Environmental Science: Nano

Supporting Information

Visualization Tool for Correlating Nanomaterial Properties and Biological Responses in Zebrafish

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Table of descriptions of the nine targeted nanomaterial characteristics

Descriptions of the targeted characteristics selected for use in the visualization tool and the number of Excel files in which that characteristic was populated are provided in the Table S1.

Table S1: Descriptions of the nine targeted characteristics used by the visualization tool and the number of Excel files in which that characteristic was populated.

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Characteristic (# populated)	Description
Surface Charge: (72)	General classification of the surface charge. Options are: "positive", "negative", or "neutral". When the field is not populated, the charge of the surface is unknown or was not specified. Nulls were replaced with "unknown".
Primary Particle Size: Avg. (nm) (117)	The primary particle size. The NBI Knowledgebase also provides a place to store the minimum and maximum particle size. For this work, the minimum and maximum values are not used as separate characteristics. In four files where a primary size was not provided, a maximum value was provided (no corresponding minimum was provided), and in those cases, that maximum value was used as the average. In the remaining cases, the primary particle size remained null.
Outermost Surface Functional Groups (89)	A layer that does not fully coat the previous layer. This can be a functional group layer covering the core (if no shell was added), or covering the shell. A list of each nanomaterial and its outermost surface functional group composition is provided on nanoHUB. Nulls were replaced with "none".
Core Atomic Composition (147)	The material of the core of the nanoparticle. A list of each nanomaterial and its core composition is provided on nanoHUB. Information from the particle descriptor was used to populate the missing value. In a few cases, two materials are combined and listed in the NBI Excel file as the core atomic composition ("gold [Au]; silver [Ag]" instead of a gold core with a silver shell). These were not changed for use in the tool.
Material Type (147)	Indicates the general type of the nanomaterial (based on the core composition). Limited to one per nanomaterial from the options: "carbon", "cellulose", "dendrimer", "metal", "metal oxide", "polymeric", or "semiconductor". Information from the particle descriptor was used to populate the missing value.
Shell Composition (48)	The material composition of a layer that fully coats the core of the nanoparticle. A null field indicates that there was no shell on the nanomaterial. Current options include: "carboxylic acid", "cetyl trimethylammonium bromide", "fluorescein isothiocyanate [FITC]", "none", "poly(amidoamine) [PAMAM]", "silica [si]", "silica [si], 98%; fluorescein isothiocyanate [FITC], 02%" (02% is shown in the text of the manuscript as 2%), "sulfate", "sulfonic acid", and "triphenyl phosphine". Nulls were replaced with "none".
Purity (107)	An indicator of the purity of the nanomaterial in regards to residual non-particle reactants. The current options are: "as synthesized" (which ranges in meaning from unknown to synthesized using a published methodology), "pure" (indicating 97% or greater), "ultra pure" (indicating 99% or greater), or "unknown". A null in this field indicates the purity is unspecified or unknown. Nulls were replaced with "unknown".
Core Shape (108)	The general shape of the core. Current options include: "cylindrical", "dendritic", "fibrous", "abnormal-angular", "regular-angular", "rod", or "spherical". A null in this field indicates the shape is unknown. Nulls were replaced with "unknown".
Core Structure (69)	The core structure field is a catch-all field capturing important information about the core. The current options include: "120nm fiber width by TEM, length unknown", "hollow", "solid", "solid 3% Mn doped", "solid, 1% Mn doped", "tube, OD=8nm ID=2-5nm Length= 0.5-200 um", "Zinc nanoparticles doped with Aluminum oxide". Nulls were replaced with "unknown".

With the exceptions of the shell and outermost surface compositions, characteristics were selected for use in the visualization tool if meaningful information was provided in more than 60 of the 148 Excel files. More information regarding what is provided in the Excel files is available on nanoHUB [Sandra Karcher (2016), "Informatics Tool to Explore the Nanomaterial-Biological Interactions Knowledgebase," https://nanohub.org/resources/23991].

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The concentration gradient heat maps (visualization option 2) for mortality at 120 hpf (B) and abnormalities (C) aggregated by the combination of core, shell, and surface composition and by surface charge

The B (mortality at 120 hpf) and C (abnormalities) concentration gradient heat maps for all nanomaterials and all responses are provided in Figure S1.

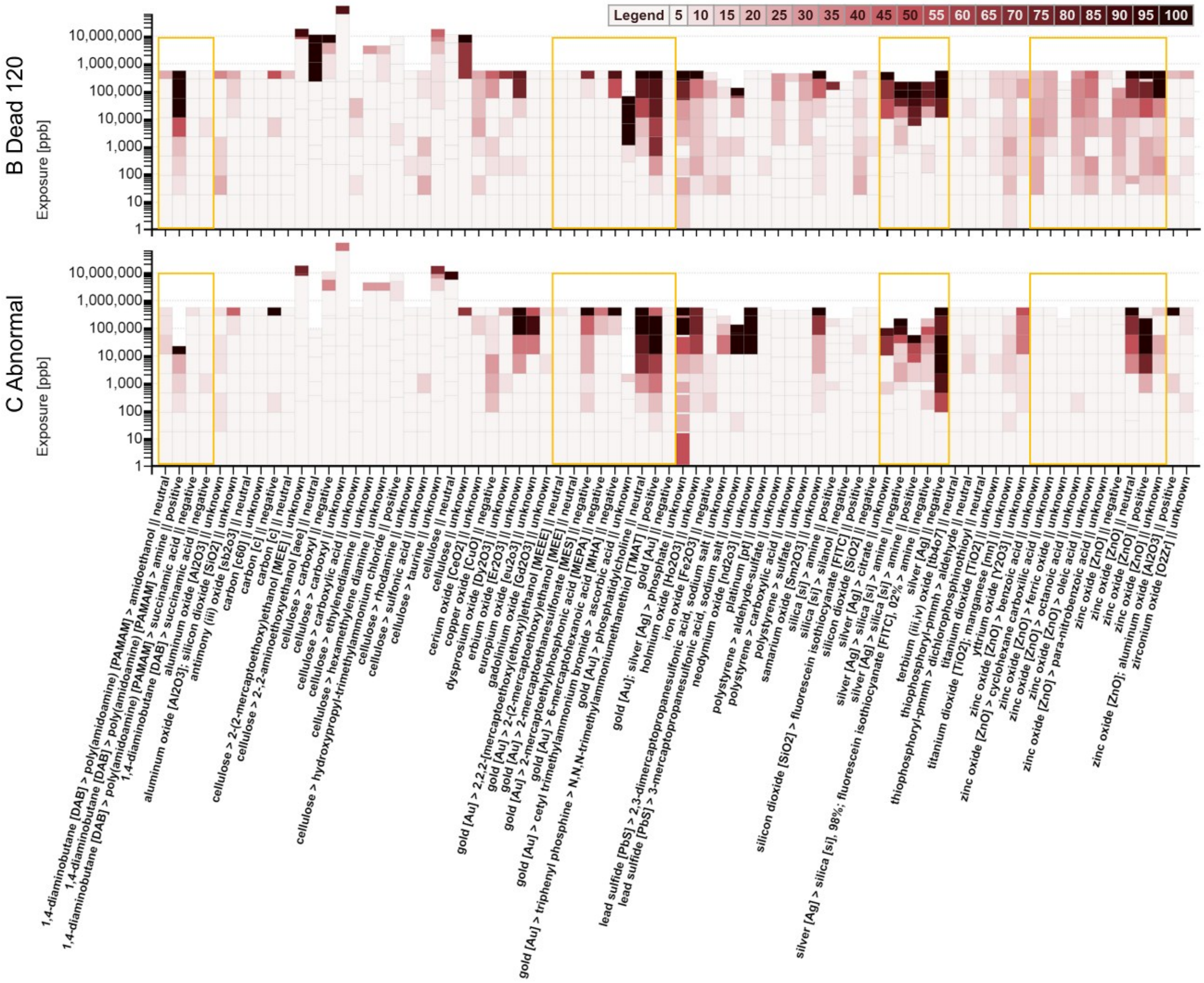

Figure S1: The concentration gradient heat maps (visualization option 2) for mortality at 120 hpf (B) and abnormalities (C) aggregated by the combination of core, shell, and surface composition and by surface charge. All sublethal biological responses and nanomaterials are included. Cores of like composition are grouped in boxes for easier visual comparison.

The concentration gradient heat maps (visualization option 2) for mortality at 120 hpf (B) and abnormalities (C) aggregated by surface charge and by the combination of core, shell, and surface composition

Based on the observations within core compositions groups, the graphs were sorted, first by surface charge, then by core, shell, and surface composition. These graphs are shown in Figure S2.

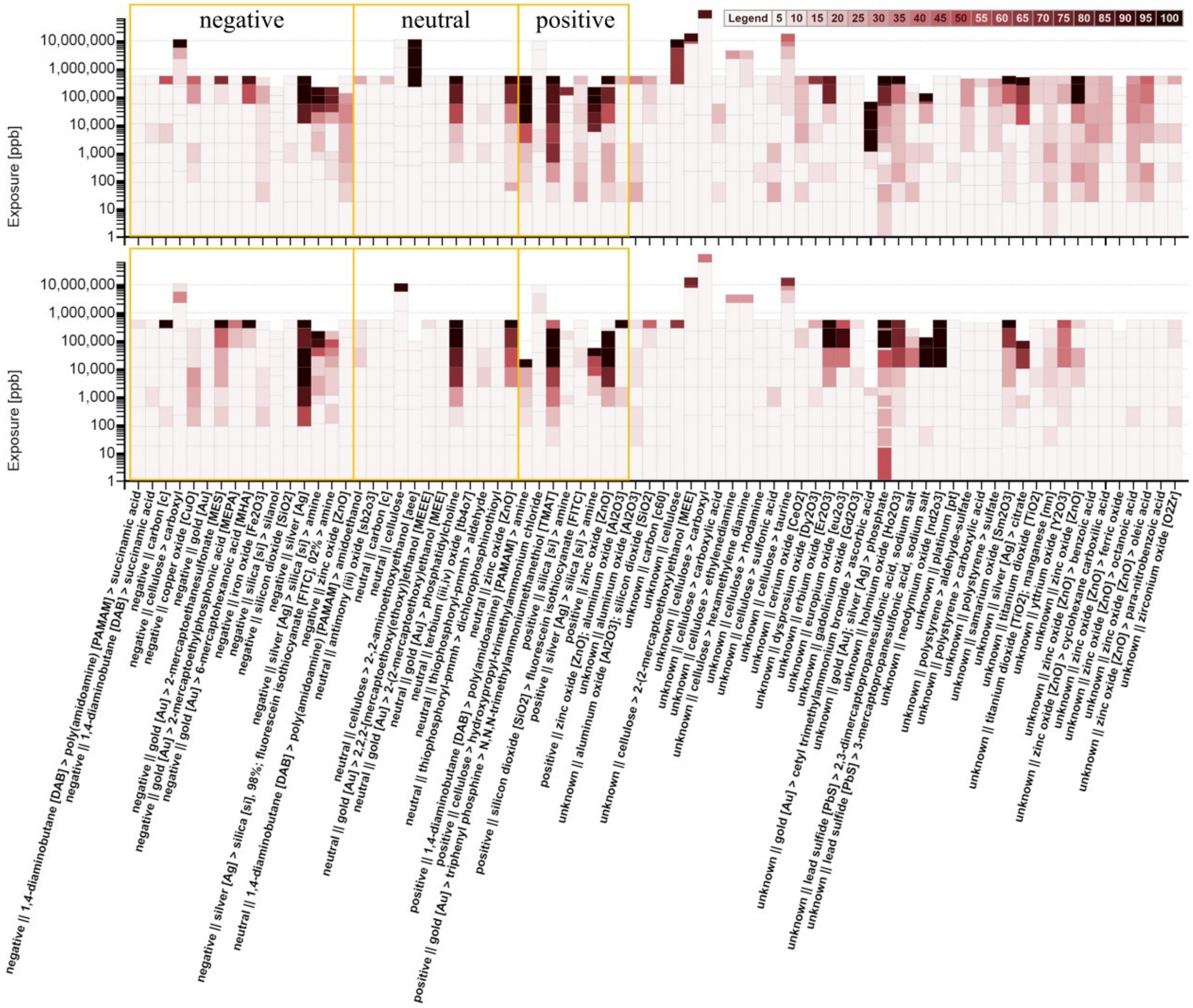

Figure S2: The concentration gradient heat maps (visualization option 2) for mortality at 120 hpf (B) and abnormalities (C) aggregated by surface charge and by the combination of core, shell, and surface composition. All sublethal biological responses and nanomaterials are included. In the mortality graph (B), particle charges are grouped in boxes for easier visual comparison.

Figure S2 confirms observations from Figure S1 with regard to surface charge, that there is some visual evidence to suggest that positively charged materials might be more deadly than neutral and negatively charged particles.

The response gradient heat maps (visualization option 3) for abnormalities (C) aggregated by the combination of surface, shell, and core

The maximum response (percentages shown in boxes) gradient heat map is shown in Figure S3 for selected nanomaterials aggregated by the combination of surface, shell, and core across the x-axis, with sublethal abnormalities over the y-axis.

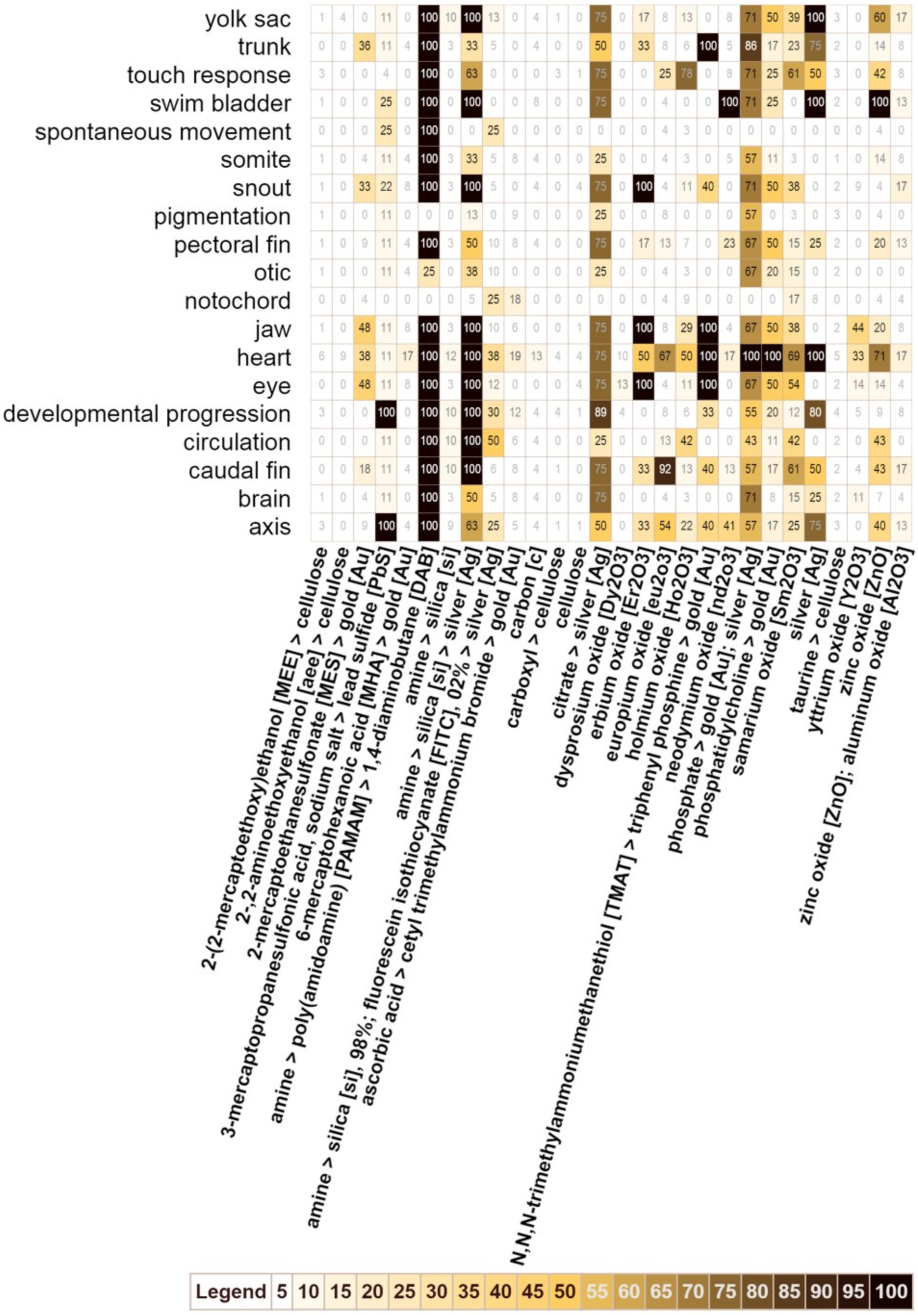

Figure S3: The response gradient heat maps (visualization option 3) for abnormalities (C) aggregated by the combination of surface, shell, and core showing the results using selected nanomaterials and all responses meeting the threshold target exposure concentration of 100,000 ppb.

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The concentration gradient heat maps (visualization option 2) for mortality at 120 hpf (B) and abnormalities (C) aggregated by the combination of core, shell, and surface composition and by particle size

Figure S4 shows the mortality at 120 hpf (B) and abnormalities (C) concentration heat maps for all nanomaterials and all responses grouped by core, shell, and surface composition and then by size.

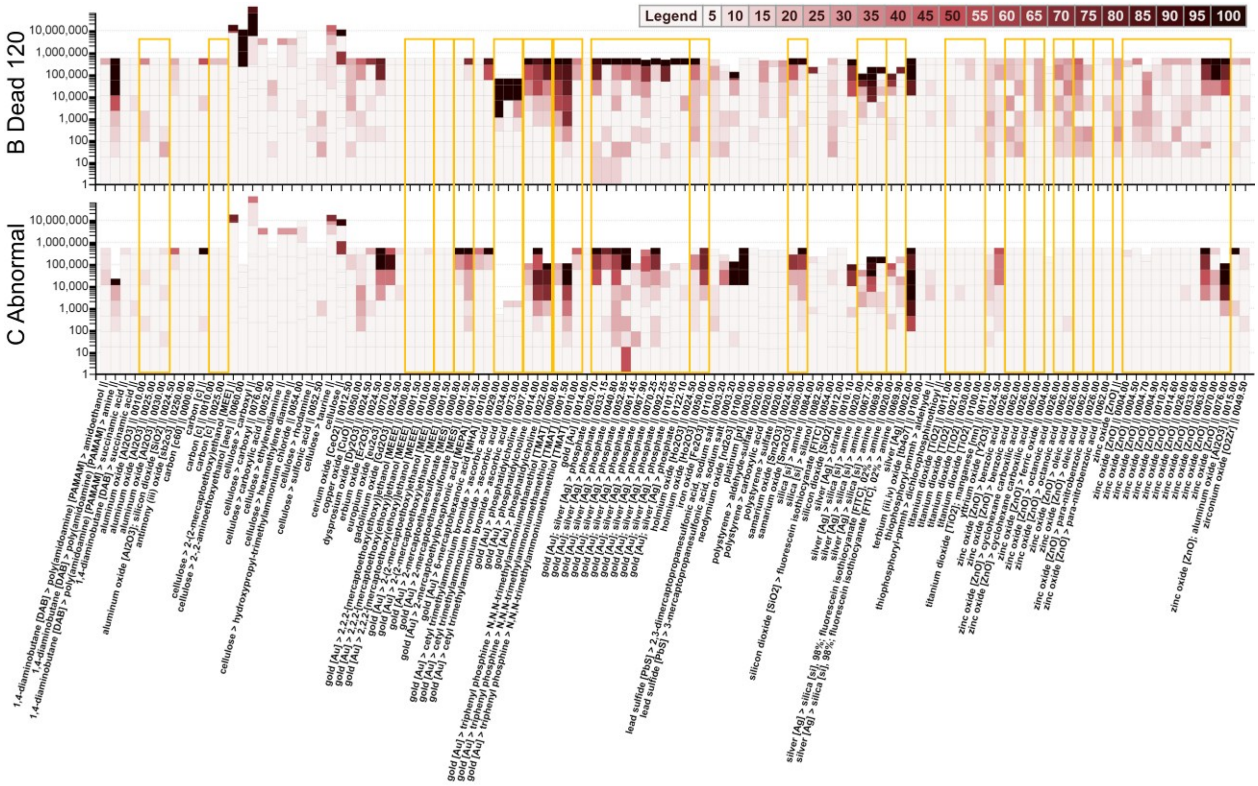

Figure S4: The concentration gradient heat maps (visualization option 2) for mortality at 120 hpf (B) and abnormalities (C) aggregated by the combination of core, shell, and surface composition and by particle size. All sublethal biological responses and nanomaterials are included. Groups of core, shell, and surface composition are boxed together for easier visual comparison.

In Figure S4, the same combinations of materials, split by different particle size, are shown with bands around the group. Differences in toxicity can be seen within a group, but a clear trend with size across the groups is not evident.