

## Compliance Level Scores

**YOUR CURRENT KEYWORD SEARCH**

TiO2

Also search within words, phrases, or formulas.

16 RESULTS FOUND FOR TiO2

Arrange by ▶ ◀ Prev 1 2 of 2 Next ▶

	COMPLIANCE LEVELS	PGC COMPLIANCE	PARTICLE SIZE	SIZE DISTRIBUTION	AGGREGATION/ AGGLOMERATION STATE	SURFACE AREA	SHAPE	COMPOSITION	PURITY	SURFACE CHARGE	SURFACE CHEMISTRY	SURFACE REACTIVITY	SOLUBILITY	STABILITY	ENVIRONMENTAL	BIOLOGICAL
NR68 - TiO2 NF	Gold	Bronze		Silver		Gold	Gold								No	No
NR91 - TiO2 NP	Gold			Silver	Gold		Gold								No	No
NR467 - TiO2 NP	Gold	Silver				Gold	Gold								Yes	Yes
NR809 - TiO2 NP	Gold	Silver			Gold		Gold								No	No
NR810 - TiO2 NP	Gold	Bronze			Gold		Gold								No	No
NR811 - TiO2 NP	Gold	Bronze			Gold		Gold								No	No
NR932 - TiO2 NP	Gold					Gold	Gold								No	No
NR933 - TiO2 NP	Gold					Gold	Gold								No	No
NR968 - TiO2 NP	Gold	Gold		Silver	Gold	Gold	Gold	Gold	Gold				Bronze		No	No
NR1076 - TiO2 NP	Gold	Silver					Gold	Gold							No	Yes
NR1102 - TiO2 NP	Bronze	Merit					Gold								No	Yes
NR1278 - TiO2 NP	Gold	Silver		Gold	Gold		Gold								No	No

Compare Selected ▶

## Project Overview





***“Provide  
Comprehensively  
curated, validated  
data on a scale  
suitable for  
decision making”***

The screenshot shows the Nanomaterial Registry website. At the top, there is a navigation bar with links for 'ABOUT THE REGISTRY', 'RESOURCES', and 'CONTACT US'. A search bar is located on the right with the text 'Search by keyword' and an 'Advanced Search' button. Below the navigation bar is a large banner with the heading 'WELCOME TO THE NANOMATERIAL REGISTRY!' and a paragraph of introductory text. Below the banner is a horizontal menu with six items: 'Nanomaterial Registry', 'Minimal Information About Nanomaterials', 'Compliance Levels', 'Instance of Characterization', 'Nanomaterial Similarity', and 'Comparison'. The main content area is divided into three columns. The left column has a 'BROWSE NANOMATERIALS' section with four categories: 'Material Type', 'Size', 'Shape', and 'Surface Area'. Below this is a 'THE REGISTRY RECORDS' section showing '1200 Nanomaterials as of 9/9/2013' and a 'Visualize Data - Click Here' link. The middle column has a section titled 'A tool for the nanomaterial community' with two paragraphs of text. The right column has a 'LATEST NEWS' section with two news items, each with a date and a 'Read more' link.

# 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

↓  
**A COMPLIANCE LEVEL SCORE** is a quantitative value calculated by an algorithm

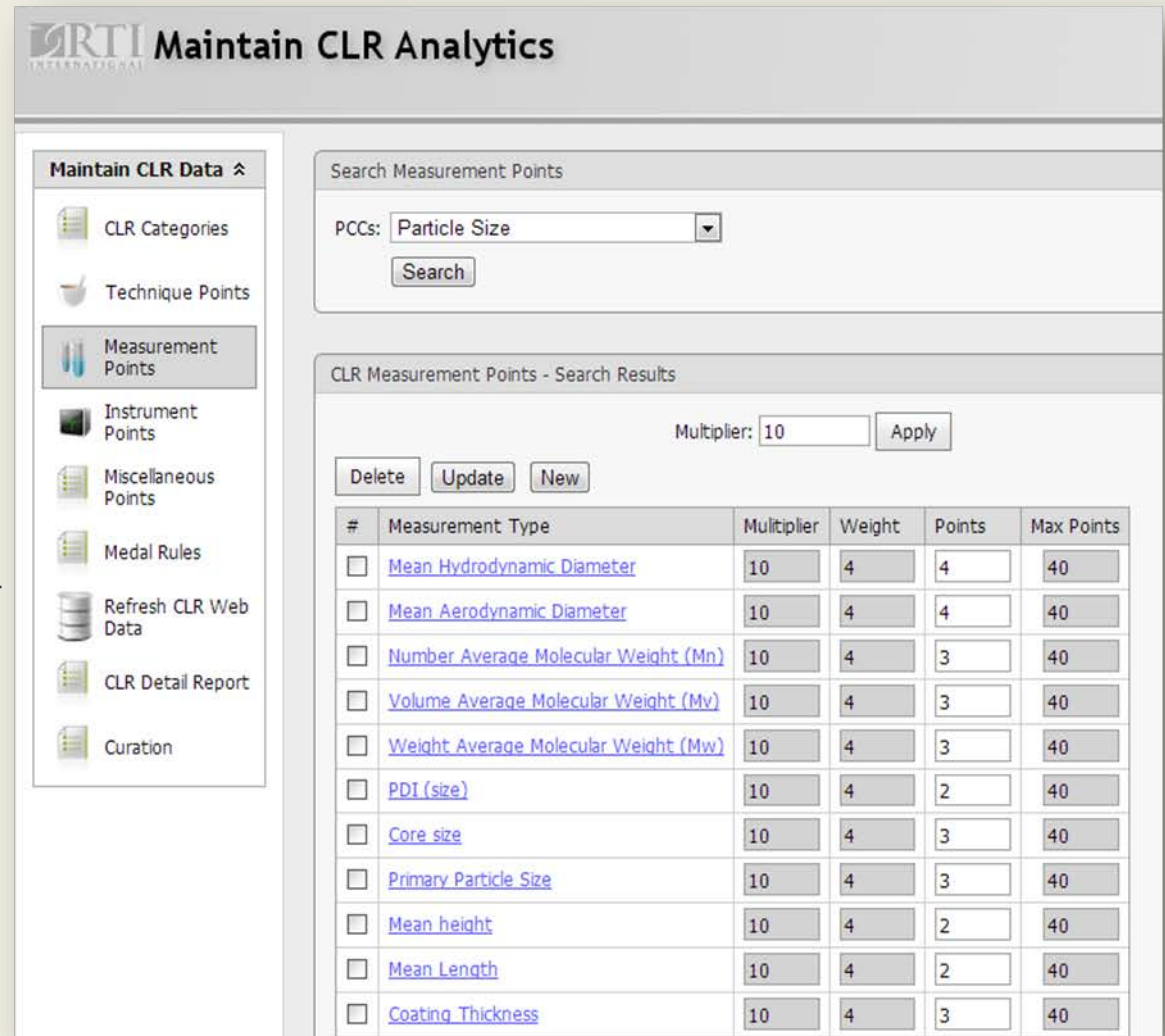
# Compliance Level Scores

	Scenario 1	Scenario 2	Scenario 2	Scenario 4
<b>Curated Data:</b>	<b>Size= 37.5 nm</b>	<i>Size= 37.5 nm</i>	<i>Size= 37.5 nm</i>	<i>Size= 37.5 nm</i>
		<b>Mean Hydrodynamic Diameter</b>	<i>Mean Hydrodynamic Diameter</i>	<i>Mean Hydrodynamic Diameter</i>
			<b>Dynamic Light Scattering</b>	<i>Dynamic Light Scattering</i>
			<b>Malvern ZetaSizer Nano ZS</b>	<i>Malvern ZetaSizer Nano ZS</i>
				<b>11 of 12 measurement parameters reported</b>
				<b>Protocol: ASTM E2490 - 09</b>
<b>Compliance Level:</b>	<b>Merit</b>	<b>Bronze</b>	<b>Silver</b>	<b>Gold</b>

Records with more specific measurement data (e.g. “Mean Hydrodynamic Diameter” are awarded more points than those with less specific data (e.g. “Size”)

# Compliance Level Scores

- CL calculation assigns weights to each value that might appear in a curated record
- Weights are motivated by specificity and are fixed by consensus-based standards arising from collaboration between our scientists and Advisory Board
- For each PCC, the weights for a given record are transformed via a mathematical formula to give a rational number between 0 and 1, the record's CL for that PCC
- Based on the CL obtained, a record is awarded one of four medals (from best characterized to least): Gold, Silver, Bronze, or Merit



#	Measurement Type	Multiplier	Weight	Points	Max Points
<input type="checkbox"/>	<a href="#">Mean Hydrodynamic Diameter</a>	10	4	4	40
<input type="checkbox"/>	<a href="#">Mean Aerodynamic Diameter</a>	10	4	4	40
<input type="checkbox"/>	<a href="#">Number Average Molecular Weight (Mn)</a>	10	4	3	40
<input type="checkbox"/>	<a href="#">Volume Average Molecular Weight (Mv)</a>	10	4	3	40
<input type="checkbox"/>	<a href="#">Weight Average Molecular Weight (Mw)</a>	10	4	3	40
<input type="checkbox"/>	<a href="#">PDI (size)</a>	10	4	2	40
<input type="checkbox"/>	<a href="#">Core size</a>	10	4	3	40
<input type="checkbox"/>	<a href="#">Primary Particle Size</a>	10	4	3	40
<input type="checkbox"/>	<a href="#">Mean height</a>	10	4	2	40
<input type="checkbox"/>	<a href="#">Mean Length</a>	10	4	2	40
<input type="checkbox"/>	<a href="#">Coating Thickness</a>	10	4	3	40

# CALCULATING COMPLIANCE LEVEL

- The database field categories utilized in Compliance Level (CL) calculation are identified as **“GROUPS”**
- For any given GROUP, the set of possible entries is called the set of **ELEMENTS** in that group
- The CL score for each PCC for a given record is the sum of the scores awarded to each measurement, capped at the maximum value a single measurement can obtain

NRID	PCC	“GROUP”		Measurement Value	“GROUP”		Technique
		Measurement Type	Sub-type 1		Uncertainty Value	Uncertainty Units	
NR1010	Particle Size	Mean Hydrodynamic Diameter	Intensity Weighted	53.2			DLS
NR1010	Particle Size	Mean Hydrodynamic Diameter	Intensity Weighted	55.8			DLS
NR1010	Particle Size	PDI (size)		0.154			DLS
NR1010	Particle Size	PDI (size)		0.161			DLS
NR1010	Particle Size	Mean Diameter		41.71	6.28	nm	TEM

} ELEMENTS

*(selection of data output from the Registry)*

# CALCULATING COMPLIANCE LEVEL

## The CLR Algorithm

- **Group:** data associated with a given PCC are broadly categorized into groups: Measurement Type, Technique, Instrument, and various Meta-data groups (uncertainty, replicates, etc.)
- **Element:** each group consists of elements; data which are categorized into a given group are called that group's elements
- **Points:** each element of each group is assigned an integer called its points value
- **Multiplier:** each group has associated with it an integer value called its multiplier
- **Weight:** For each group within a given PCC, the weight is the product of the group multiplier and the largest points value assigned to any element in the group
- **Measurement:** a measurement is a single characterization of a particle

$$CL_{PCC} = \sum_{Measurements} \left\{ \frac{\sum_G M_G * P_G}{\sum_G M_G * W_G} \right\}$$

$G$  = group

$M_G$  = group multiplier

$P_G$  = points awarded to element  $P$  of group  $G$

$W_G$  = weight assigned to group  $G$

# CALCULATING COMPLIANCE LEVEL

## The CLR Tool

The screenshot displays the 'Maintain CLR Data' interface. On the left is a navigation menu with options: CLR Categories, Technique Points, Measurement Points (selected), Instrument Points, Miscellaneous Points, Medal Rules, Refresh CLR Web Data, CLR Detail Report, and Curation. The main area is titled 'Search Measurement Points' and shows a search for 'Particle Size'. Below this is a section for 'CLR Measurement Points - Search Results' which includes a 'Multiplier' input field with an 'Apply' button, and buttons for 'Delete', 'Update', and 'New'. A table with columns '#', 'Measurement Type', 'Multiplier', 'Weight', 'Points', and 'Max Points' is shown, but it contains no data, displaying 'No data to display'.

- The CLR tool allows us to **ADJUST** multipliers and points for all groups and group elements
- We can then **APPLY** the changes to all records and see the **IMPACT** on CL score on the website

- This gives us the necessary **FLEXIBILITY** to address dynamic nanomaterial characterization standards as well as to tailor CL calculation to specific stakeholder groups



# CALCULATING COMPLIANCE LEVEL

## The CLR Tool

CLR Detail Report

Generate Report

TOTAL PTS	TOTAL POSSIBLE	Measurement Pts	Meas Poss	Sub Meas. Pts	Sub Meas Poss	Technique Pts	Technique Poss	Graph
43	70	20	40	0	0	20	20	
0	7	0	0	0	0	0	0	
43	60	20	30	0	0	20	20	
0	7	0	0	0	0	0	0	
60	67	40	40	0	0	20	20	
30	37	30	30	0	0	0	0	
0	7	0	0	0	0	0	0	
0	7	0	0	0	0	0	0	
0	7	0	0	0	0	0	0	
0	7	0	0	0	0	0	0	
0	7	0	0	0	0	0	0	
0	7	0	0	0	0	0	0	
0	7	0	0	0	0	0	0	

The tool also supports **DETAILED REPORT** views which

- ✓ help us ensure that the algorithm mechanics are sound
- ✓ explicitly show the contribution of each group to the PCC CL scores

# CALCULATING COMPLIANCE LEVEL

EXAMPLE: Particle Size calculation for NR50, a silicon nanoparticle, curated from NIL

1 RESULT FOUND FOR NR50

Arrange by ▶

COMPLIANCE LEVELS ?

- Gold
- Silver
- Bronze
- Merit

NR50 - Si NP

PCC COMPLIANCE	PARTICLE SIZE	SIZE DISTRIBUTION	AGGREGATION / AGGLOMERATION STATE	SURFACE AREA	SHAPE	COMPOSITION	PURITY	SURFACE CHARGE	SURFACE CHEMISTRY	SURFACE REACTIVITY	SOLUBILITY	STABILITY	ENVIRONMENTAL	BIOLOGICAL ?
												No	No	

Compare Selected ▶

Medal Rules (Use decimals to represent percentages - Example: .50 = 50%)

Gold Medal given for a CLR	>	0.90	
Silver Medal given for a CLR	>	0.70	(assumes less than gold value)
Bronze Medal given for a CLR	<	0.70	(assumes less than silver value)
Merit Medal given for a CLR	<	.50	

# CALCULATING COMPLIANCE LEVEL

**PHYSICO-CHEMICAL CHARACTERISTICS** | **BIOLOGICAL INTERACTIONS**

**Particle Size**

Mean Primary Particle Size: **59 nm**  
*Transmission Electron Microscopy* ✓

Mean Primary Particle Size: **graphically represented**  
*Scanning Electron Microscopy* ✓

**Aggregation/Agglomeration State**

State: **Not Aggregated/Agglomerated**  
*Transmission Electron Microscopy* ✓

**Shape**

Nanoscale Dimensionality: **3D**  
*Transmission Electron Microscopy* ✓

Nanoscale Dimensionality: **3D**  
*Scanning Electron Microscopy* ✓

**Composition**

● **CORE** (hover over circle for proportion of material)

**COATING**

**COMPONENT 1**

**SHELL**

Material Type: **Group IV - non C**

Molecular Identity: **Si**  
*X-ray Photoelectron Spectroscopy* ✓

Crystallinity: **Crystalline**  
*Transmission Electron Microscopy* ✓

View of particle size information from the details page of the website

**NR50, a silicon nanoparticle, curated from NIL**

# CALCULATING COMPLIANCE LEVEL

Group	Mult.	Weight
Measurement	10	4
Technique	4	5
Instrument	3	1
Uncertainty	1	2
Replicates	1	2
Graph. Rep.	1	3

(TABLE 1)

Group	Element	Points
Measurement	Mean Primary Particle Size	3
Technique	TEM	5
Instrument		
Uncertainty		
Replicates		
Graph. Rep.	yes	3

(TABLE 2)

The data relevant to Particle Size CL calculation for NR50 are tabulated below:

Msrmt. awd.	Msrmt. poss.	Tech. awd.	Tech. poss.	Inst. awd.	Inst. poss.	Uncrty. awd.	Uncrty. poss.	Repl. awd.	Repl. poss.	Graph. awd.	Graph. poss.
30	40	20	20	0	3	0	2	0	2	3	3

(TABLE 3)





# CALCULATING COMPLIANCE LEVEL

## Algorithm:

$$CL_{PCC} = \sum_{Measurements} \left\{ \frac{\sum_G M_G * P_G}{\sum_G M_G * W_G} \right\}$$

## Algorithm applied to NR50:

$$CL_{Particle\ Size} = \frac{(10)*(3)+(4)*(5)+(1)*(3)}{(10)*(4)+(4)*(5)+(3)*(1)+(1)*(2)+(1)*(2)+(1)*(3)} = \sim 0.75$$

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

# CALCULATING COMPLIANCE LEVEL

## Curation and CL Scores

The method of reporting can change the resulting CL score!

**Example:** A researcher measured a distribution of particles with TEM

**Data:**

Mean Diameter = 45.9 nm +/- 3.1 nm

Measured on TEM

CL = **Silver**

**Reported in Paper:**

Diameter = 50 nm

Measured on TEM

CL = **Bronze**