

Data, Metadata and “Data Quality” for Databases

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# Confidence & Purpose

- Reproducibility instills confidence;
- Protocols and metadata are other tools;
- Legal certainty is not scientific certainty;
- Relevance implies purpose;
- Explanations encompassing protocols, controls and metadata choices are preferred when setting acceptable reproducibility.

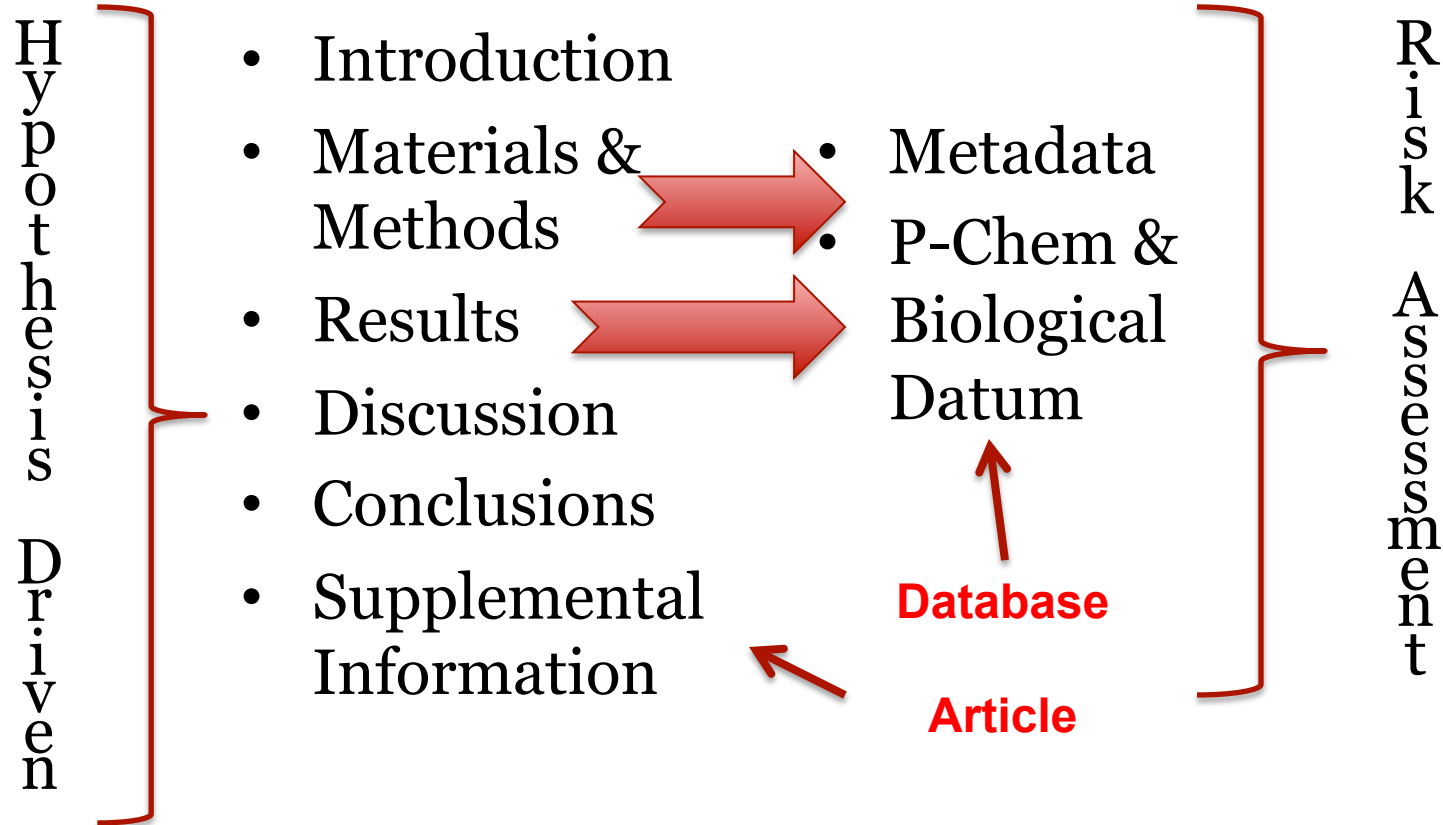
## Outline of talk:

1. Illustrate divide between scientific and legal purposes;
2. Examine effect of a nascent MOA on metadata ; and
3. Differentiating roles and responsibilities of curator and database user.



Braque: Guggenheim

# Mixing Hypotheses & Risk Assessment Purposes



Risk Assessment Avoids False Positives for Legal Reasons  
Hypotheses Balance False Positives & False Negatives

# *Daphnid Constipation*

- **EPA poster:** protocol adjustment (static renewal) and controls lead to whole organism Mode of Action (MOA) useful to risk assessment: gut obstruction ;
- **MOA focuses on:** ingestible particles (<30  $\mu\text{m}$  in *Daphnids*) & suspended solids literature for ecological insight; and
- **Recent articles:** nanoTiO<sub>2</sub> ~ clay and possible size distinctions based on cell entry (<500 nm for viruses; FK).

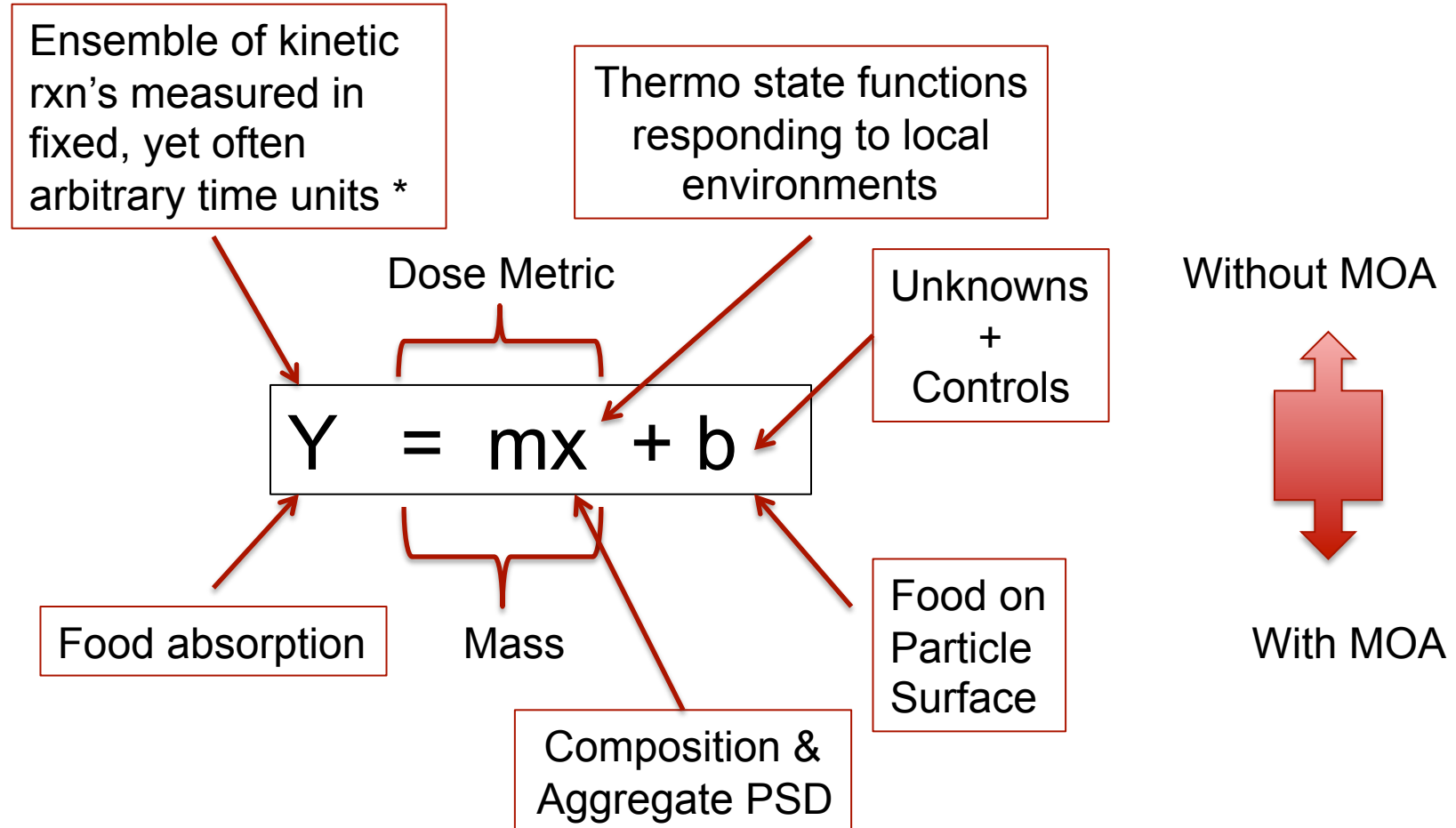
Pursuing reproducibility with current metadata would not reduce test variability;

Static renewal might lower variability; and

For MOA, needed dosing technique and added controls.

*See references for additional commentary*

# Independent & Dependent Variables



*\* See Theophel reference for continuous growth discussion*

## Recommendations

Database Curator (or Administrator) has a different role and responsibility from the Database User

These can be expressed in a description of the database, its purpose, sources & operation:

1. The selection criteria regarding data sources;
2. “Study evaluation” criteria (a.k.a. compliance or Klimisch scores), & their breadth & function, plus articles illustrating these preferences; and
3. Database boundaries, such as raw vs. processed data or publication dates covered or confidentiality requirements, etc.



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*See Leonelli reference*

# Thank You

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## Acknowledgements:

- Marty Fritts
- Sharon Ku
- John Rumble



# Citations

Slide	Reference(s)
4	<ul style="list-style-type: none"><li>• Sayre &amp; Kennedy, “Carbon Nanotube (CNT) Nanomaterial Eco- logical Risk Assessment Trends, and Recent Protocol Needs as seen under the Toxic Substances Control Act,” SETAC 2014 Conference Poster.</li><li>• Edgington, Aaron J., Aaron P. Roberts, Leigh M. Taylor, Matt M. Alloy, Jason Reppert, Apparao M. Rao, Jingdong Mao, and Stephen J. Klaine, “The Influence of Natural Organic Matter on the Toxicity of Multiwalled Carbon Nanotubes,” <i>Environmental Toxicology and Chemistry</i>, 2010, 29 (11): 2511–2518</li><li>• Alloy, Matthew M., Aaron P. Roberts, “Effects of suspended multi-walled carbon nanotubes on daphnid growth and reproduction,” <i>Ecotoxicology and Environmental Safety</i>, 2011, 74: 1839–1843</li><li>• Robinson, Sarah E., Neil A. Capper and Stephen J. Klaine, “The Effects of Continuous and Pulsed Exposures of Suspended Clay on the Survival, Growth, and Reproduction of <i>Daphnia Magna</i>,” <i>Env. Tox. and Chem.</i>, 2010, 29(1): 168–175</li><li>• Zhang, Xiaoyan, Peiyong Guo, Jinxiu Huang, Xiufu Hou, “Effects of suspended common-scale and nanoscale particles on the survival, growth and reproduction of <i>Daphnia magna</i>,” <i>Chemosphere</i>, 2013, 93: 2644–2649</li></ul>
5	<ul style="list-style-type: none"><li>• Theophel K, Schacht VJ, Schlüter M, Schnell S, Stingu C-S, Schaumann R and Bunge M, “The importance of growth kinetic analysis in determining bacterial susceptibility against antibiotics and silver nanoparticles,” <i>Front. Microbiol.</i>, 2014, 5:544</li></ul>
6	<ul style="list-style-type: none"><li>• Leonelli, Sabina, “Data Interpretation in the Digital Age,” <i>Perspectives on Science</i>, 2014,22(3): 397-417</li></ul>