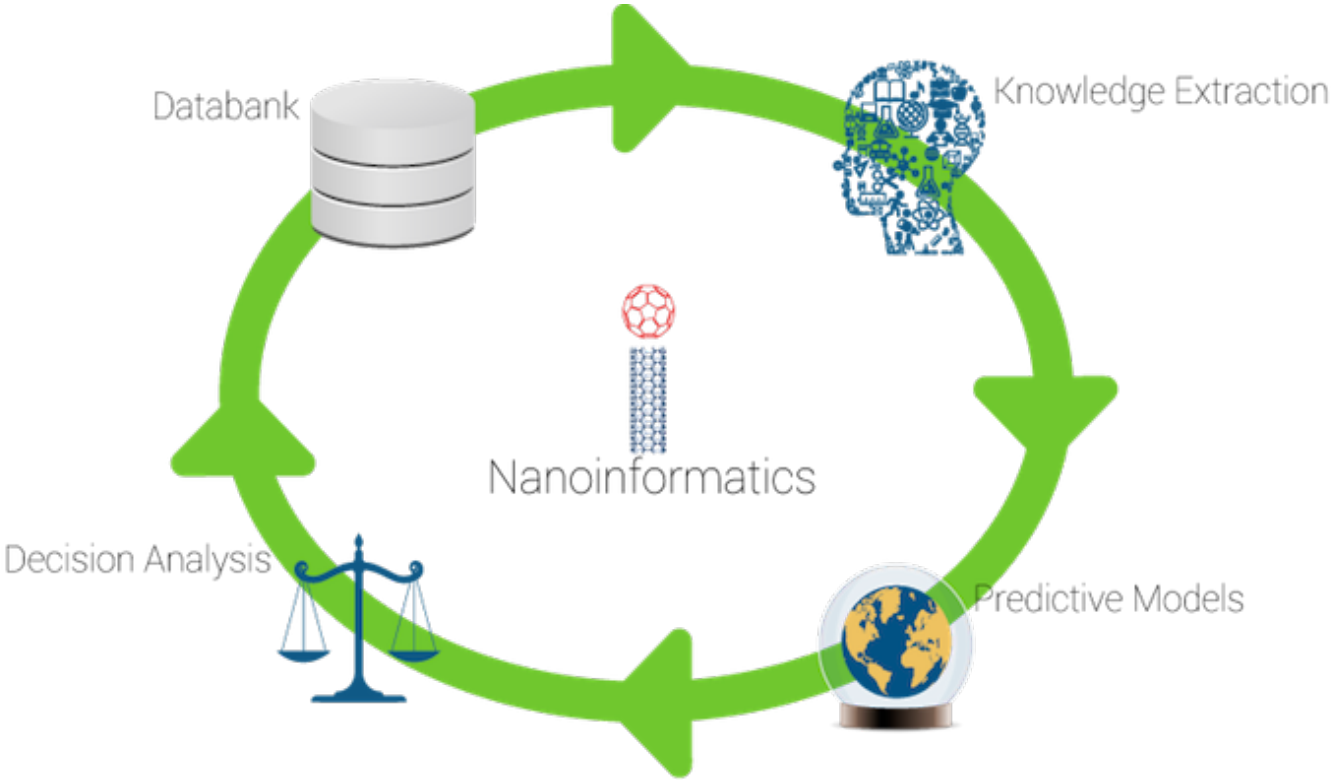
NanoInfo.Org

CEIN Integrated Nanoinformatics Web-Portal



Dennis Bacsafra, *Muhammad Bilal, Dr. Yoram Cohen, Haven Liu, Rong Liu, Michelle Romero*

http://www.nanoinfo.org

Is this Engineered Nanomaterial Environmentally Safe?

Information/Data Management

Experimental Studies / Models

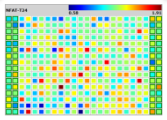
Hazard Identification

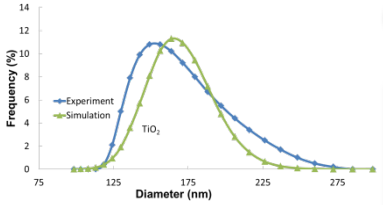
Physicochemical Characterization

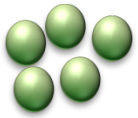
Exposure Assessment

In Vitro In Vivo Toxicity

In Silico Toxicity







Transport and Fate studies/ Modeling

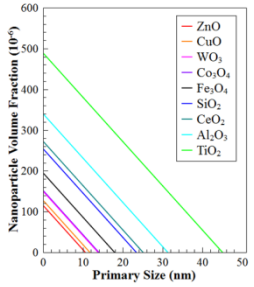
Monitoring

HT Exp.

LT Exp.

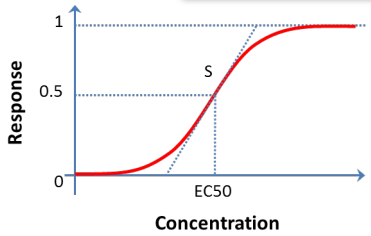
Mechanistic Conceptual

Quantitative Nano-SAR



Environmental Concentrations

- Dose- Response
- Hazard Thresholds



Environmental Impact Assessment

Decision Analysis

Product manufacturing & use approval

Product/process redesign

Exposure control

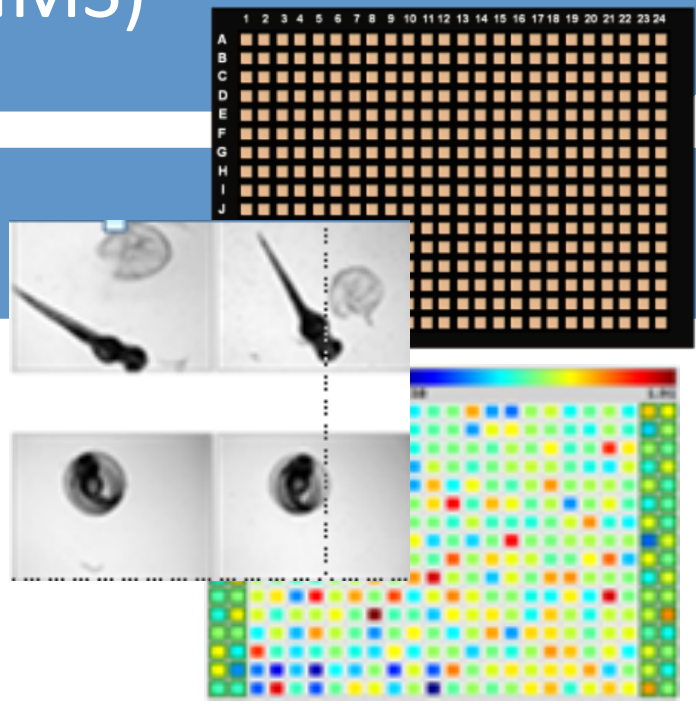
Cohen et al., ACR, 46, 802-812 (2013)

Overall Goal

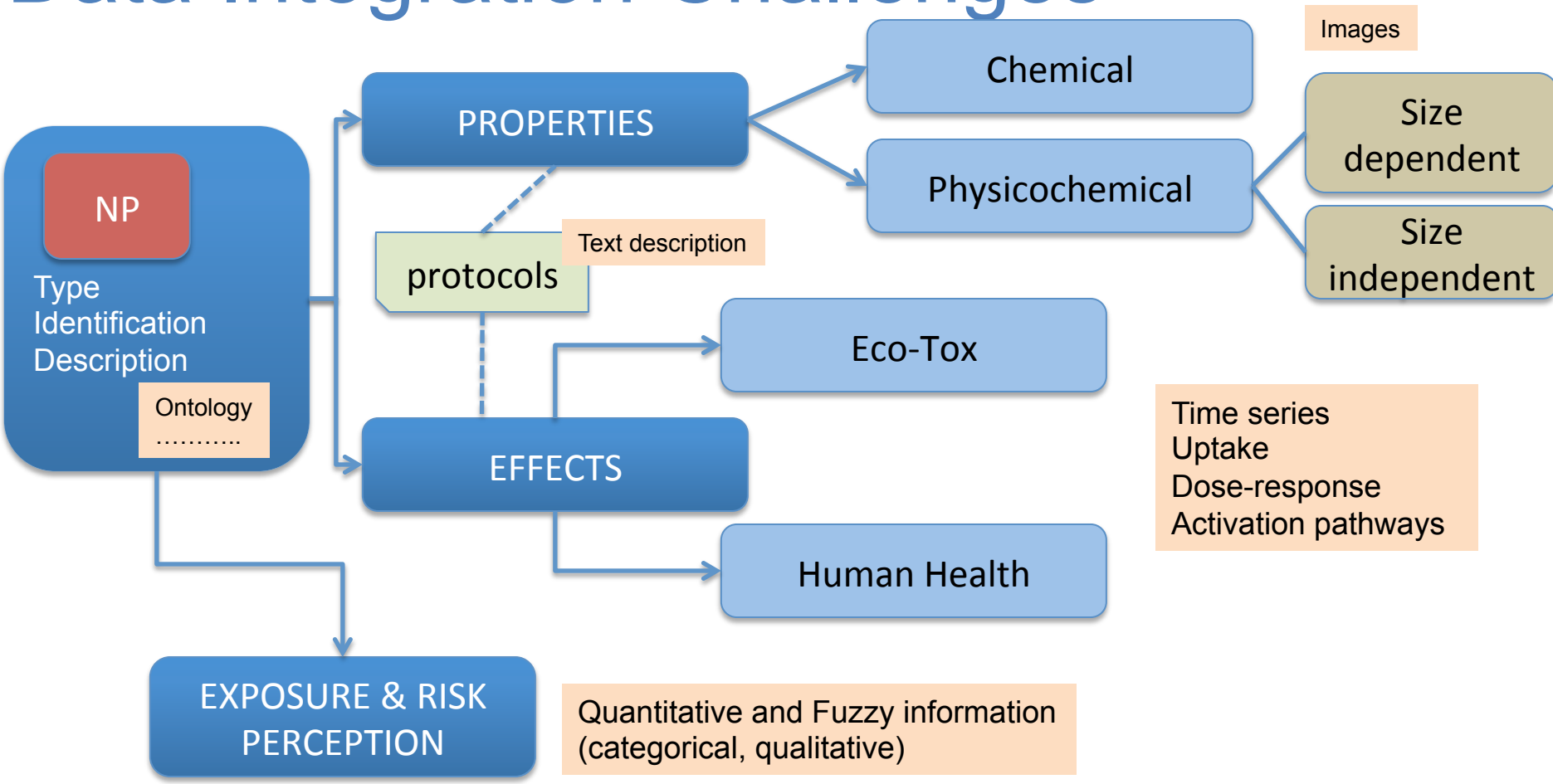
Develop the means to perform a comprehensive environmental impact assessment for Engineered Nanomaterials (ENMS)

Requires data on:

- Physicochemical properties
- Toxicity
- Potential release to environment
- Fate and transport



Data Integration Challenges

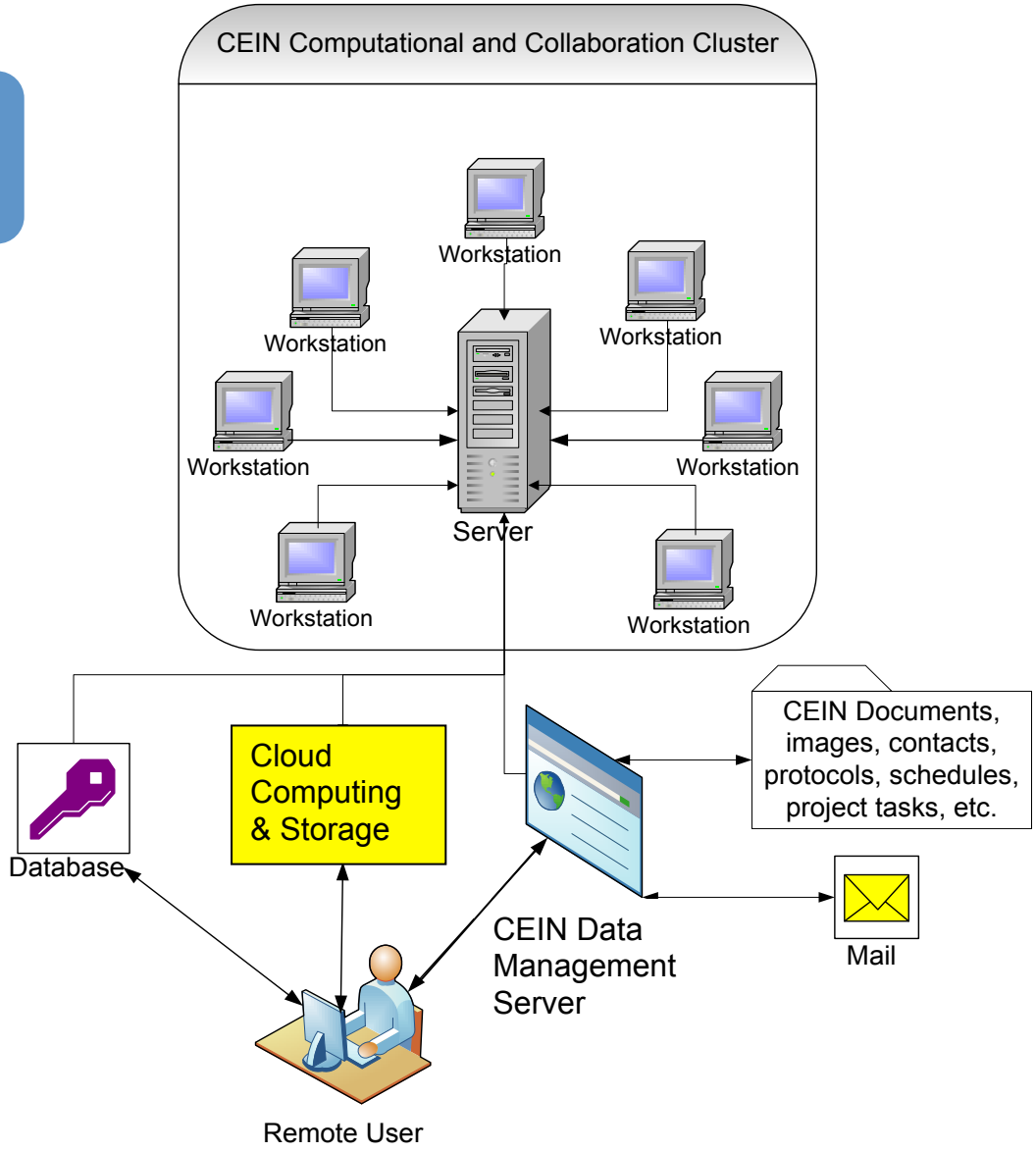


- Interoperability of data repositories containing heterogeneous datasets (structured and unstructured)
- Common vocabulary (i.e., ontology) to unambiguously describe NPs
- Standard formats for data exchange

NanoInfo.org Approach

Infrastructure

- NanoInfo.org is a cloud based platform that is physically hosted in a server cluster behind CEIN's network platform.
- Storage and processing capacity is scalable as demand increases.



Nanoinformatics Tools

Developed for environmental impact analysis of ENMs

LearNano

Estimate release of ENM via life cycle assessment

MendNano

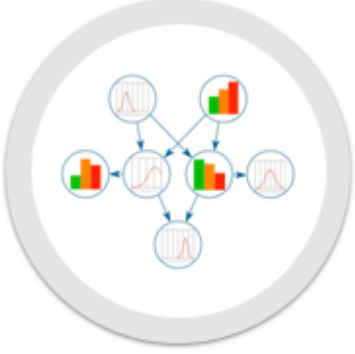
Predict environmental distribution of ENMs via multimedia compartmental modeling

ToxNano

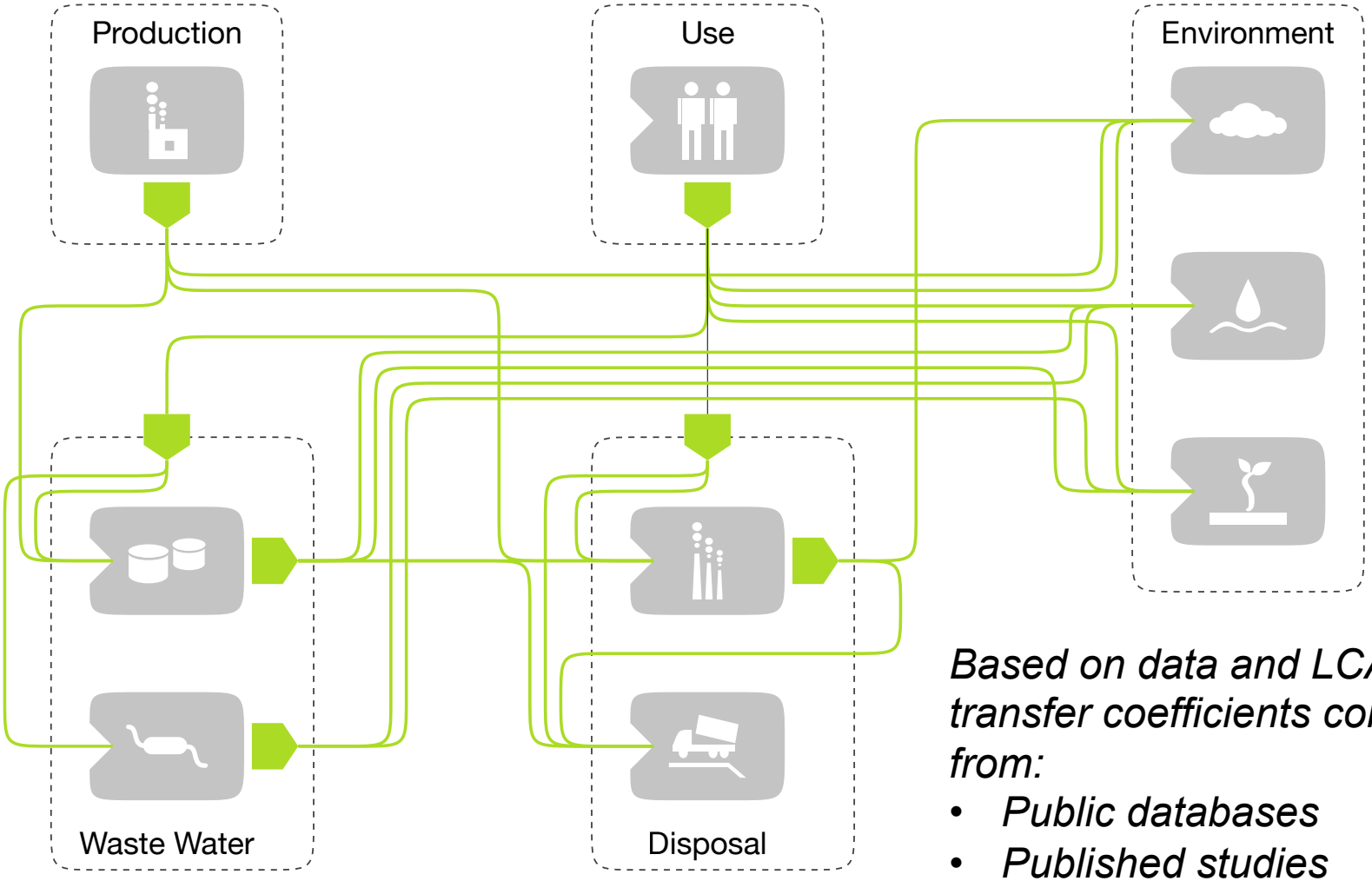
Toxicity Screening for Nanomaterials

NanoDatabank

NanoEIA



Lifecycle environmental assessment for the release of nanomaterials (LearNano)

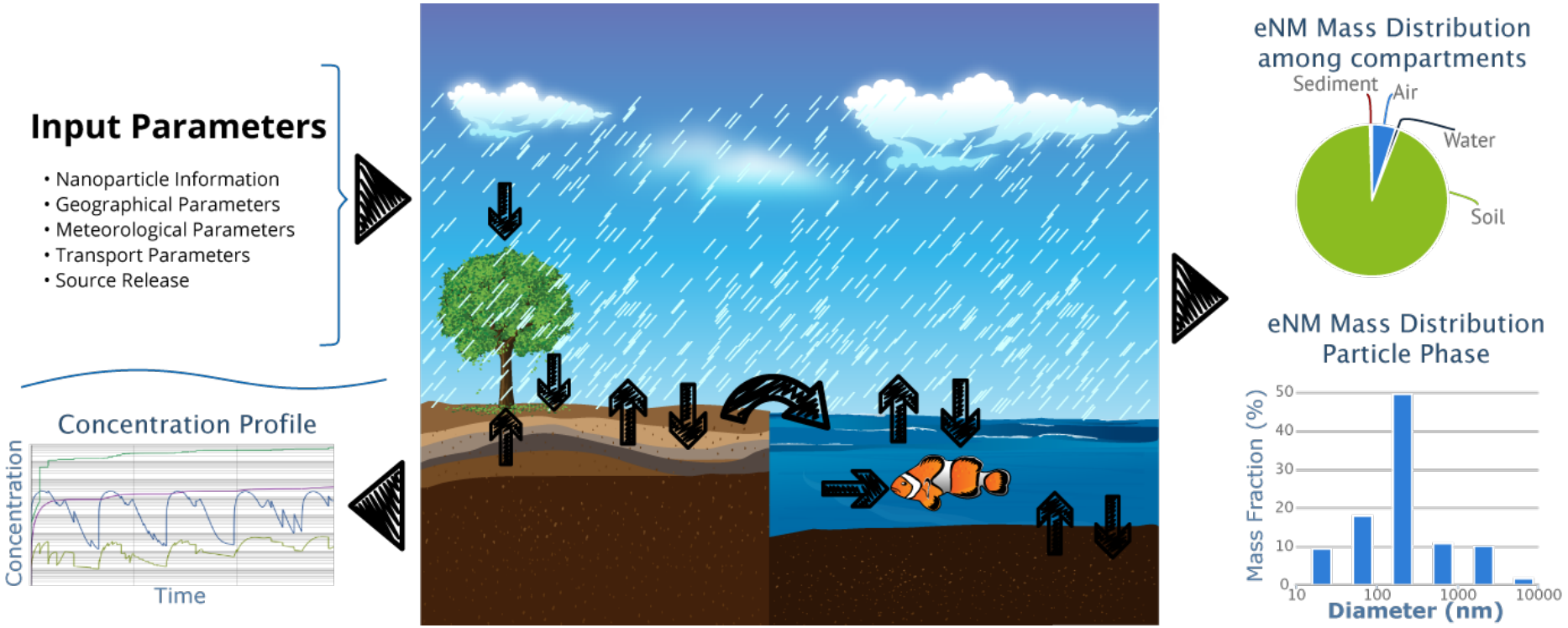


Based on data and LCA transfer coefficients compiled from:

- *Public databases*
- *Published studies*
- *Market research*
- *Economic indicators*

Keller, et al., *Predicted releases of engineered nanomaterials: From global to regional to local,* Environ. Sci. Tech. Letters. 2013.

MendNano is a first-tier model for analysis of the potential environmental distribution and “chronic” exposure concentrations associated with engineered nanomaterial



Liu, et al., Multimedia Environmental Distribution of Engineered Nanomaterials. Environ. Sci. Tech. 2014.

Plate Configuration

<config:Config_ID>

Configuration starts

0	-1	A	A	...	...	...	...	B	B	1	0
0	-1	A	A	...	...	...	...	...	...	1	0
0	-1	...	...	...	...	...	...	...	...	1	0
0	-1	...	...	0	...	...	...	...	...	1	0
0	-1	...	...	...	...	...	...	...	...	1	0
0	-1	...	...	...	...	...	...	0	...	1	0
0	-1	...	...	...	...	...	...	...	...	1	0
0	-1	...	...	...	...	B	...	...	B	1	0

</config>

Configuration ends

- ... Sample well
- -1 Negative control
- 1 Positive control
- 0 Ignored well

Replicates of sample A Replicates of sample B

a

Plate Data

<plate:Plate_ID>

Plate data starts

2.3	1.9	3.0	1.6	1.7	3.1	4.8	2.4	2.5	2.1	3.5	3.1
1.8	0.7	2.7	2.6	7.5	4.4	4.1	1.9	2.8	2.1	2.2	2.8
2.2	3.8	2.2	11.6	6.9	4.3	7.4	6.3	3.5	3.3	6.1	1.7
4.1	9.2	2.3	2.9	8.1	0.2	7.7	4.3	8.7	8.3	6.7	3.8
3.9	1.1	1.7	2.0	1.7	2.0	1.1	1.2	0.9	1.1	1.4	1.9
0.5	0.2	1.5	1.2	2.2	1.2	0.9	1.3	1.8	0.9	1.3	1.4
0.9	6.1	5.2	5.7	1.0	7.6	4.9	18.3	5.6	8.7	9.4	5.4
3.9	6.2	5.6	8.4	5.9	4.8	2.3	5.7	5.2	9.5	7.0	9.7

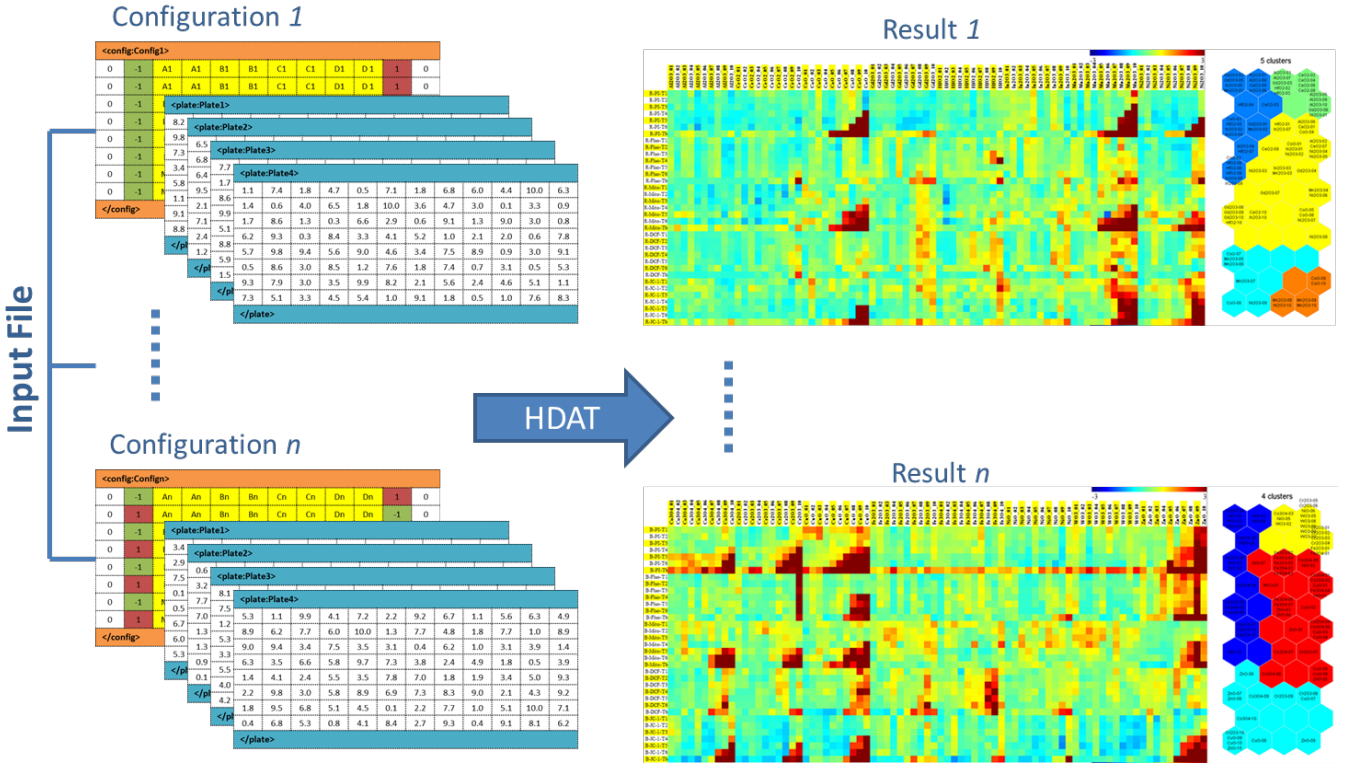
</plate>

Plate data ends

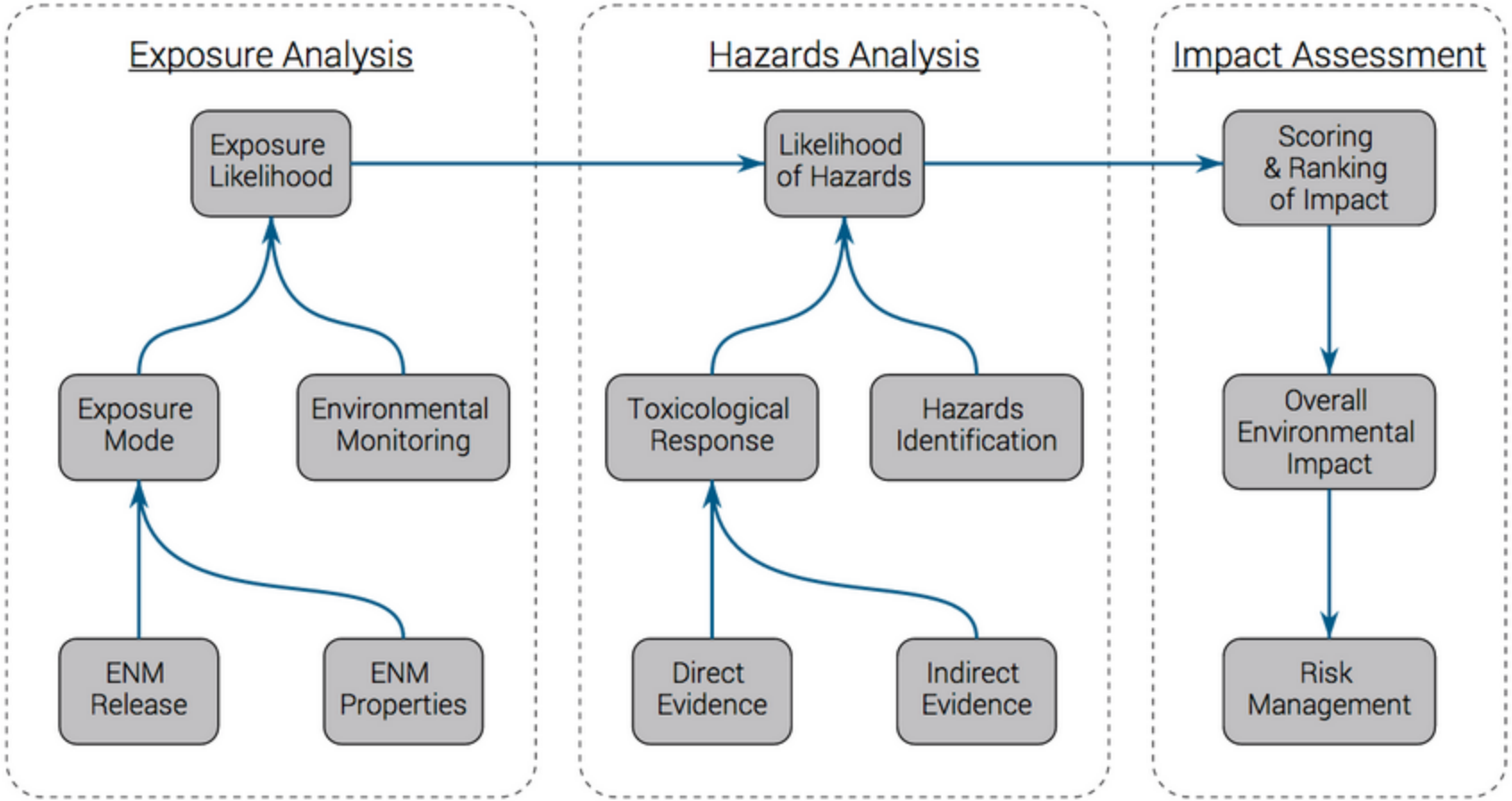
b

ToxNano provides tools for analysis and visualization (e.g., heat maps and self-organizing maps) of HTS data. It also provides QSAR s for predicting toxicity of ENMs

Standardized data format for flexible plate configuration



NanoEIA utilizes ENMs toxicity information to define suitable environmental/toxicity metrics for assessing environmental impacts



NanoDatabank

- Full integration of all the NanoInfo.org tools and data
- Essential for systematic identification and consistent retrieval of data
- Storage of files that are compatible with the NanoInfo.org tools

NanoDatabank

Provide data input for models/tools

Assessment of data completeness

Organization of large amounts of ENMs related data

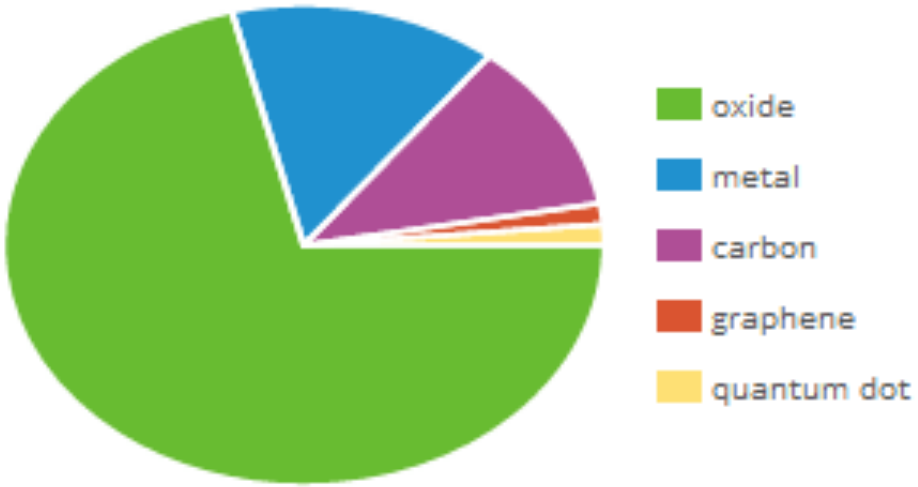
Archive/retrieve documents and publications

Storage of experimental data and simulation results

Contents of NanoDatabank

205 Nanomaterials	208 Characterizations
325 Publications	525 Contributions

Amorphous	Crystalline	Unknown
27% 56	68% 139	5% 9



CEIN Data

- >200 nanomaterial types
  - Physicochemical characterization
  - Toxicity data for various cell lines, zebrafish and bacterial strains
  - Various toxicity assays

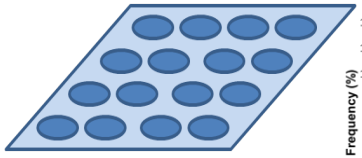
External Data

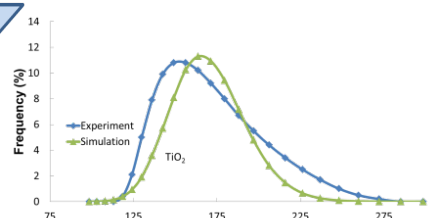
- HTS toxicity for Iron oxide/ surface modified NPs
- Quantum Dots – Literature mined data from 0ver 400 publication/sources
- Cell association with gold/ surface-modified NPs

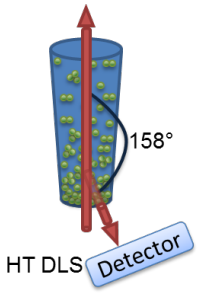
Experimental Data

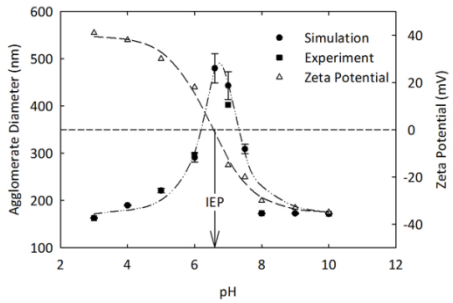
Nanoparticle size characterization:

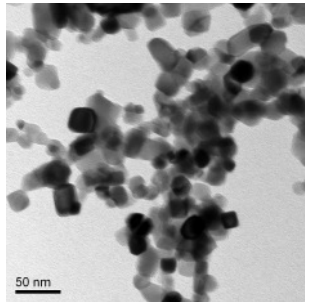
- DLS
- imaging
- zeta potential
- temporal variability
- etc…





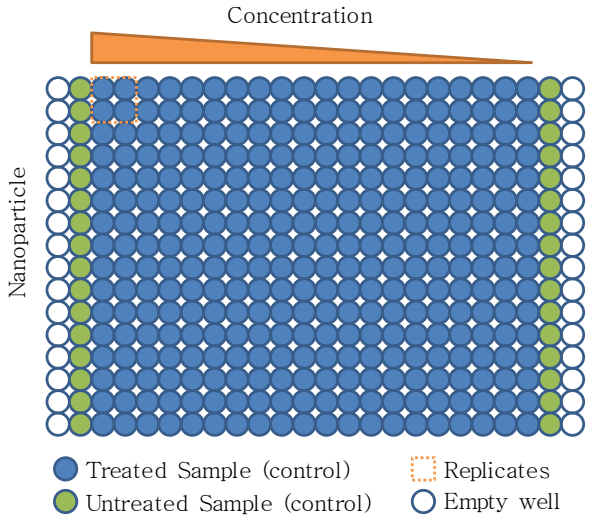


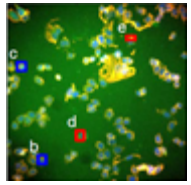


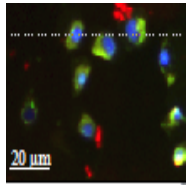


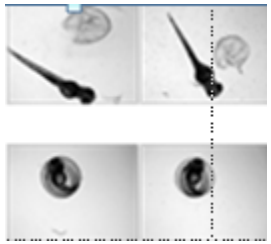
Nanoparticle toxicity screening:

- Different particle types and properties
- Multiple Assays (e.g., cytotoxicity, cell signaling pathways)
- Multiple cell lines
- Various environmental conditions; temporal variability)









Processed Data

Turbidity measurements

System: Kaolinite Al2Si2O5(OH)4 0.005g and with ZnO 30nm, in 10g Nanopure water in a vial

Into a 20
Kaolinite
A small p
pH: 8.91
ZnO30nm
Settling ti

Record	Type	Sample Name	Measurement Date and Time	T (°C)	Z-Ave (d.nm)	Num...
Pk 1 Area Int (%)		Pk 2 Area Int (%)	Peak 3 Area Intensity (%)		Attenuation	
3845	Size	TiO2 - pH8 NaHCO3	Friday, August 27, 2010 1:12:45 PM	23.0	157	
3846	Size	TiO2 - pH8 NaHCO3	Friday, August 27, 2010 1:13:48 PM	23.0	171	
3847						
3848						
3849						
3850						
3851						
3852						
3853						
3854						
3855						
3856						
3857						
3858						

P2 SWNT 1mMK pH7 10mg/L	"08/25/11"	"15:30:20"	0	183.5	0.318
P2 SWNT 1mMK pH7 10mg/L	"08/25/11"	"15:29:50"	0	184.2	0.388
P2 SWN		:29:19"	0	164.6	0.299
P2 SWN		:28:48"	0	162.5	0.334
P2 SWN		:28:18"			
P2 SWN		:27:47"			
P2 SWN		:27:16"			
P2 SWN					
P2 SWN					

B4 | BioSpec-1601

	A	B	C	D
1	Experimer	Differing Concentrations of TiO2 in Seawater With Cou		
2	Date	6/9/11-6/14/11		
3	Notes	Bottles put on shaker table under UV light. Samples fil		
4	Equipmen	BioSpec-1601		
5				
6	Sample	Time (hr)	A	
7	0 mg/L	0		
8		0.25		
9		1		
10		23		
11		24		
12		118		
13		119		
14	1 mg/L	0		
15		0.25		
16		1		
17		23		
18		24		
19		118		
20		119		
21	3 mg/L	0		

TiO2F_10_pH7_100mM CaCl2_1

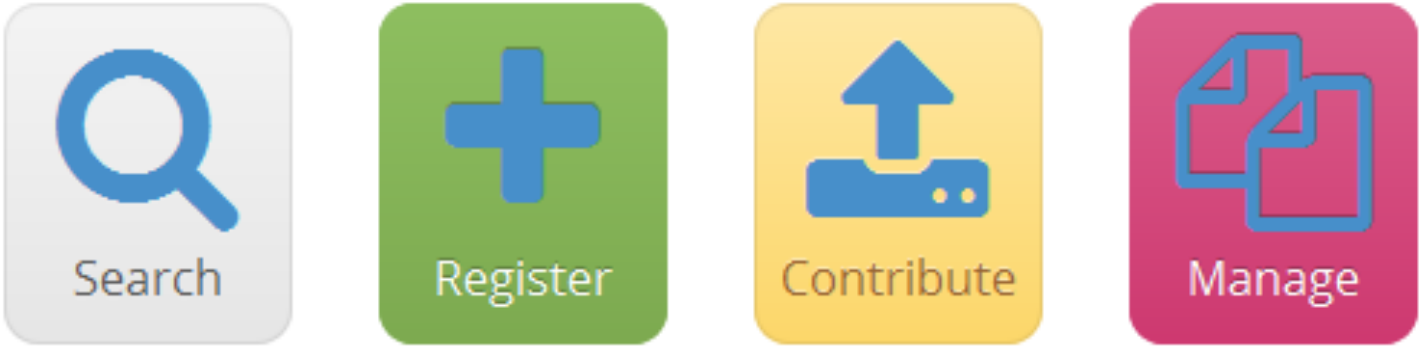
Runs	Mobility	Zet
1	-0.83	
2	0.16	
3	0.38	
4	0.37	
5	-0.44	
6	0.31	
7	0.64	
8	-0.15	
9	-0.19	
10	1.4	
average	0.165	
stdev	0.618371517	7.

Table S1. Agronomic parameters in radish plants 12 days after planting in soil treated with *n*CeO_2 at different concentrations. Data are means of four replicates ± standard deviation.

Parameter*	mg *n*CeO_2 kg^{-1} soil 0	62.5	125	250	500
Plant length (cm)	11.68±0.90	13.03±0.95	11.54±2.17	10.93±1.51	11.29±0.90
Root length (cm)	2.21±0.35	3.02±0.44	2.47±0.21	2.40±0.21	2.52±0.16
Leaf length (cm)	6.72±1.00	7.88±0.16	6.58±0.28	6.16±0.18	6.79±0.13
Shoot length (cm)	2.75±0.95	2.13±0.16	2.50±0.28	2.37±0.18	1.98±
Number of true leaves	2.00±0	2.00±0	2.00±0	2.00±0	2.00±0
Roots dry weight (mg)	1.05±0.14	1.44±0.48	1.21±0.19	0.96±0.48	1.17±0.25
Shoots dry weight (mg)	3.19±0.42	3.34±0.88	2.94±0.94	2.98±0.69	3.10±0.45
True leaves dry wt (mg)	12.98±6.94	20.53±4.79	17.25±8.10	13.48±5.16	15.64±0.96
Cotyledon leaves d wt (mg)	14.79±2.45	17.48±2.33	15.51±5.18	14.79±3.12	15.50±1.32

NanoDatabank Features

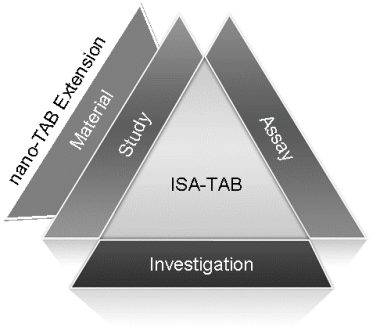
Standard Features



Search	Register	Contribute	Manage
Search for a particular nanomaterial	Register a unique nanomaterial	Upload, classify and link files	Manage files and records

What makes it unique?

- You can customize settings for your organization, manage/ create own metadata dictionary, define own configuration
- Export nanomaterial data into ISA-TAB-Nano format
- Integrate additional tools via NanoInfo API and automatically trigger files that are compatible



Our Configuration

Similarity Threshold *= 75%*

Similarity Score *= IF(a_formula==b_formula) { .50 + IF (a_shape==b_shape) {return .20;} + IF (a_crystalstructure=b_crystalstructure) {return .10;} + (1-(ABS(a_size-b_size)/ MAX(a_size,b_size)) * **.10**; + IF (a_source=b_source) {return .10;} } ELSE {return 0};*

Nanomaterial Details

Name	Titanium Dioxide P25
Formula	TiO2
Shape	irregular
Primary Size	21
Crystal Structure	rutile; anatase
Phase	mix
Source	Dorsett & Jackson Inc.
Registered By	Taimur Hassan on 6/28/2010 14:36

Similarity

None

Our score weight for nanomaterial size is **0.0**

Titanium Dioxide P25 from our view

Your Configuration

Similarity Threshold *= 75%*

Similarity Score *= IF(a_formula==b_formula) { .50 + IF (a_shape==b_shape) {return .20;} + IF (a_crystalstructure=b_crystalstructure) {return .10;} + (1-(ABS(a_size-b_size)/ MAX(a_size,b_size)) * **0.0**; + IF (a_source=b_source) {return .10;} } ELSE {return 0};*

Nanomaterial Details

Name	Titanium Dioxide P25
Formula	TiO2
Shape	irregular
Primary Size	21
Crystal Structure	rutile; anatase
Phase	mix
Source	Dorsett & Jackson Inc.
Registered By	Taimur Hassan on 6/28/2010 14:36

Similarity

TiO2 P25 with anionic coating, 50 mg/mL in water	9
TiO2 P25 with cationic coating, 50 mg/mL in water	12
AML Anatase 021710 #17, 0.40 wt.% in water	3
AML TiO2 Rutile 021710 #1, 3.02 wt.% in water	21
AML TiO2 718 #4, 2.4 wt.% in water	30
HOMBIKAT UV 100, Uncoated TiO2	11

Your score weight for nanomaterial size is **0.0**

Titanium Dioxide P25 from your view

Custom Settings

Lab Administration » Manage laboratory specific settings

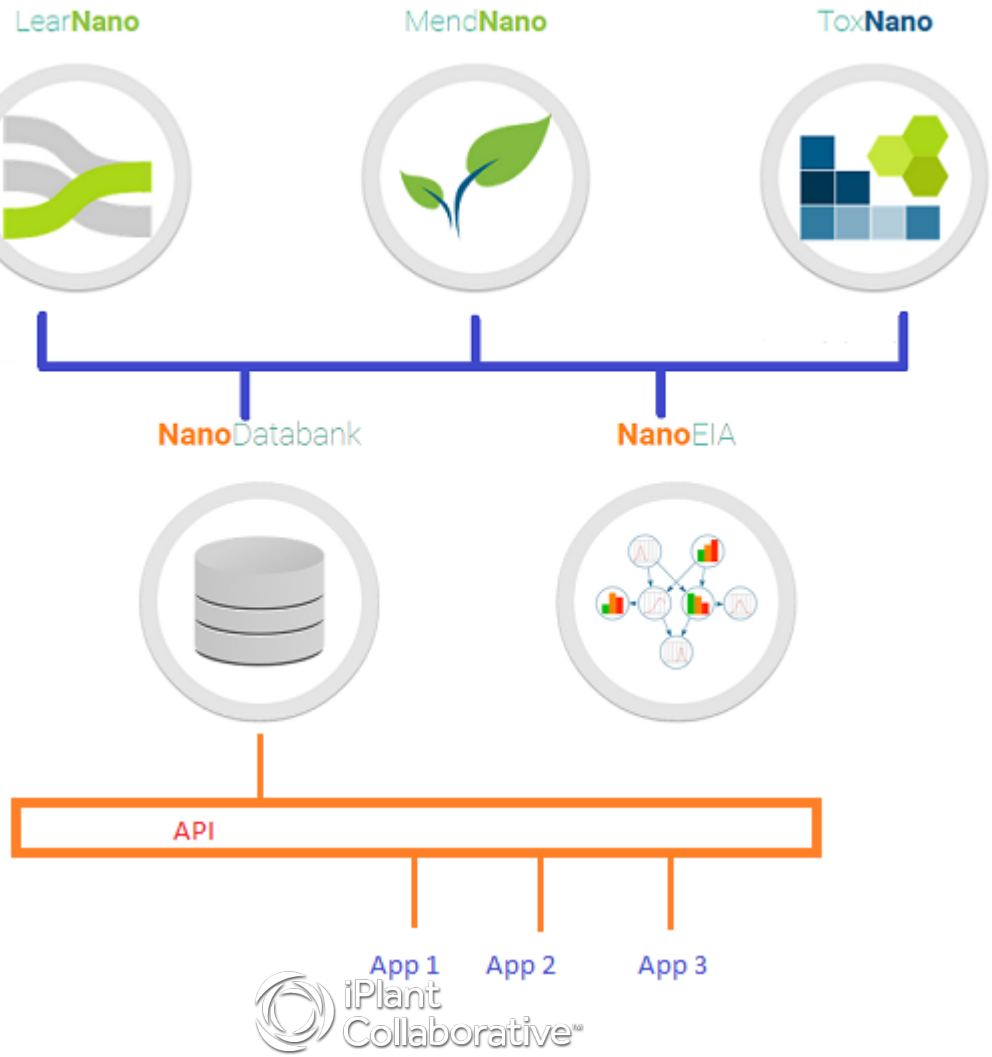
Formula | Inventory | Material Type | Shapes | Settings | Metadata

	MetaKey ID	MetaKey Name	Display Text	File Classification	Field Type	Options	Expired?
	10	processdescription	Process Description	processed data	1		0
	11	processingdate	Processing Date	processed data	4		0
	12	contents	Contents	processed data	1		0
	13	concentration	Concentration	raw data	3		0
	14	medium	Medium	raw data	1		0
	15	duration	Duration	raw data	3		0
	16	ph	pH	raw data	3		0
	17	sampletemperature	Sample Temperature	raw data	3		0
	18	target	Target	raw data	1		0
	19	analysistype	Analysis Type	raw data	3	,quantitative,qualitative	0
	20	instrument	Instrument	raw data	3	,JEM 1200-EX,CM 120,T12,TF20,Titan Krios,Mervyn,Other	0

Expandable System

Currently useable on mobile platforms, but support is being expanded for increased usability

NanoInfo API as a connector for other ENMs tools external to NanoInfo.org



Conclusion

An integrated nanoinformatics platform addresses the challenges of managing complex data for ENMs research

Using the fully integrated NanoInfo.org platform leads to flexible and more effective utilization of information, data analysis, and interfacing with decision analysis tools aimed at assessing the environmental impacts of engineered nanomaterials

It is envisioned that NanoInfo.org will emerge as a support system that could potentially be useful in various applications related to the production, use and disposal of engineered nanomaterials

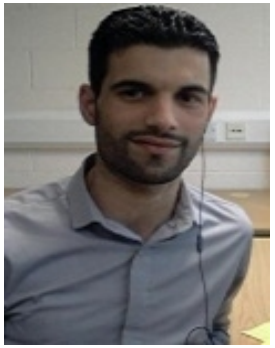
NanoInfo.Org Team

Prof. Yoram Cohen

Rong Liu

Haven Liu

Muhammad Bilal



Michelle Romero

Dennis Bacsafra

Acknowledgements: UC CEIN, Ivy Ji

Questions