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Evaluating chemical contaminants in biosolids: A collaboration between EPA's Center for Computational Toxicology and Exposure and EPA's Office of Water

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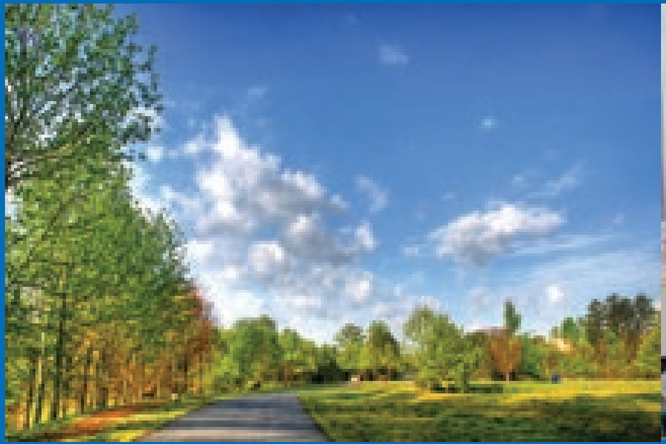

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Overview

- What are biosolids?
- How EPA evaluates biosolids contaminants under the Clean Water Act
- Risk screening & assessment for biosolids contaminants has been slowed by lack of available data regarding hazard & exposure
- EPA Office of Water (OW) proposes a new process to increase efficiency
- Researchers from EPA Office of Research & Development (ORD) Center for Computational Toxicology & Exposure (CCTE) are working closely with OW to develop and adapt data & tools to support OW's decision-making process
  - CCTE collaboration: Curation of list of chemicals found in biosolids
  - CCTE collaboration: Chemical prioritization workflow
  - CCTE collaboration (work in progress): High-throughput model of biosolids chemical occurrence

What are biosolids?

- Biosolids are treated sewage sludge.
- During wastewater treatment process, solids and liquids are separated
- Solids are treated physically and chemically to produce a semisolid, nutrient-rich product known as *biosolids*
- Biosolids are used or disposed in one of several ways:
  - Land application: Biosolids may be used as fertilizer on agricultural land, soil amendment on non-agricultural land, etc
  - Landfill
  - Incineration
  - Other

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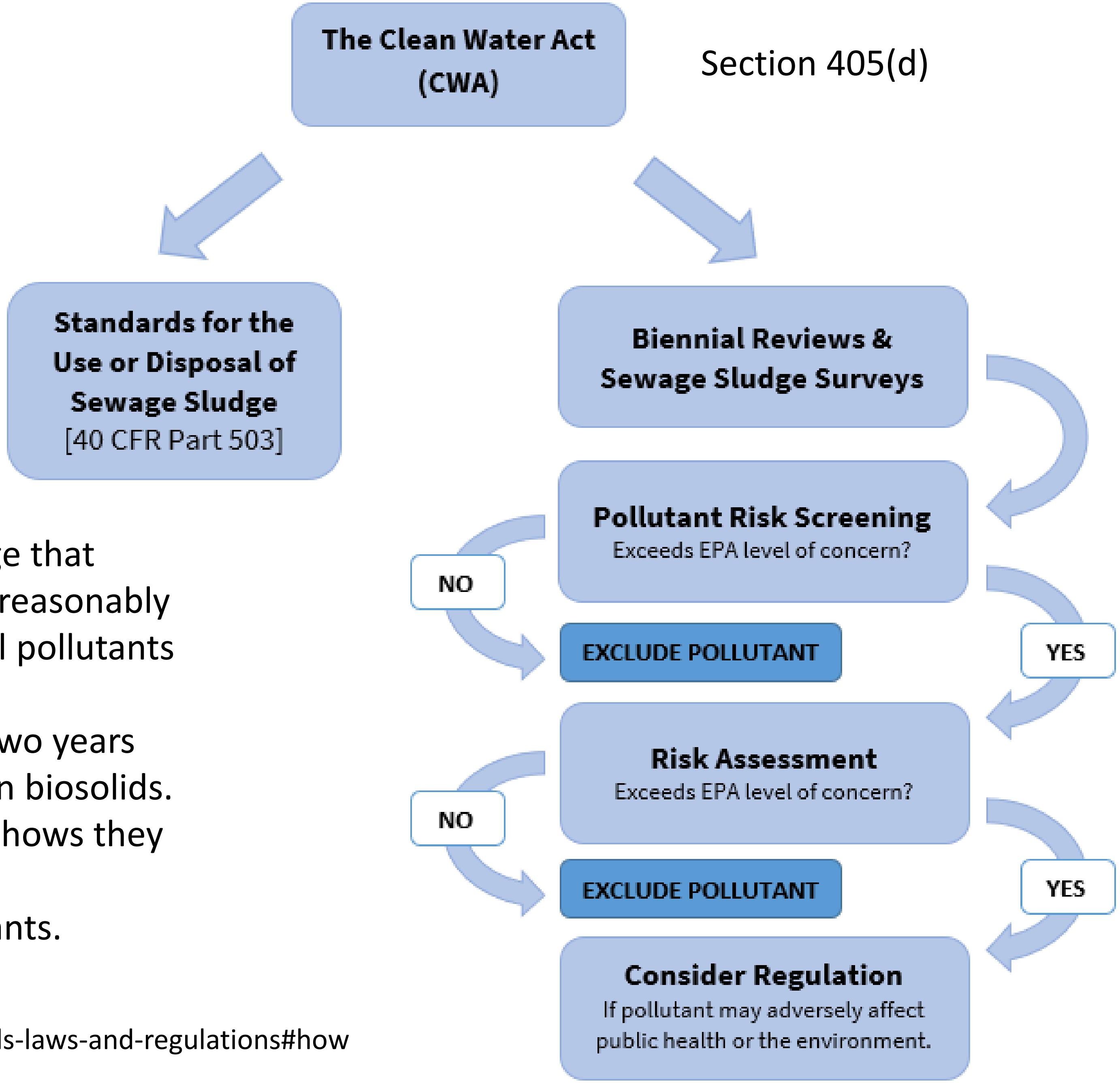
EPA and biosolids under the Clean Water Act

Section 405(d) of the CWA requires EPA to:

- Set standards for the use or disposal of sewage sludge that protect public health and the environment from the reasonably anticipated adverse effects of chemical and microbial pollutants (40 CFR Part 503)
- Review sewage sludge (biosolids) regulations every two years to identify any additional pollutants that may occur in biosolids.
  - Evaluate whether sufficient scientific evidence shows they may harm human health or the environment.
  - If so, then consider regulations for those pollutants.



Source: https://www.epa.gov/biosolids/biosolids-laws-and-regulations#how

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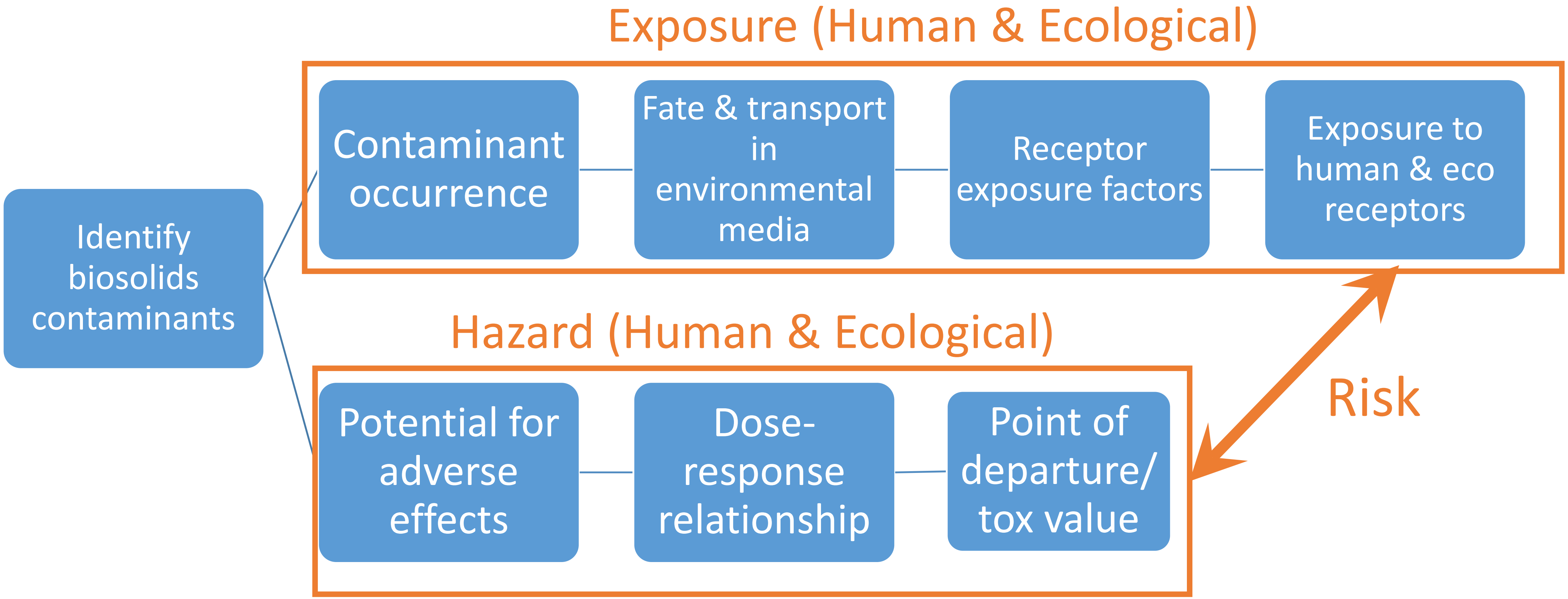
Risk screening & assessment for biosolids contaminants has been slowed by gaps in both exposure and hazard data.

[NRC 2002; USEPA 2018]



EPA's Office of Water proposes a new approach for increased efficiency

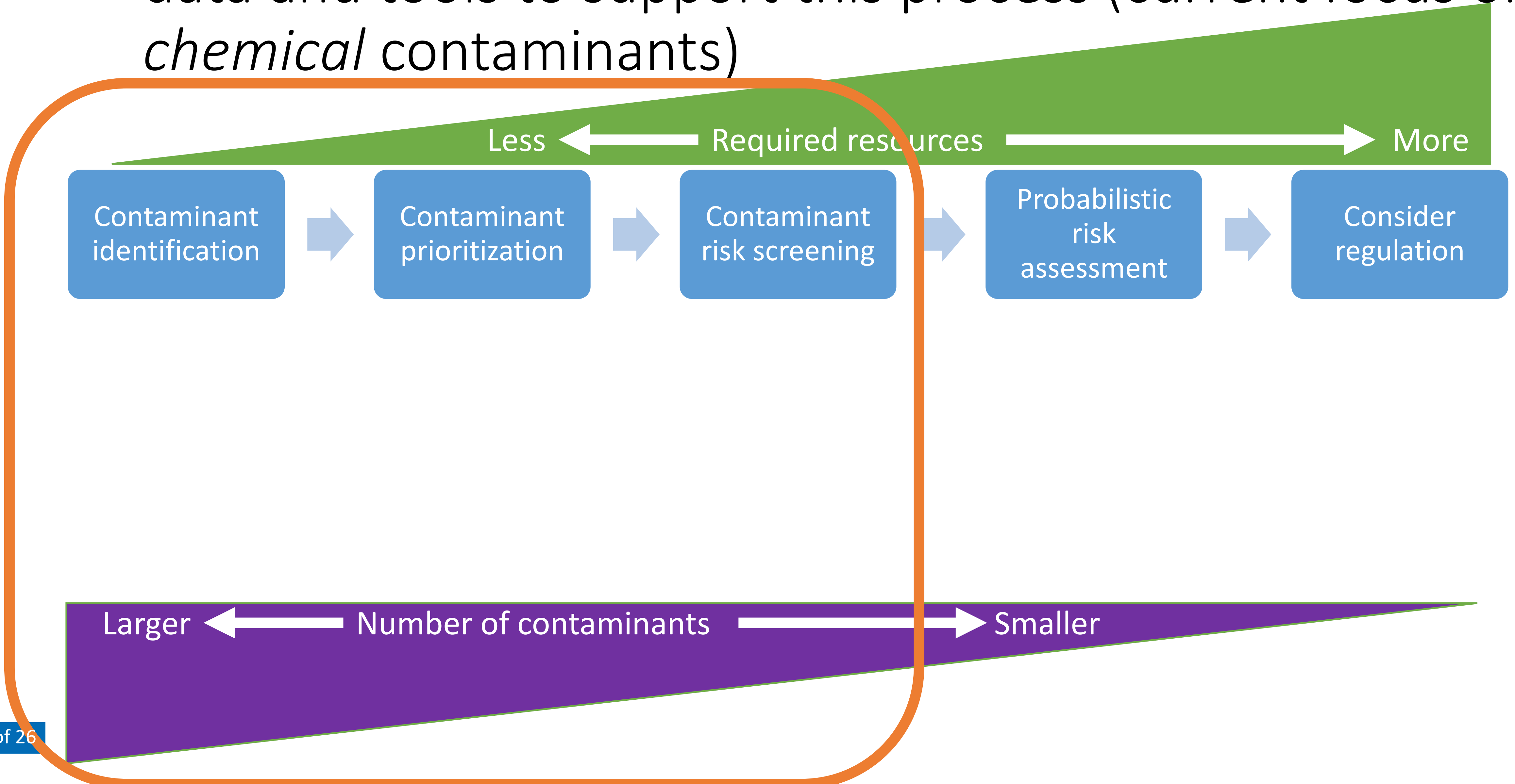
Less ← Required resources → More

Contaminant identification → Contaminant prioritization → Contaminant risk screening → Probabilistic risk assessment → Consider regulation

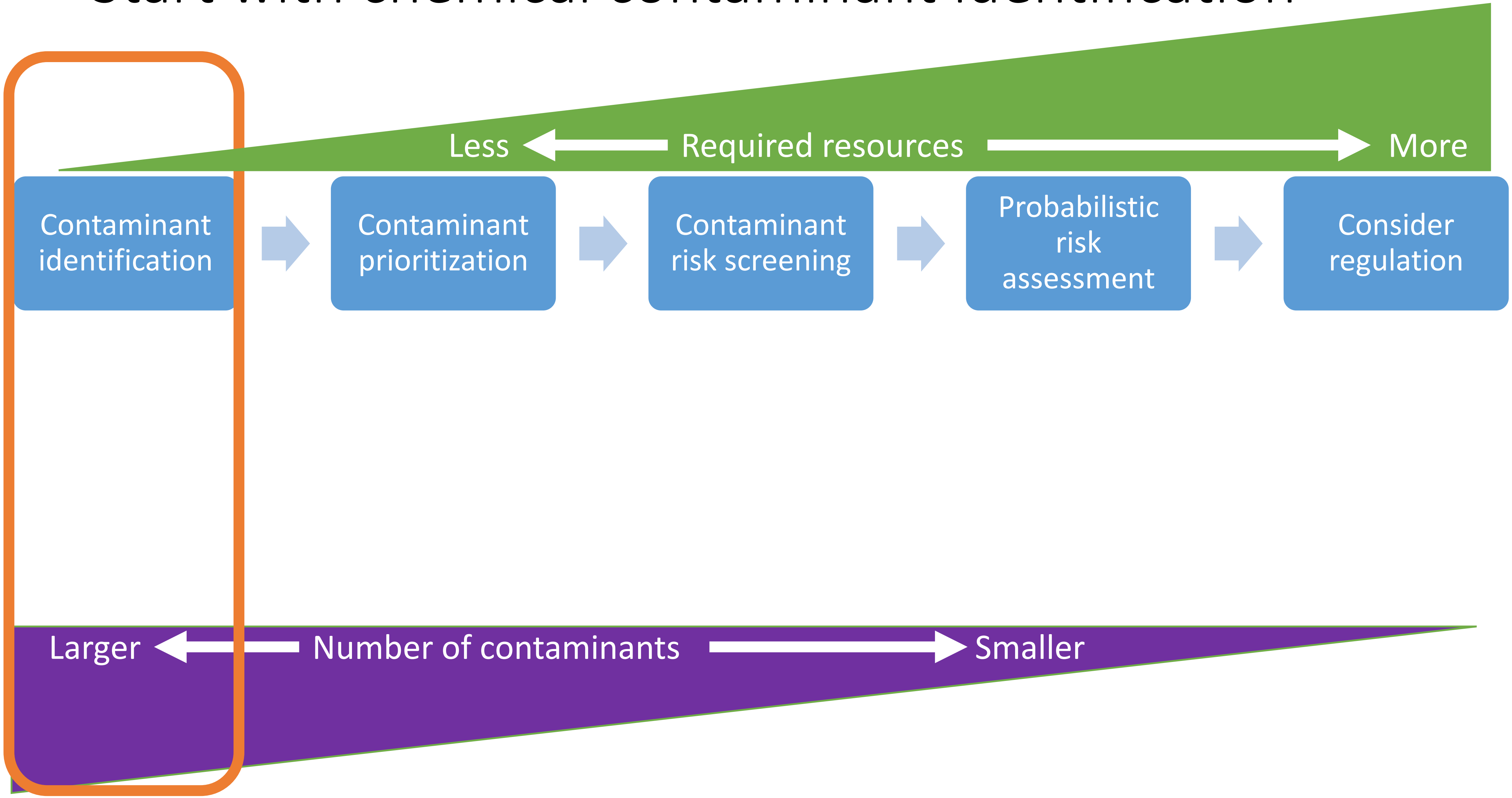
- **Contaminant identification**: Based on data from biennial reviews & national sewage sludge surveys
- **Contaminant prioritization**: Use available information to determine which contaminants may be of greater concern
- **Contaminant risk screening**: For prioritized contaminants first: Apply screening-level risk model. If high, proceed.
- **Probabilistic risk assessment**: Detailed probabilistic risk assessment. If high risk, proceed.
- **Consider regulation**: If sufficient evidence shows that contaminant may harm human health or environment, set appropriate regulations

Larger ← Number of contaminants → Smaller

ORD-CCTE researchers are working with OW to develop data and tools to support this process (current focus on *chemical* contaminants)



Start with chemical contaminant identification



ORD-CCTE & OW collaborated to curate a list of chemical substances found in biosolids [Richman & Williams, in prep]

Multiple reports listing chemicals found in biosolids:

- National Sewage Sludge Surveys (1988, 2001, 2009)
  - nationwide monitoring surveys of biosolids from wastewater treatment facilities
- Biennial Reports (2004-2019)
  - biosolids monitoring data found in the published literature

Problem:

- Each of these reports was a totally separate effort
- Data formats and reporting standards changed between reports
- Chemical identifiers (names, CASRNs) were not standardized among reports

Difficult to combine data from different reports, let alone connect to other chemical data necessary for risk screening and assessment

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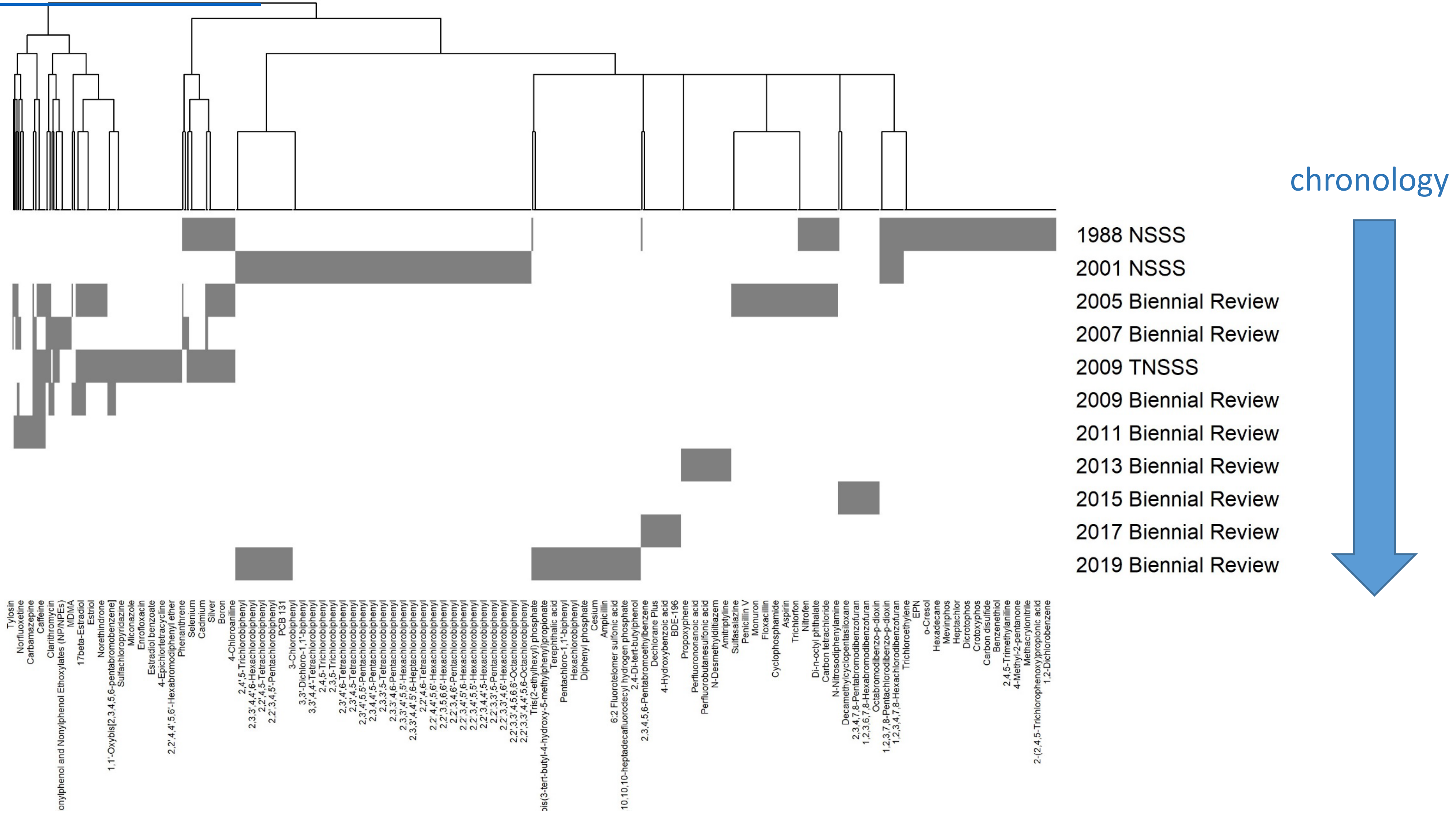
ORD-CCTE & OW collaborated to curate a list of chemical substances found in biosolids [Richman & Williams, in prep]

Solution: Data curation

- Extract data from reports & harmonize formatting
- Standardize chemical names
  - Fix misspellings & typos
  - Identify synonyms
  - Identify neutral forms of salts & charged anionic perfluorinated compounds
- Identify individual components of chemical combinations
  - e.g., chemicals that can't be separated by standard analytical chemistry methods, such as co-eluting PCBs
- Identify correct CASRNs (ensure Active CASRNs)
- Map to DSSTox Substance IDs [Grulke et al. 2019]

Chemical identification result: Curated list of chemicals found in biosolids in each Biennial Review and National Sewage Sludge Survey

On Comptox Chemicals Dashboard! https://comptox.epa.gov/dashboard/chemical-lists/BIOSOLIDS2021



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Chemical curation allows OW and ORD researchers to…

[Richman & Williams, in prep]

- Correctly determine when each chemical was identified
  - For example, the 2018-2019 Biennial Report reported 116 “newly identified” chemical pollutants in biosolids.
  - After curation, it turns out 41 of 116 had actually been identified previously!
- Query hazard-, exposure-, and risk-relevant data sources for biosolids chemicals, e.g., data available through the CompTox Chemicals Dashboard [Williams et al. 2017] https://comptox.epa.gov/dashboard/chemical-lists/BIOSOLIDS2021
  - Structure
  - Physicochemical properties
  - Chemical categories
  - Chemical functional use
  - High-throughput exposure predictions
  - ToxCast/Tox21 high-throughput *in vitro* screening data
  - Existing *in vivo* toxicology data

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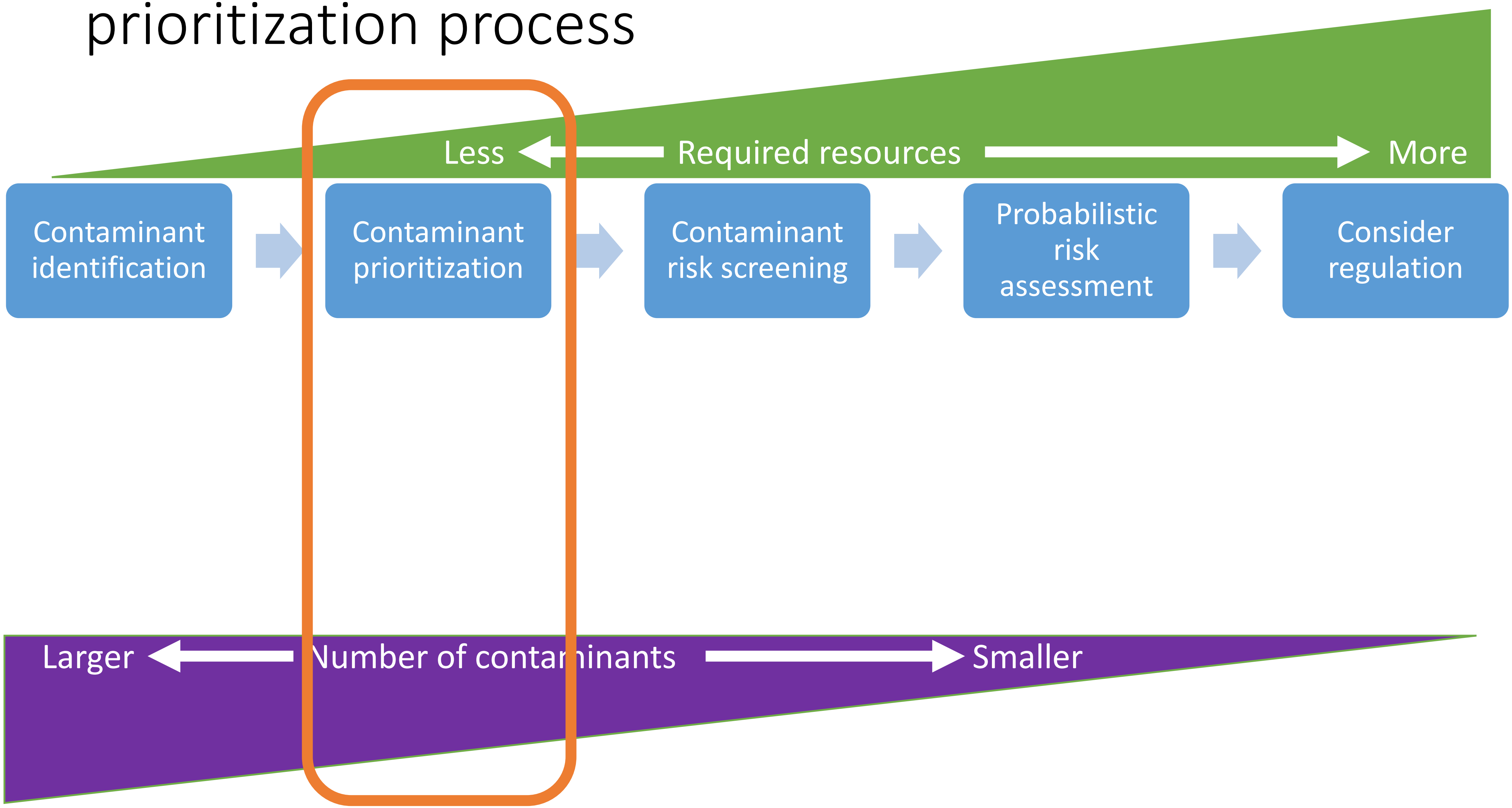
Curated chemical list can be used to apply a chemical prioritization process



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ORD-CCTE worked with OW to adapt a prioritization workflow originally developed in the context of TSCA prioritization as an ORD-CCTE/OCSPP collaboration:

PICS (Public Information Curation and Synthesis) [USEPA 2021c]

[previously presented to CSS BOSC by Dr. Richard Judson in February 2021]

To prioritize chemical substances, PICS integrates publicly available information from multiple domains:

- hazard
- exposure
- persistence & bioaccumulation

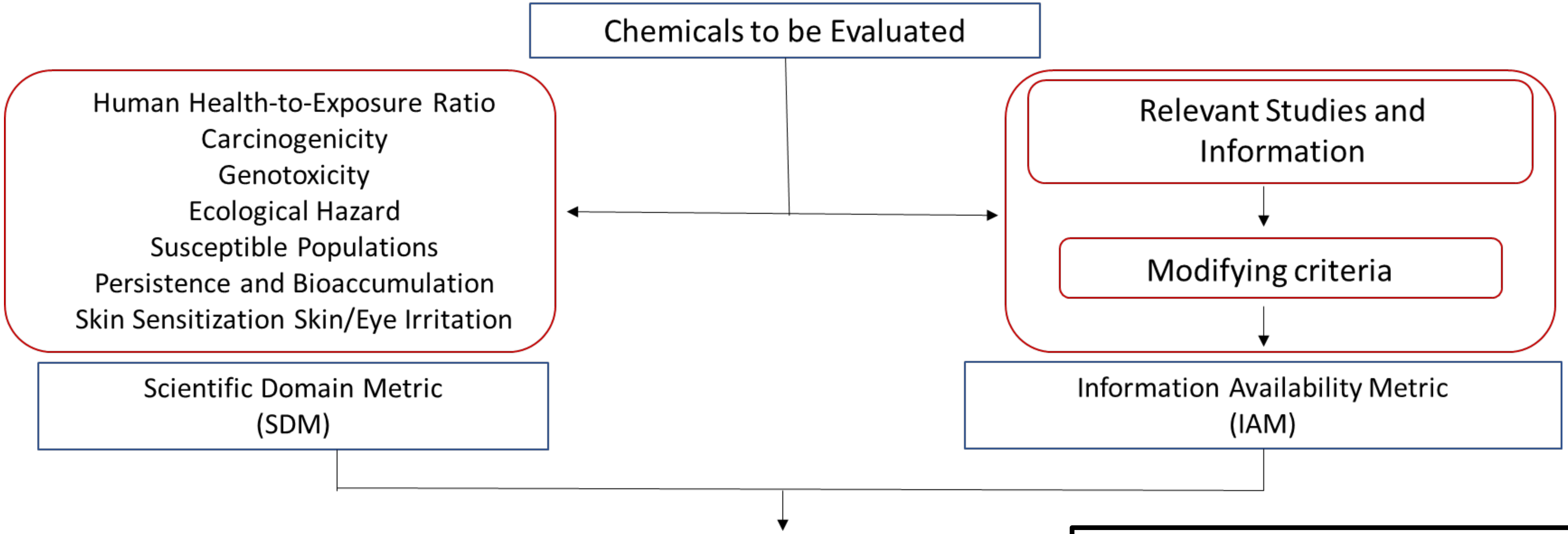
PICS synthesizes information from traditional methods and New Approach Methodologies

PICS was designed to:

- understand the overall **degree of potential concern** related to human health and the environment, based on available information
- understand the **relative coverage of potentially relevant information** about human health and ecological toxicity and exposure
- inform **level of effort and resources** that may be needed to evaluate a specific substance
- be **readily adaptable to address prioritization needs** under other mandates (not just TSCA!)

PICS workflow: chemicals are scored on two metrics, Scientific Domain Metric & Information Availability Metric

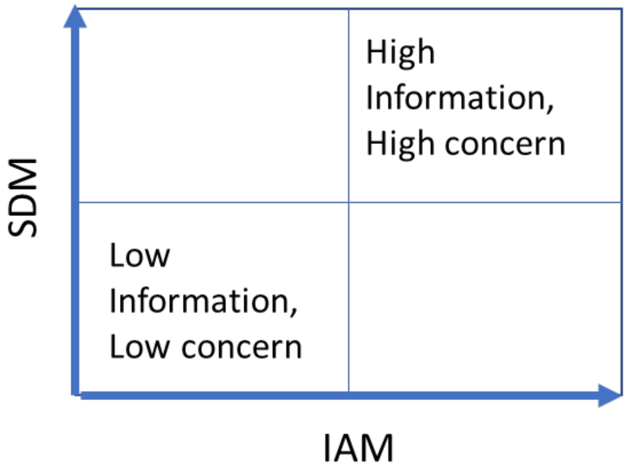
Score = concern for potential risk



Score = how much relevant information is available?

SDM & IAM originally developed to be TSCA-relevant

e.g., current exposure estimates are aggregate daily intake from *all* pathways – conservative with respect to biosolids

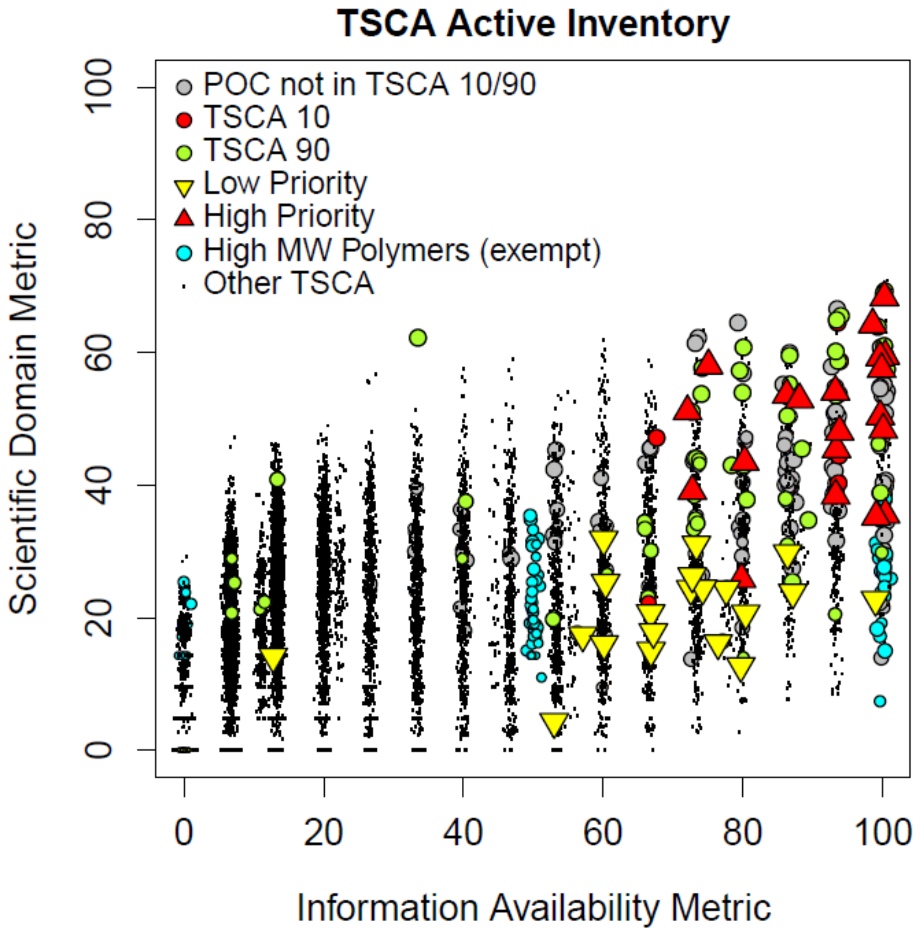


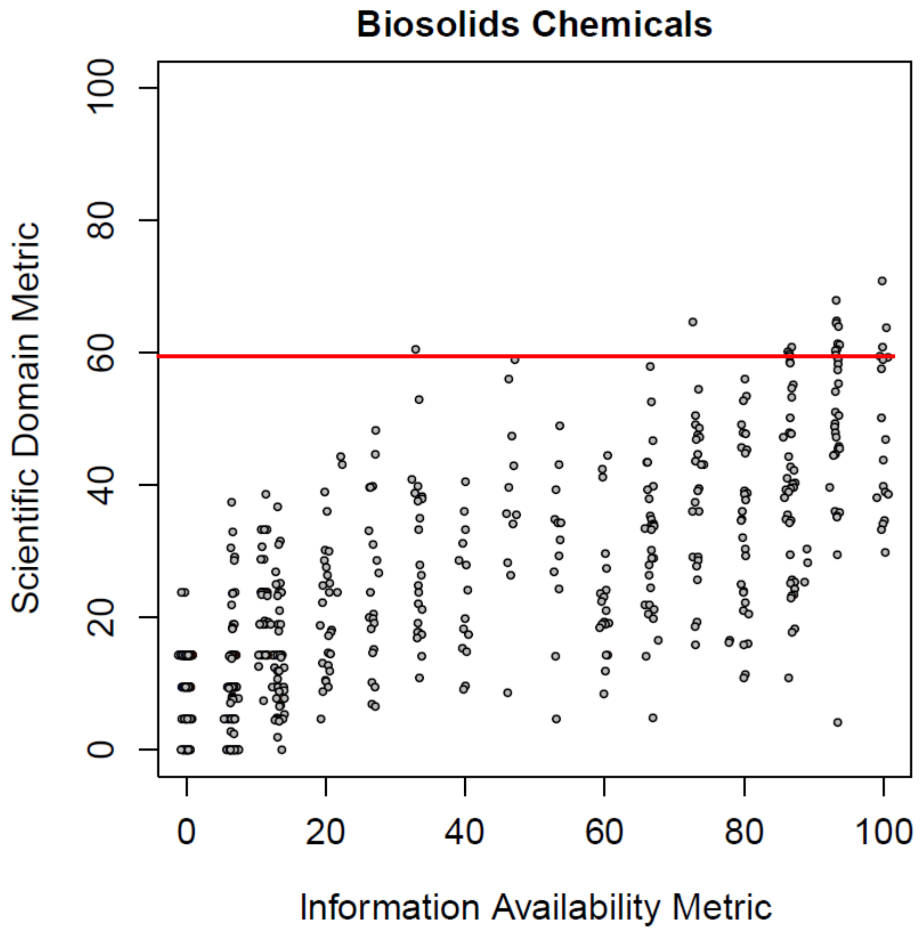
But PICS framework is modular & flexible –

based on feedback from stakeholders, could modify specific domains as needed

Figure courtesy of Dr. Richard Judson

PICS TSCA case study results vs. Biosolids preliminary results





Left: For TSCA prioritization, PICS generally agreed with previously-identified high- and low-priority chemicals

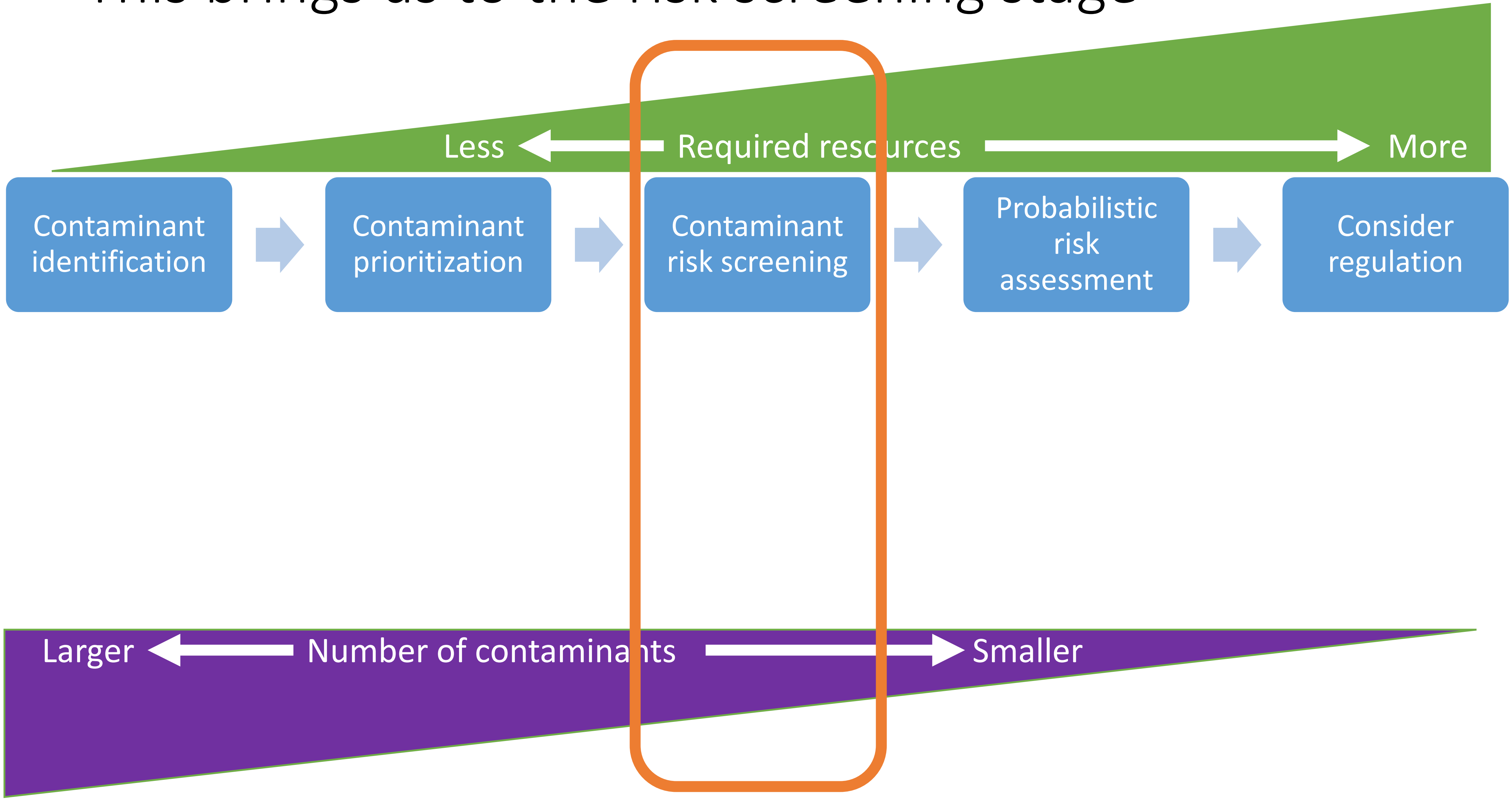
Right: Distribution of SDM/IAM is similar in biosolids chemicals and in TSCA Active Inventory

Scientific Domain Metric criteria (red line) can be used to prioritize chemicals for risk screening

[POC = PICS Proof of Concept chemical subset]

slide adapted from Dr. Richard Judson

This brings us to the risk screening stage



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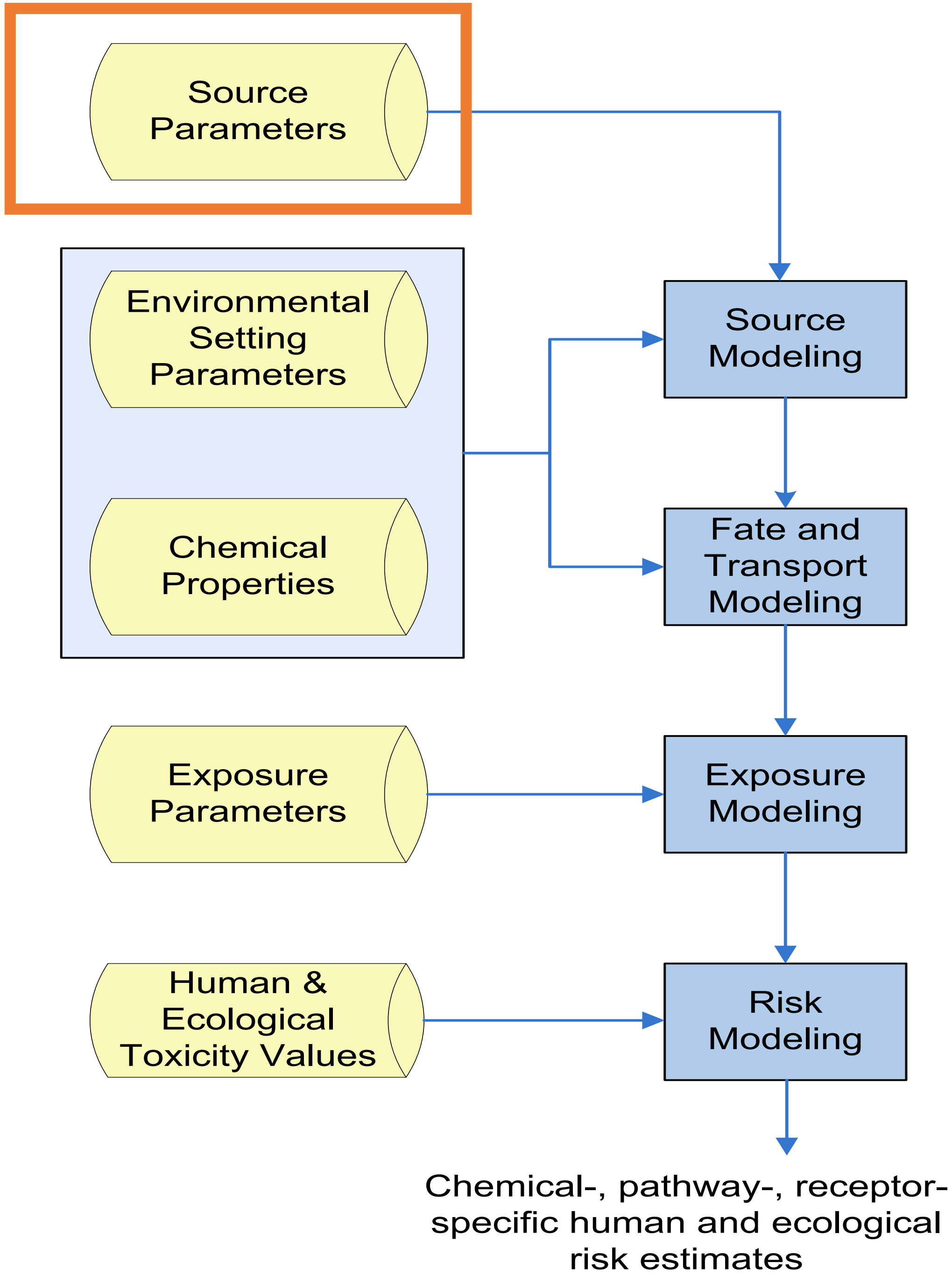
For risk screening, OW has developed Biosolids Screening Tool (BST)

But BST requires biosolids concentrations as input!

Measured biosolids concentrations are only available for about half of chemicals on the curated biosolids list.



Overview of Biosolids Screening Tool modeling framework

Simulates multiple exposure pathways relevant to land application, incineration, and surface disposal

Figure from OW

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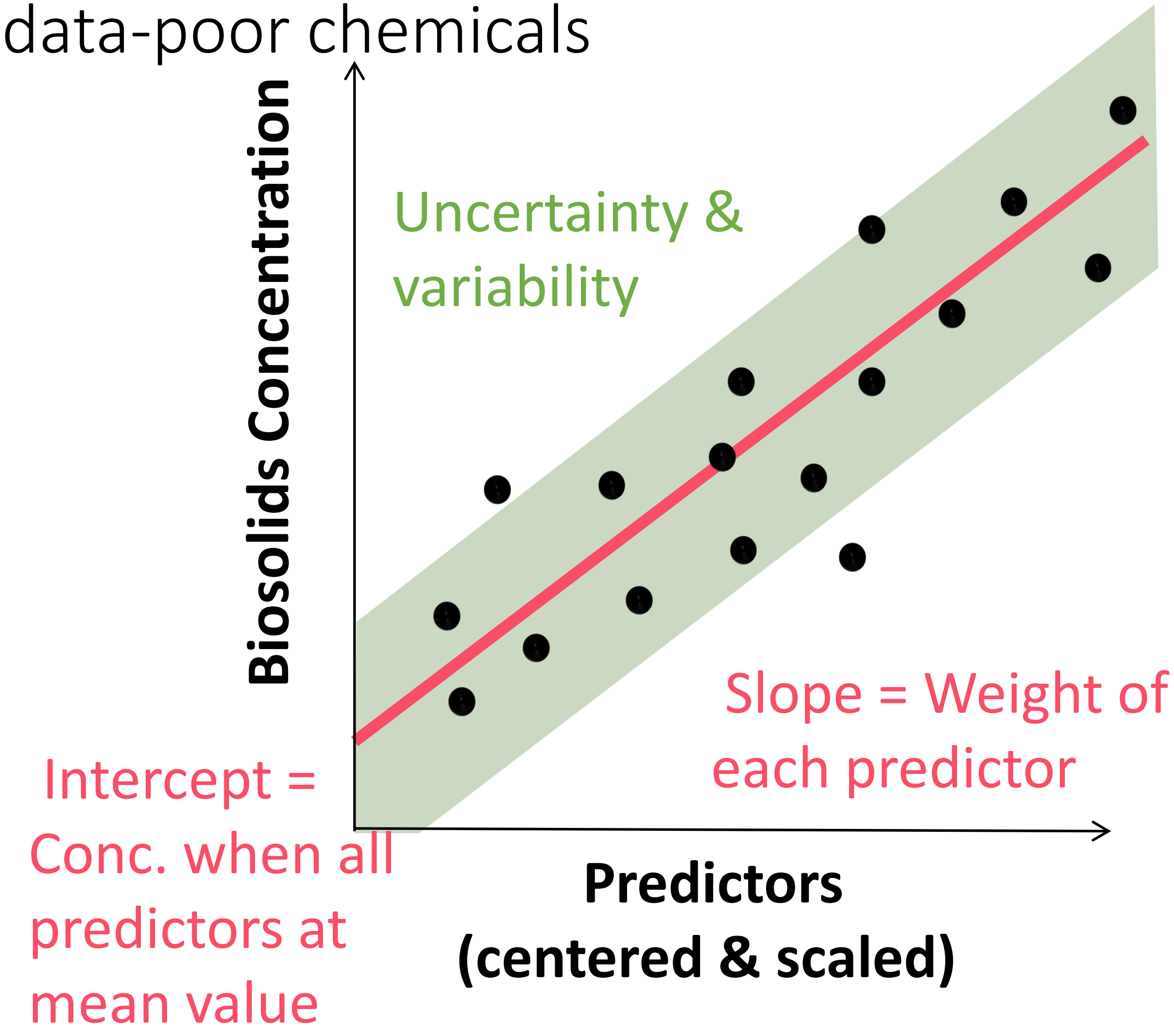
How CCTE can help: Develop a model to rapidly *predict* biosolids concentrations for data-poor chemicals

- Detailed wastewater treatment plant (WWTP) models not feasible
  - Require chemical-specific data that are not available for many chemicals
    - liquid-solid partitioning coefficients
    - biodegradation in sludge
    - **WWTP influent concentration**
  - Require plant-specific operating parameter data that are typically not available
  - Typically can't be run quickly for hundreds or thousands of chemicals
- Need a model that requires minimal chemical-specific data, but can make use of any relevant data that *are* available
- Need to characterize *variability & uncertainty* in model-predicted biosolids concentrations

Solution (work in progress): A high-throughput consensus model that combines easily-available model predictions & data to predict biosolids concentrations for data-poor chemicals

- Essentially a multiple linear regression: a weighted sum of predictor variables
- Model will be trained on National Sewage Sludge Survey monitoring data
- Predictors for each chemical will be easily-available occurrence-relevant data and existing model predictions
    - e.g., down-the-drain models; chemical production volume; presence on lists of banned chemicals; use in consumer products, industry, pesticides, food, pharmaceuticals….
    - Any missing values simply imputed with average
- Will build on existing framework from consensus model of human aggregate daily intake rates: SEEM3 (Systematic Empirical Evaluation of Models, version 3) (Ring et al. 2019)



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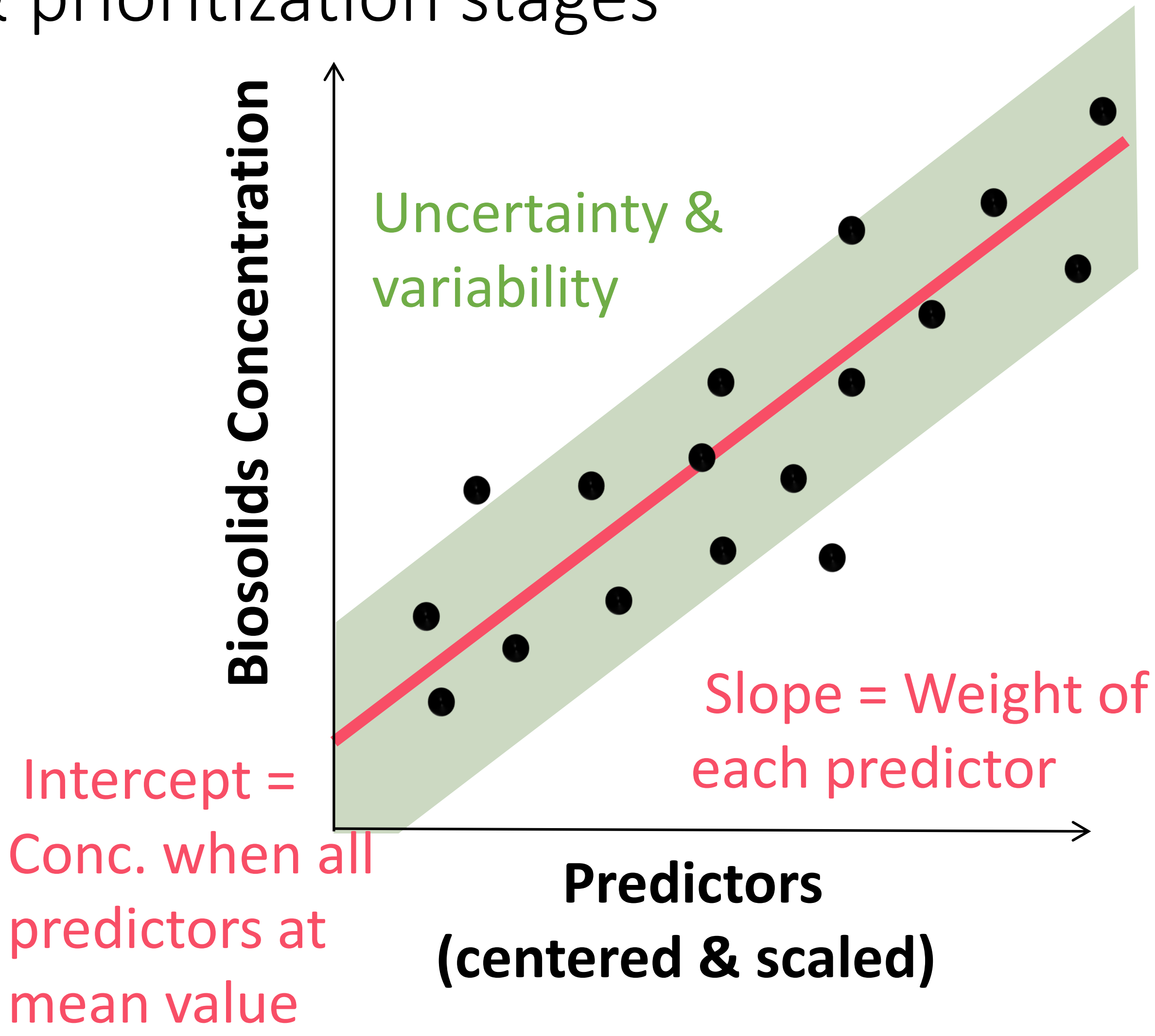
Consensus model predictions (work in progress) could also be used at identification & prioritization stages

- Consensus model could be applied to chemicals outside the curated biosolids list to identify additional chemicals with potential to occur in biosolids
- Identified chemicals could be prioritized using PICS process
- Could be used to propose candidates for new National Sewage Sludge Survey



Summary

- The Clean Water Act requires OW to evaluate chemicals and microbes that occur in biosolids for harm to human health and the environment
- OW has a need to fill data gaps to more efficiently evaluate biosolids contaminants
- CCTE researchers are working with OW Biosolids to provide data and tools to support biosolids chemical prioritization and screening
    - Curation of list of chemicals found in biosolids
    - PICS prioritization workflow
    - (Work in progress) High-throughput consensus model to predict biosolids chemical concentrations

Key People

OW Biosolids

- Liz Resek
- David Tobias
- Tess Richman (ORISE)

ORD CCTE

- Caroline Ring
- Paul Kruse (ORISE)
- Antony Williams
- Richard Judson
- PICS Proof of Concept Team (see next slide)
- Kristin Isaacs
- Marc Russell

PICS Proof of Concept Team

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- Amar Singh
- Andrew Greenhalgh
- Anita Pascocello
- Anita Simha
- Ashley Jackson
- Carlie LaLone
- Carolyn Gigot
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- David DeMarini
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- Janet Burke
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- Jeff Dean
- Jeremy Dunne
- Johanna Congleton
- John Cowden
- John Nichols
- John Wambaugh
- Katherine Phillips
- Kathie Dionisio
- Katie Paul-Friedman
- Kelly Garcia
- Kent Thomas
- Kristin Isaacs
- Lauren Koval
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- Michael Gonzalez
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- Sarah Warren
- Todd Martin
- Antony Williams
- Urmila Kodavanti
- Yu-Sheng Lin

Thank you!

Questions?

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References

Grulke, C. M., Williams, A. J., Thillanadarajah, I., & Richard, A. M. (2019). EPA's DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research. *Comput Toxicol, 12*. doi:10.1016/j.comtox.2019.100096

NRC. (2002). *Biosolids Applied to Land: Advancing Standards and Practices* (978-0-309-08486-4). Retrieved from The National Academies Press: https://www.nap.edu/catalog/10426/biosolids-applied-to-land-advancing-standards-and-practices

Ring, C. L., Arnot, J. A., et al. (2019). Consensus Modeling of Median Chemical Intake for the US Population Based on Predictions of Exposure Pathways. *Environmental Science & Technology, 53*(2), 719-732. doi:10.1021/acs.est.8b04056

USEPA. (1995). *A Guide to the Biosolids Risk Assessments for the EPA Part 503 Rule*. (EPA-832-B-93-005). Washington, DC Retrieved from https://www.epa.gov/sites/production/files/2018-11/documents/guide-biosolids-risk-assessments-part503.pdf

USEPA. (2018). *EPA Unable to Assess the Impact of Hundreds of Unregulated Pollutants in Land-Applied Biosolids on Human Health and the Environment*. (Report No. 19-P-0002). Washington, DC Retrieved from https://www.epa.gov/biosolids/office-inspector-general-reports-biosolids-program

USEPA. (2021a). Biennial Reviews of Sewage Sludge Standards. Retrieved from https://www.epa.gov/biosolids/biennial-reviews-sewage-sludge-standards

USEPA (2021b). Sewage sludge surveys. Retrieved from https://www.epa.gov/biosolids/sewage-sludge-surveys

USEPA (2021c). A Proof-of-Concept Case Study Integrating Publicly Available Information to Screen Candidates for Chemical Prioritization under TSCA. U.S. Environmental Protection Agency, Washington, DC, EPA/600/R-21-106, 2021. https://doi.org/10.23645/epacomptox.14878125

Williams, A. J., Grulke, C. M., et al. (2017). The CompTox Chemistry Dashboard: a community data resource for environmental chemistry. *J Cheminform, 9*(1), 61. doi:10.1186/s13321-017-0247-6