

Updating the NBI knowledgebase to provide design rules for safer nanotechnology



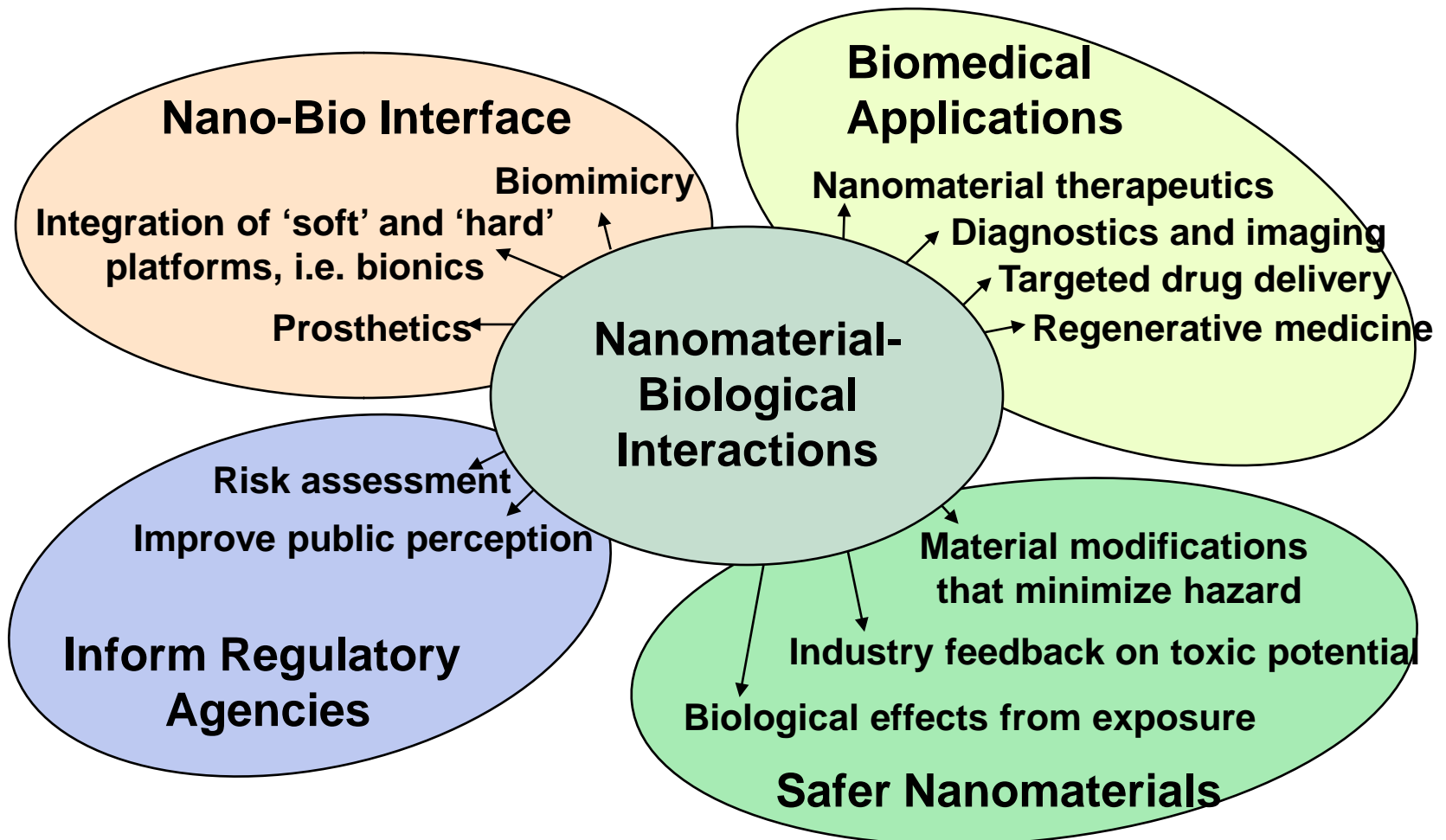
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Acknowledgements



Need to Define Nano-Bio Interactions



Rationale for the NBI Knowledgebase

Information void

Unique physicochemical properties – unique interactions with biological systems

No relative baseline for studies

Testing protocols may need to be adapted

Nanomaterials

Relative importance of nanomaterial characteristics?

Physicochemical Properties

Chemicals

Structure

pKa

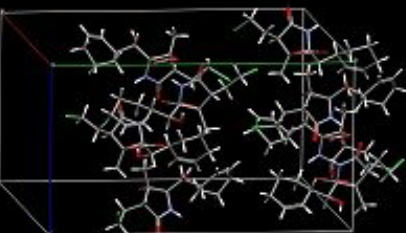
Solubility

log *P*

3-D Molecular Structure



3-D Crystal Structure



Nanomaterials

Chemical Structure

Core Particle Composition

Size

Shape

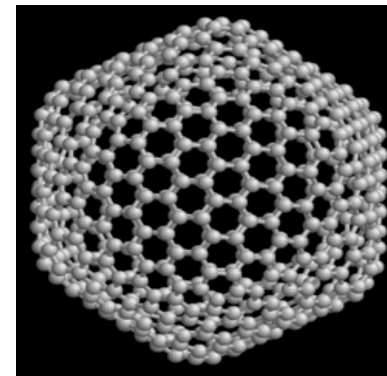
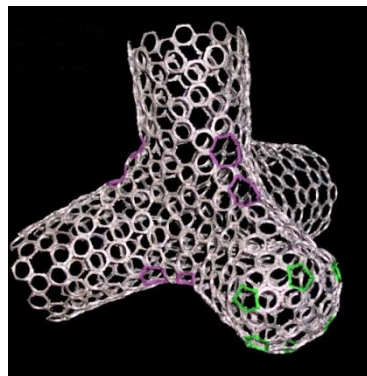
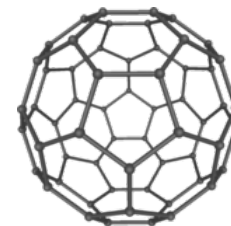
Charge

Surface Chemistry

Surface Area

Agglomeration State

Zeta Potential



Investigations to Define Nanomaterial-Biological Interactions

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Relative importance of nanomaterial characteristics?

Appropriate dose metrics?



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Dose Metrics?

Mass of core

Total mass (core + ligands)

Atoms

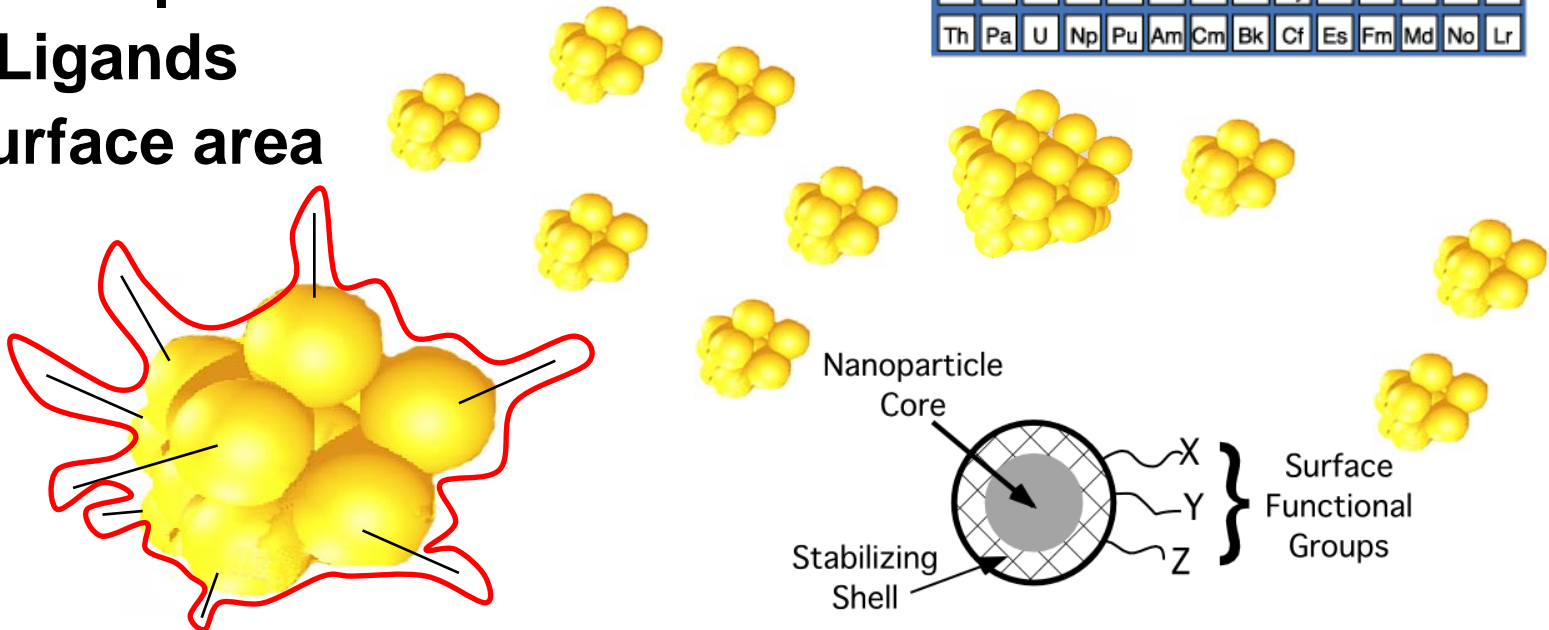
Nanoparticles

Ligands

Surface area

Periodic Table of Elements

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac	Unq	Unp	Unh	Uns	Uno	Une	Uun	Uuu	Uub	Uut	Uuq	Uup	Uuh	Uus	Uuo
		Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
		Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		



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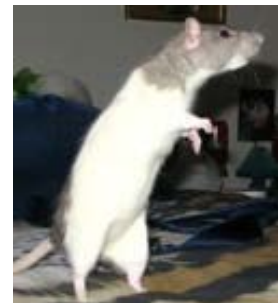
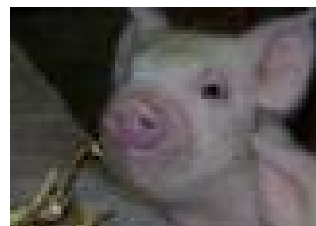
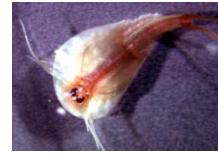
Appropriate dose metrics?

Experimental design variables

Biological test system

Biological Test System

Whole Animal
Cell Culture
Species
Age/Life Stage
Gender
Weight
Cell Line



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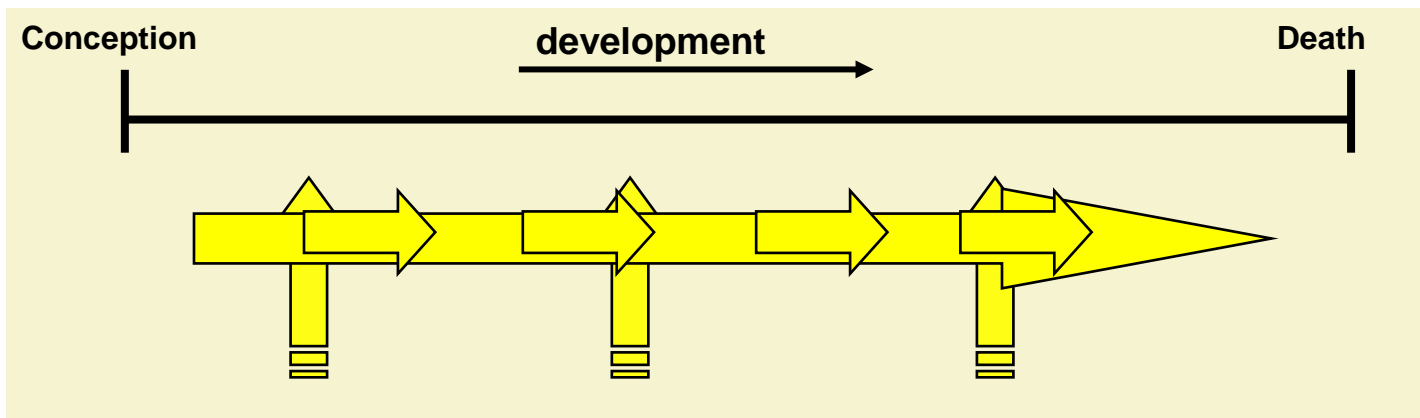
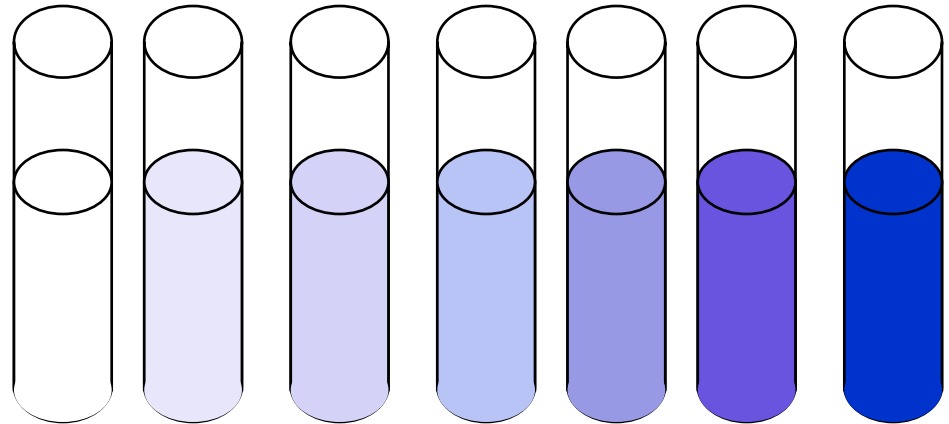
Experimental design variables

Biological test system

Exposure Scenario

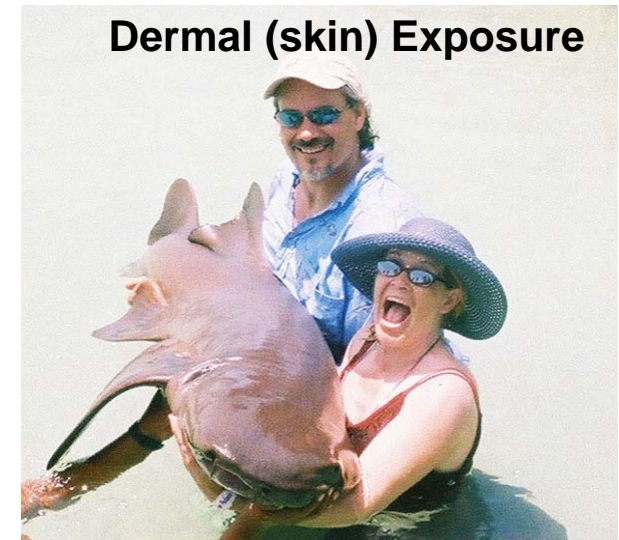
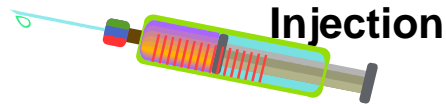
Exposure Scenario

Dose/Concentration
Timing
Duration



Exposure Scenario

Dose/Concentration
Timing
Duration
Route of Exposure



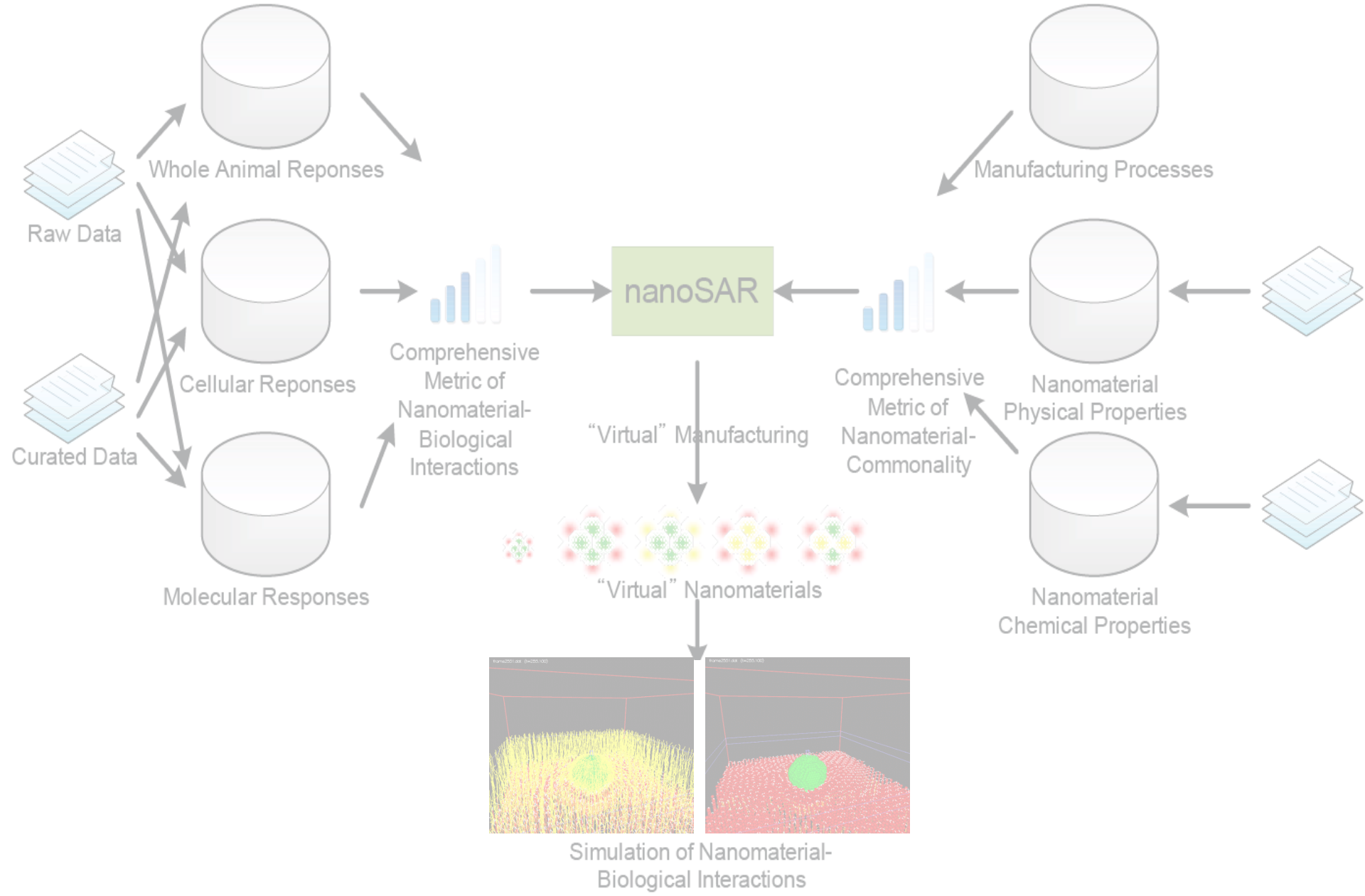
Oral Exposure



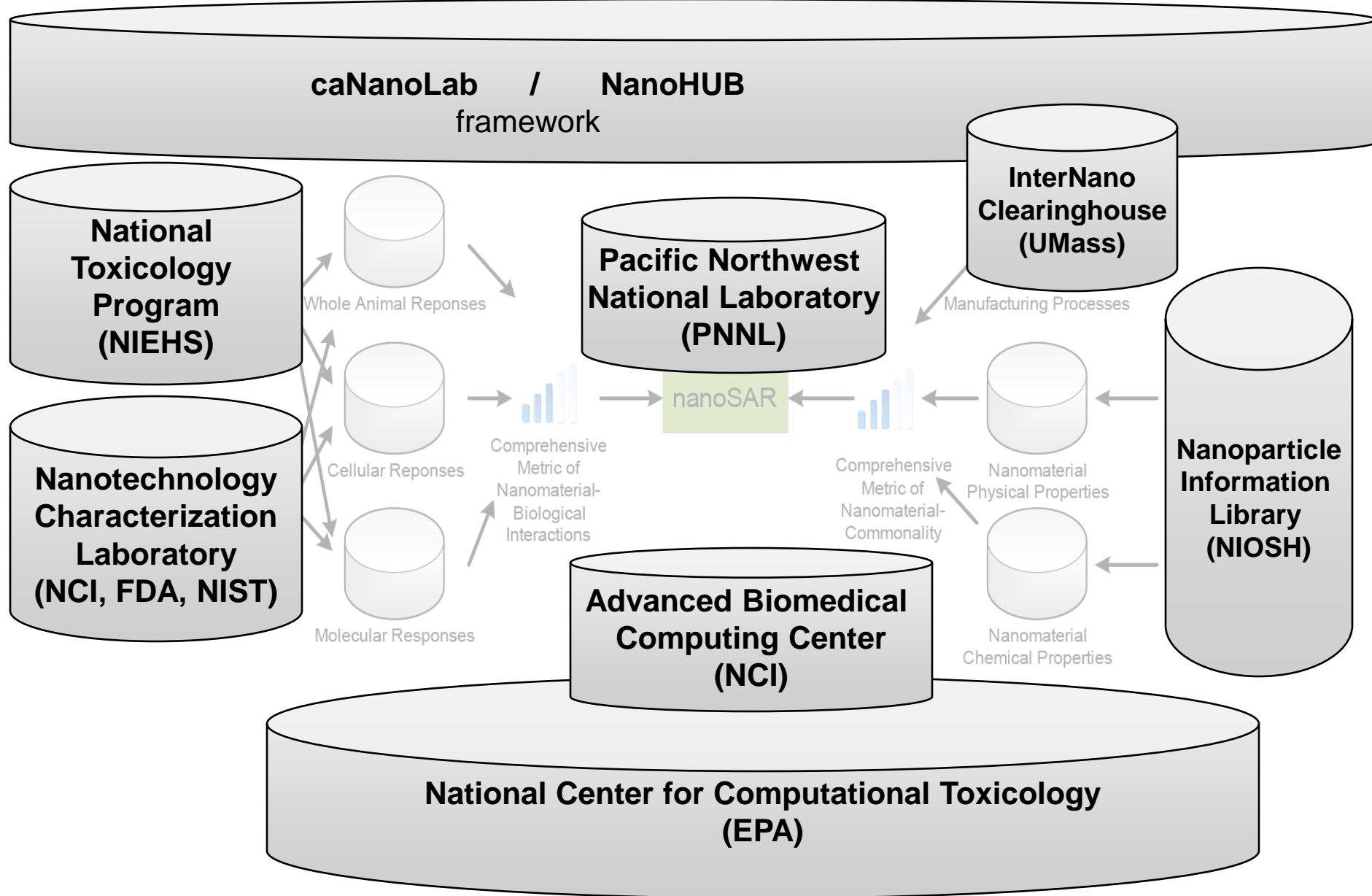
Goals of NBI Knowledgebase

- To organize and analyze data and compare results across research platforms in an effort to define robust structure-property relationships
- To identify the functional structure and design principles of high performing, environmentally-benign nanomaterials
- To predict potential biological impacts of unsynthesized nanomaterials

NBI Knowledgebase



Interoperable, Federated System of Data/Knowledgebases for Nano-Bio Informatics





NBI Updates

- User-friendly interface
- User privilege management
 - 5 user levels with different privileges
 - Now, login required
 - Multiple administrative levels
- Data management
 - Data access and input based on user privileges
 - Flexible and extendable database design
- Data analysis tools
 - Graphing and color coding data