Similar Nanomaterials



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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
- Semantic Search

Additional Opportunities

- Public data submission tool
  - Open source option for file upload
  - Wizard-style custom design

DISCUSSION

Questions for the CoR

- What are the CoR's valued endpoints for biological and environmental systems?
- What resources will the CoR use for models on nanomaterials exposure?