Using the SSD Toolbox to account for interspecific variability in toxicity

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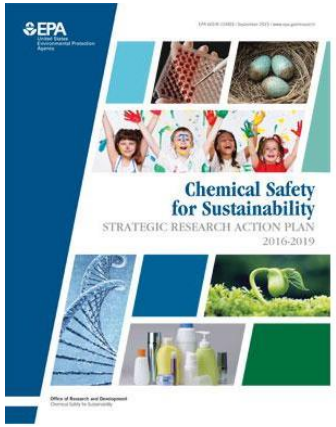
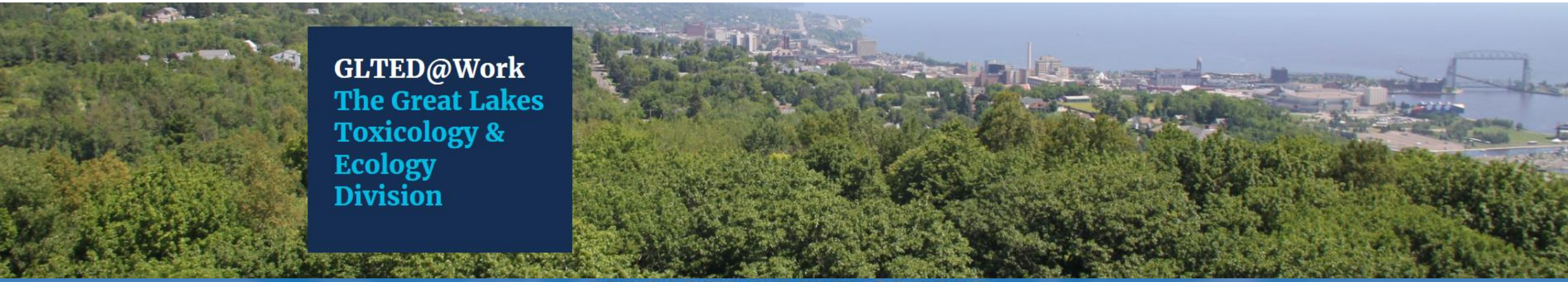


National Program: Chemical Safety for Sustainability
Research Areas: Ecotoxicological Analysis and Modeling
27 February 2020



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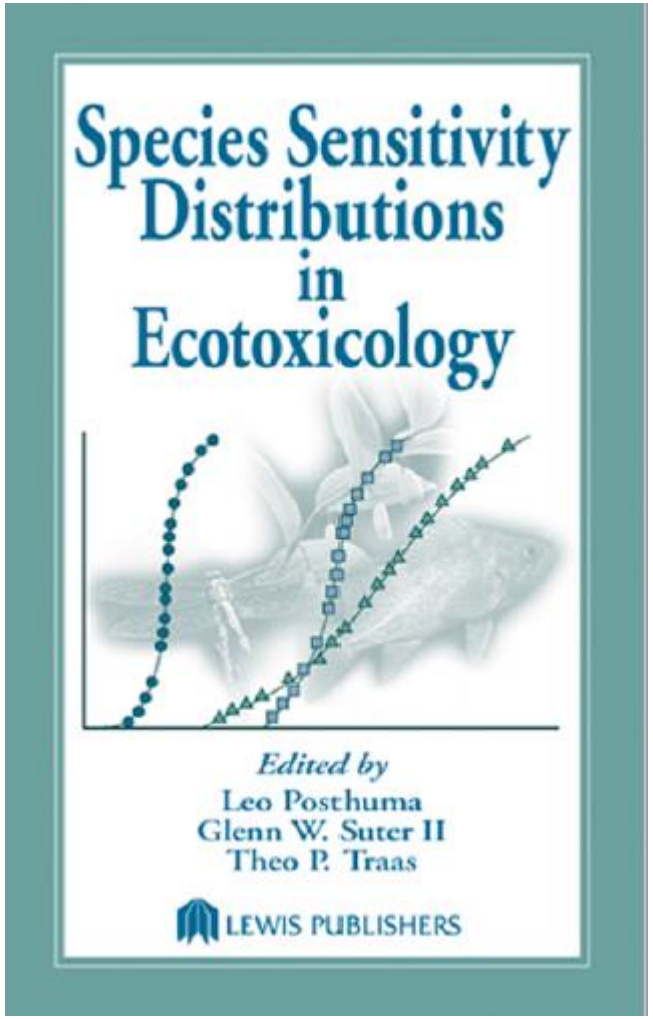
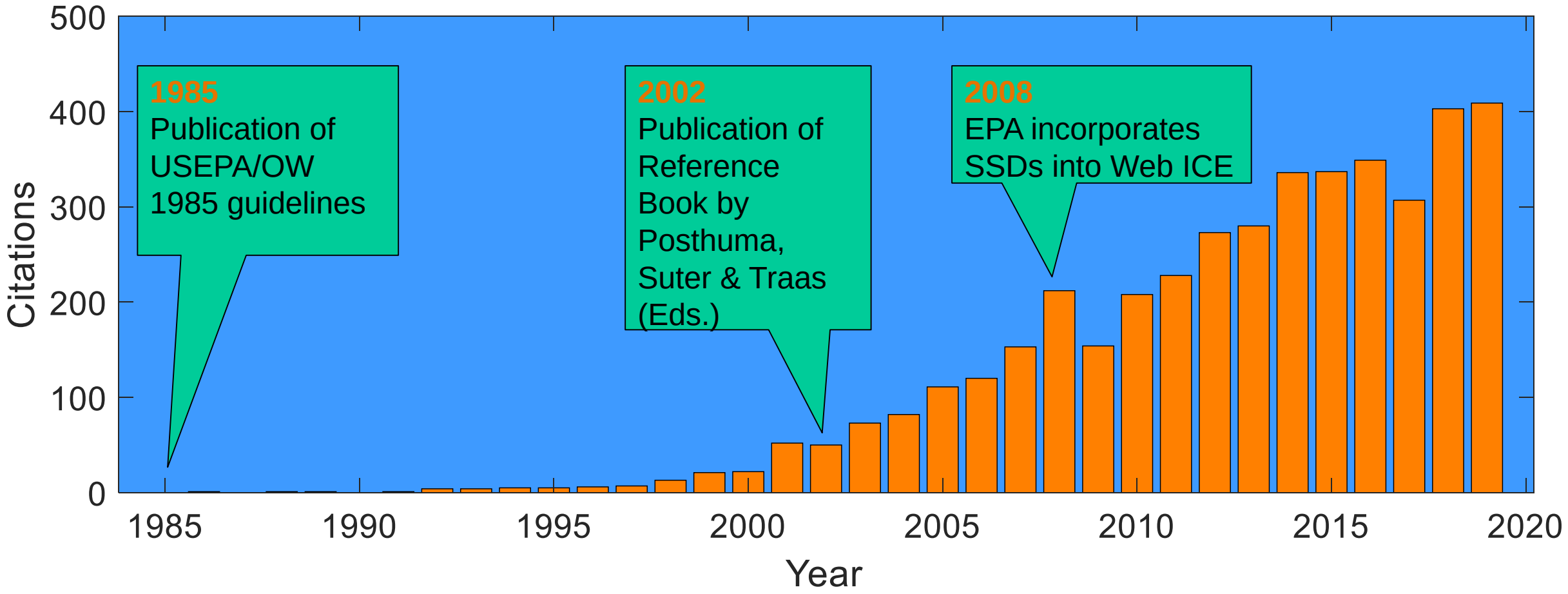
What is an SSD?

- SSD = Species Sensitivity Distribution

- “A SSD is a statistical distribution describing the variation among a set of species in toxicity of a certain compound or mixture” (Posthuma et al. 2002)

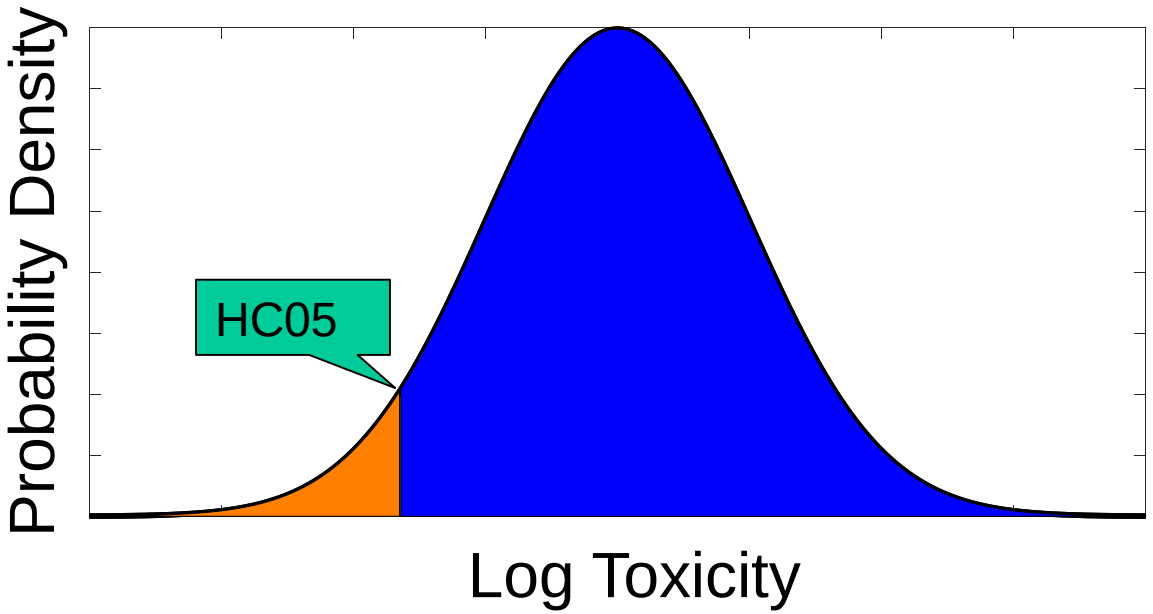


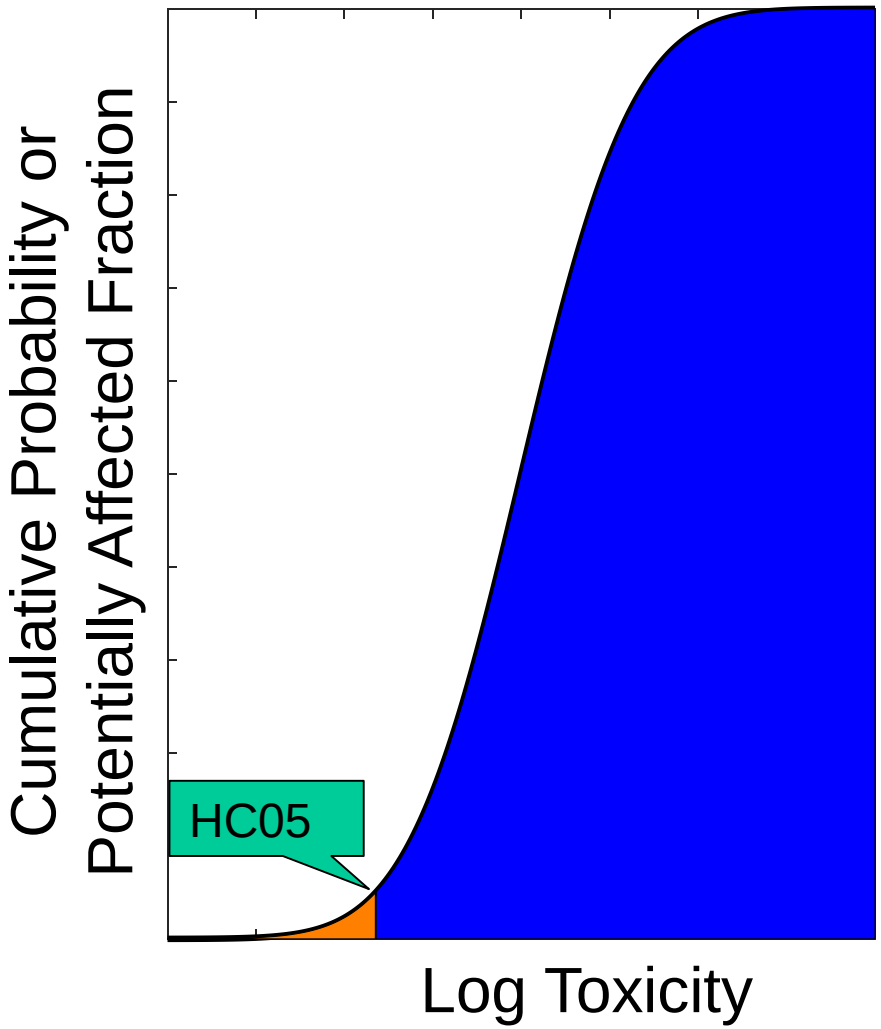
(selected) History of SSD



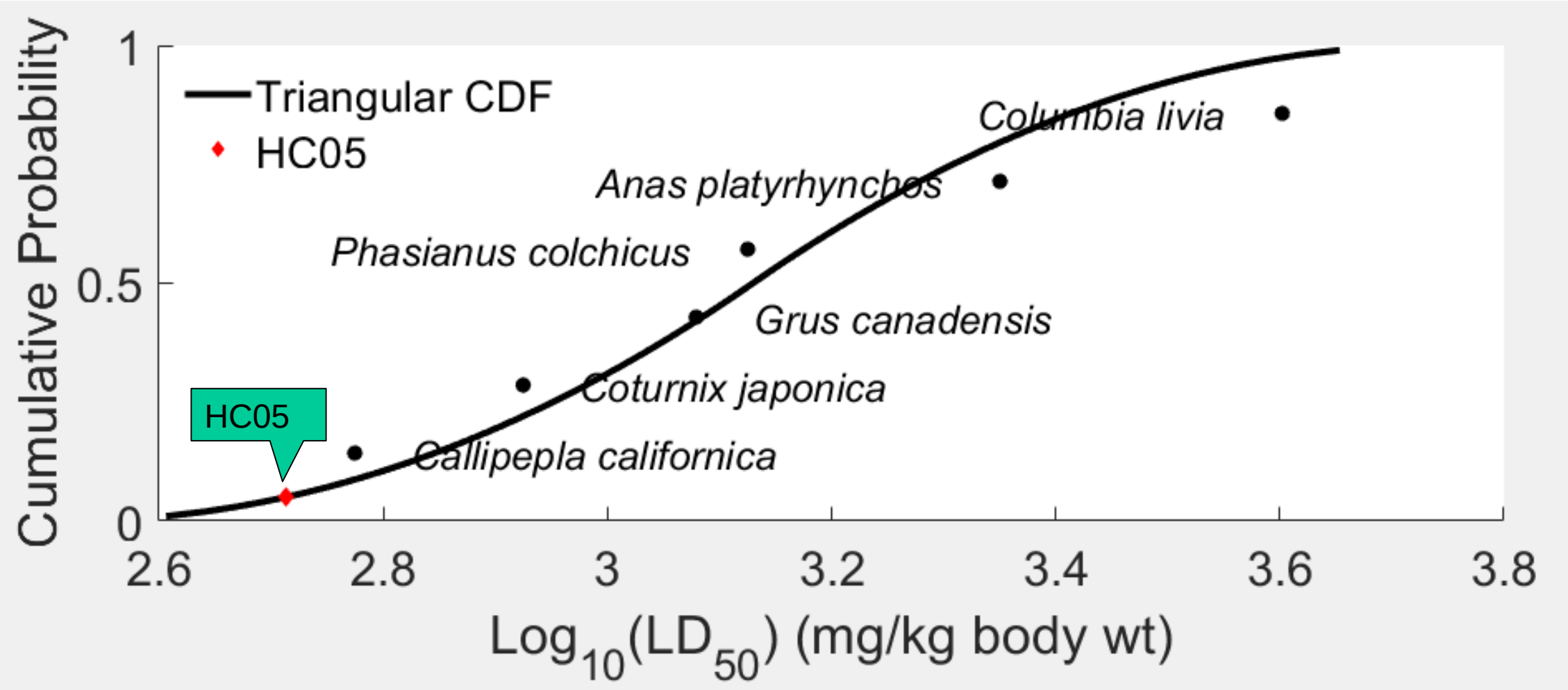
An SSD = a statistical model

- $\text{Log}_{10}(\text{LC50}) \sim N(\mu,\sigma)$
- $\text{Log}_{10}(\text{LC50}) \sim \mu + \varepsilon \;;\; (\varepsilon \sim N(0,\sigma))$
- Inference usually is made on the 5th percentile (HC05)





Example – DDT 14d avian LD50s



SSD Toolbox - genesis

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Notice of FIFRA SAP Meeting; Consultation on Common Effects Assessment Methodology Developed in the Office of Pesticide Programs and Office of Water

Docket Folder Summary View all documents and comments in this Docket

Docket ID: EPA-HQ-OPP-2011-0898 **Agency:** Environmental Protection Agency (EPA)

Summary:
For further information contact: Sharlene Matten

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Primary Documents View All (1)

N — Meetings: Federal Insecticide, Fungicide, and Rodenticide Act Scientific Advisory Panel
Notice **Posted:** 11/16/2011 **ID:** EPA-HQ-OPP-2011-0898-0001
Comment Period Closed
Jan 17, 2012 11:59 PM ET

Supporting Documents View All (22)

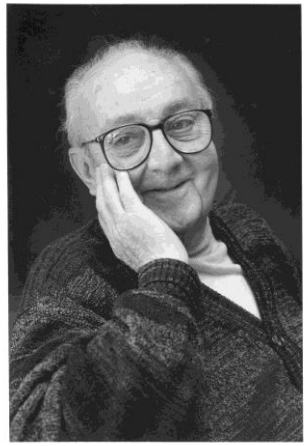
SR — FIFRA SAP Final Meeting Report-SAP Minutes No. 2012-02 A Set of Scientific Issues Being Considered
Supporting & Related Material **Posted:** 05/15/2012 **ID:** EPA-HQ-OPP-2011-0898-0027
Comments Not Accepted

SR — Background and Overview of Methods for Characterizing Effects of Pesticides on Aquatic Organisms
Supporting & Related Material **Posted:** 02/02/2012 **ID:** EPA-HQ-OPP-2011-0898-0019
Comments Not Accepted

SR — Extrapolation Factors for Estimation of HC5s
Supporting & Related Material **Posted:** 02/02/2012 **ID:** EPA-HQ-OPP-2011-0898-0022
Comments Not Accepted

2012
FIFRA Science Advisory Panel

$Log_{10}(LC50) \sim \mu + \varepsilon \quad ; \quad \varepsilon \sim N(0,\sigma)$
Assumptions:



- *All* variation in sensitivity is *random*
- Toxicity data are an *unbiased sample* that is *representative* of the set of species for which regulatory protection is intended
- Toxicity test results for species in SSD are *accurate* measurements of toxicity
- *Field responses* to exposure would be *similar* to laboratory test results

Questions we should ask about SSDs

- How does sample size influence bias and variance of the estimated HC05?
- How do different estimation methods influence properties of the estimated HC05?
- Is Akaike's Information Criterion a useful method for identifying the best distribution?
- Are goodness-of-fit tests reliable measures of performance?
- Does model-averaging across distributions improve estimates of the HC05?

SSD Toolbox - exodus

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Endangered Species

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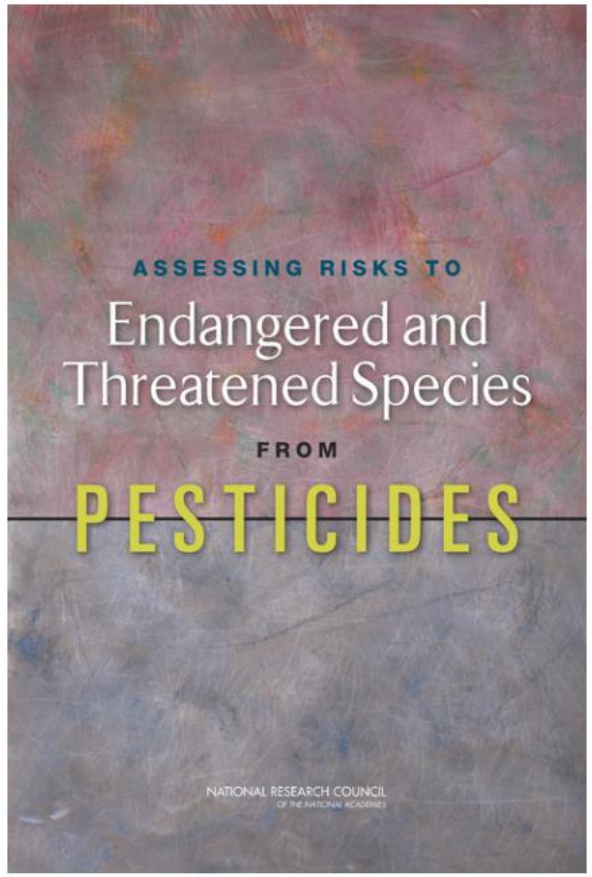
- Assessing Pesticides Under the Endangered Species Act
- Endangered Species: Information For Pesticides Users
- Litigation on Endangered Species and Pesticides
- Bulletins Live!
- For Kids

Interim Approaches for Pesticide Endangered Species Act Assessments Based on NAS Report Recommendations

EPA worked with the Departments of Agriculture, Commerce and the Interior to develop the following Interim Approaches for Pesticide Endangered Species Act Assessments based on National Academy of Sciences Report Recommendations[06][06]. The interim approaches were used by EPA to finalize biological evaluations for the three pilot chemicals: chlorpyrifos, diazinon and malathion in 2017. The Draft Revised Method for National Level Endangered Species Risk Assessment Process for Biological Evaluations of Pesticides released in May 2019 is an important step in further refining the interim approaches.



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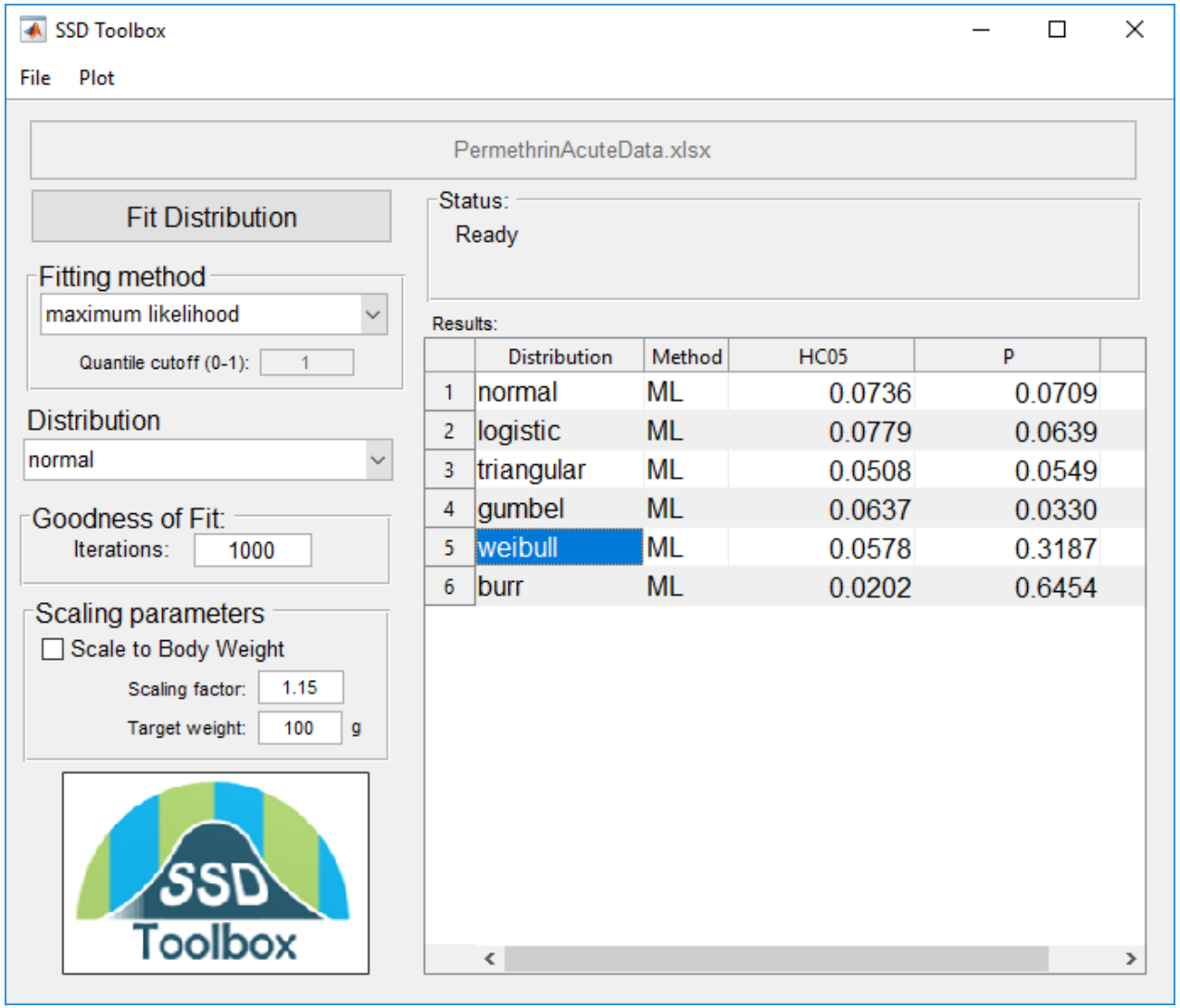
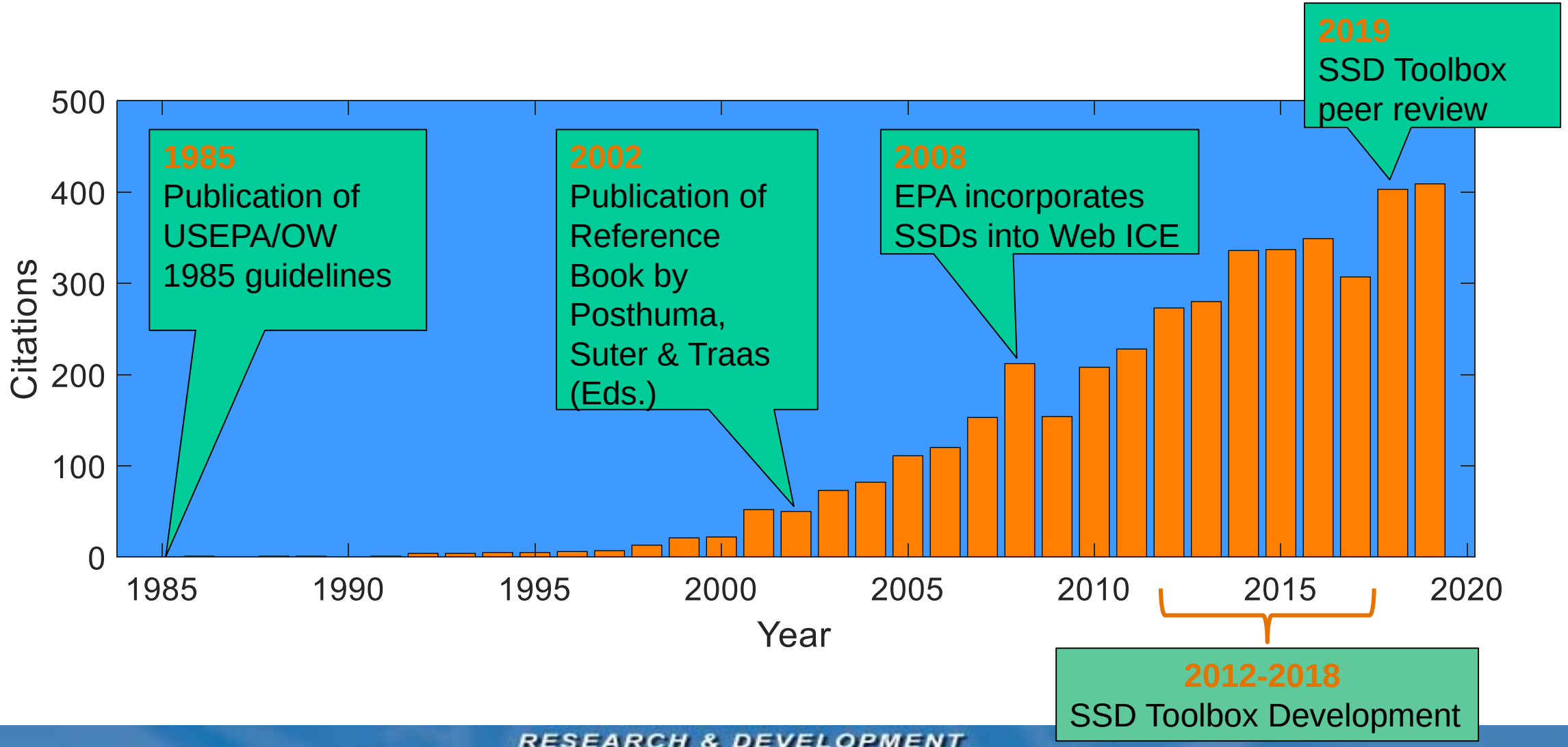
Standalone Software



Design Criteria:

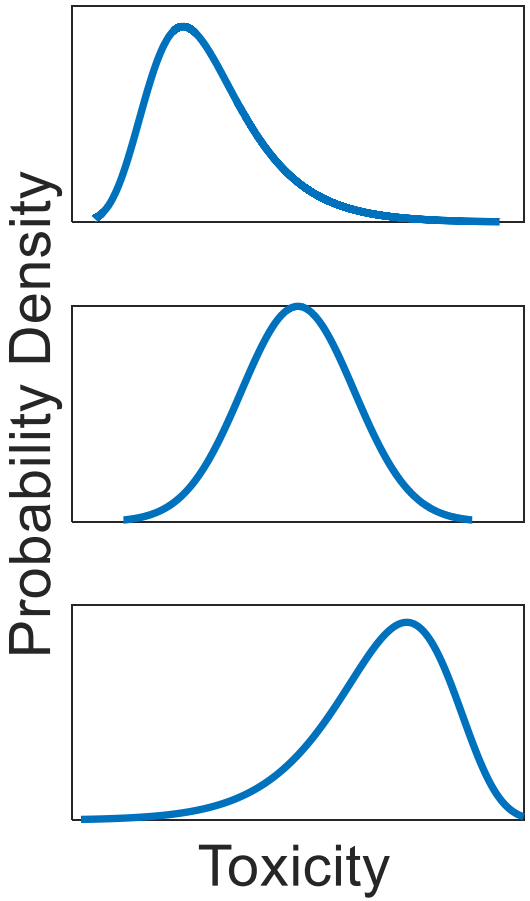
- Intuitive decision process for model-fitting
- Methods vetted through peer-review
- Standardized QA/QC
- Extensive help in User's Guide and Technical Manual
- Easy to use!

(selected) History of SSD



SSD Toolbox Features

- Ability to fix six distributions accommodating differently “shaped” data (normal, logistic, triangular, Gumbel, Weibull, & $Burr_{III}$)
- AIC_c methods for distinguishing among distributions
- Post-hoc Goodness of Fit (GoF) tests
- Extensive graphing and visualization tools
- Distribution-averaging of HC05 estimates
- Ability to use non-definitive toxicity values (e.g., LC50 > x)

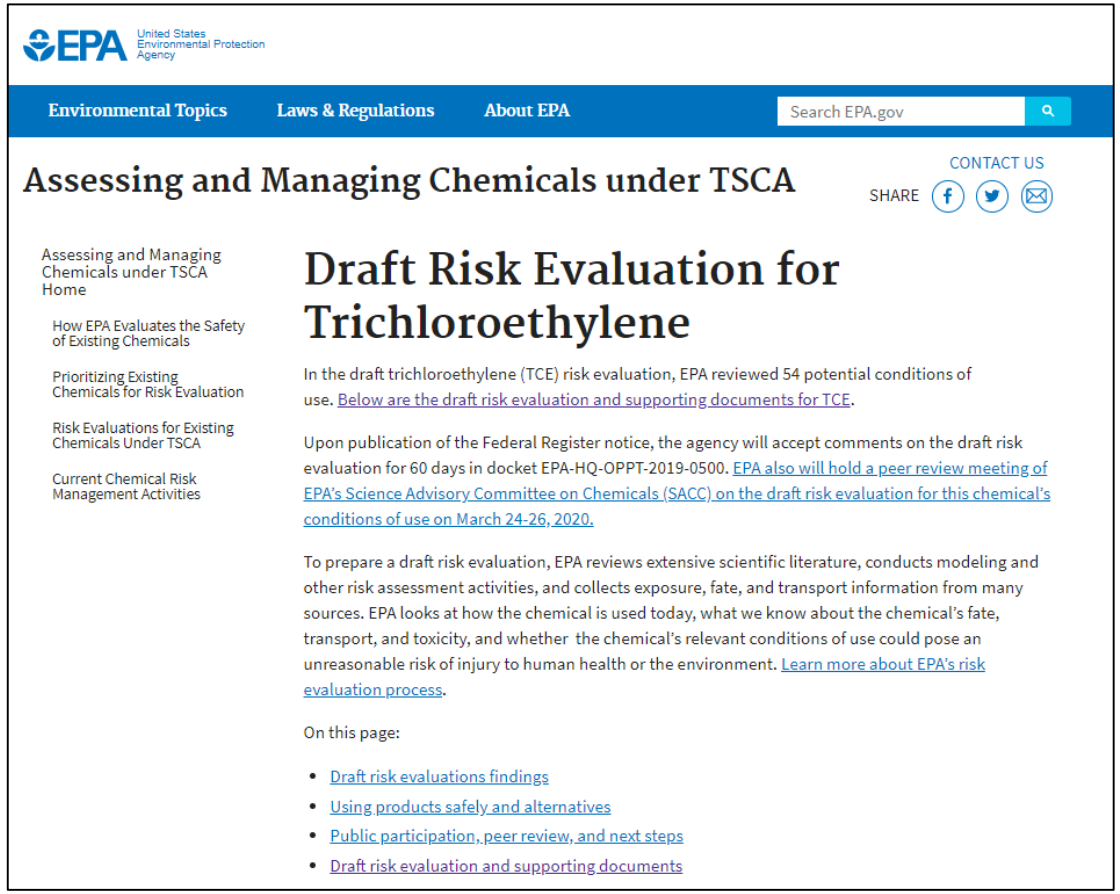


Software Demo!

SSD Toolbox

Using SSD Toolbox for the TSCA Risk Evaluation for TCE

- TSCA Background:
  - Under TSCA, OPPT evaluates and regulates, as appropriate, the full life cycle of a chemical, *i.e.*, manufacture (import), distribution in commerce, use and disposal.
  - In 2016, TSCA was amended by the Frank R. Lautenberg Chemical Safety for the 21st Century Act
  - Currently OPPT is drafting risk evaluations for the first 10 chemicals, including TCE, since the Lautenberg Act was signed.
- Used SSD Toolbox for aquatic toxicity data: algae data and acute toxicity data



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Assessing and Managing Chemicals under TSCA

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How EPA Evaluates the Safety of Existing Chemicals

Prioritizing Existing Chemicals for Risk Evaluation

Risk Evaluations for Existing Chemicals Under TSCA

Current Chemical Risk Management Activities

Draft Risk Evaluation for Trichloroethylene

In the draft trichloroethylene (TCE) risk evaluation, EPA reviewed 54 potential conditions of use. Below are the draft risk evaluation and supporting documents for TCE.

Upon publication of the Federal Register notice, the agency will accept comments on the draft risk evaluation for 60 days in docket EPA-HQ-OPPT-2019-0500. EPA also will hold a peer review meeting of EPA's Science Advisory Committee on Chemicals (SACC) on the draft risk evaluation for this chemical's conditions of use on March 24-26, 2020.

To prepare a draft risk evaluation, EPA reviews extensive scientific literature, conducts modeling and other risk assessment activities, and collects exposure, fate, and transport information from many sources. EPA looks at how the chemical is used today, what we know about the chemical's fate, transport, and toxicity, and whether the chemical's relevant conditions of use could pose an unreasonable risk of injury to human health or the environment. Learn more about EPA's risk evaluation process.

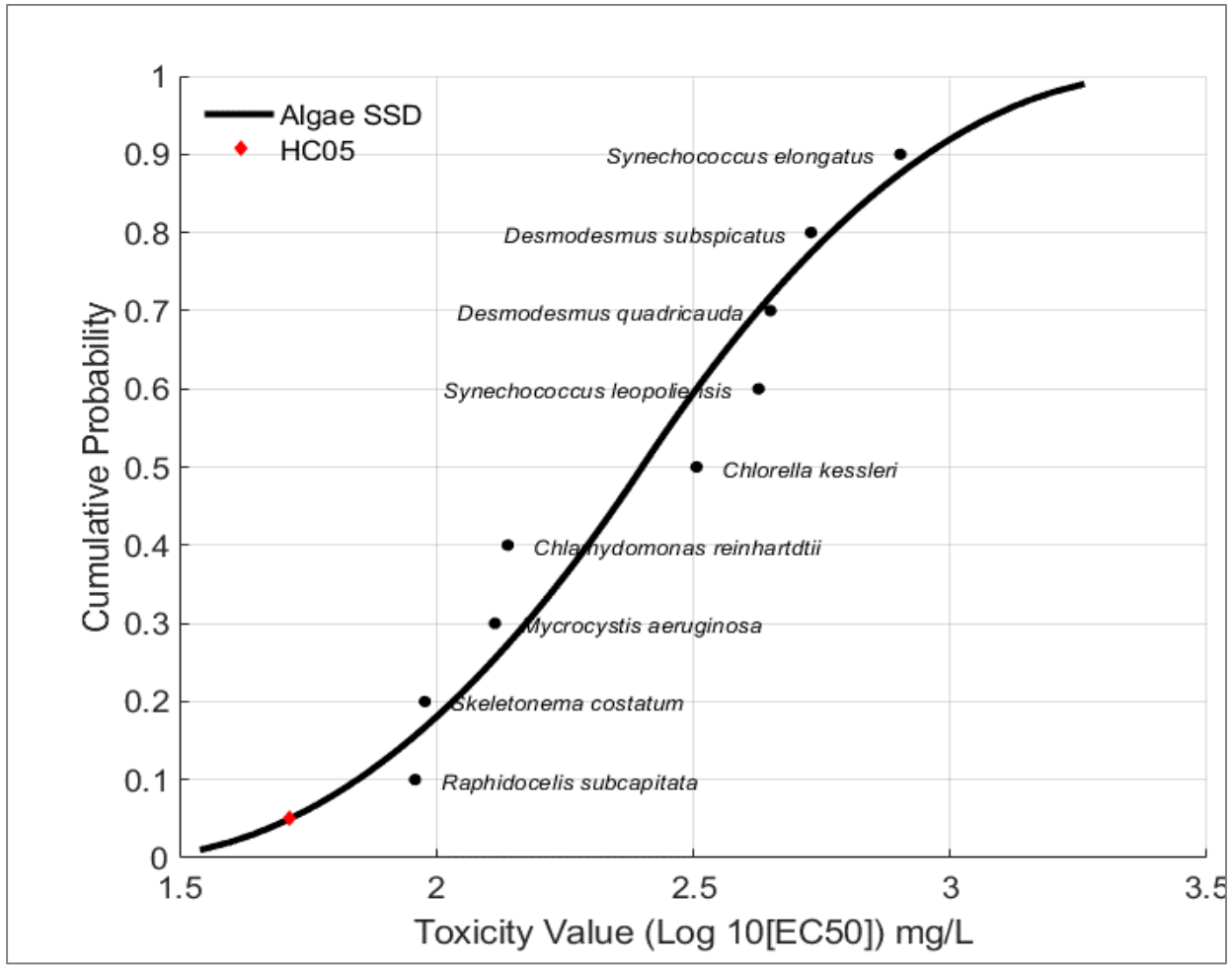
On this page:

- Draft risk evaluations findings
- Using products safely and alternatives
- Public participation, peer review, and next steps
- Draft risk evaluation and supporting documents

Algae toxicity data for TCE

- Algae toxicity data on TCE had a wide range of values.
- SSD was used as a line of evidence for assessing algae in this assessment.
- The resulting SSD calculated an HC_{05} of 52 mg/L or 52,000 µg/L.

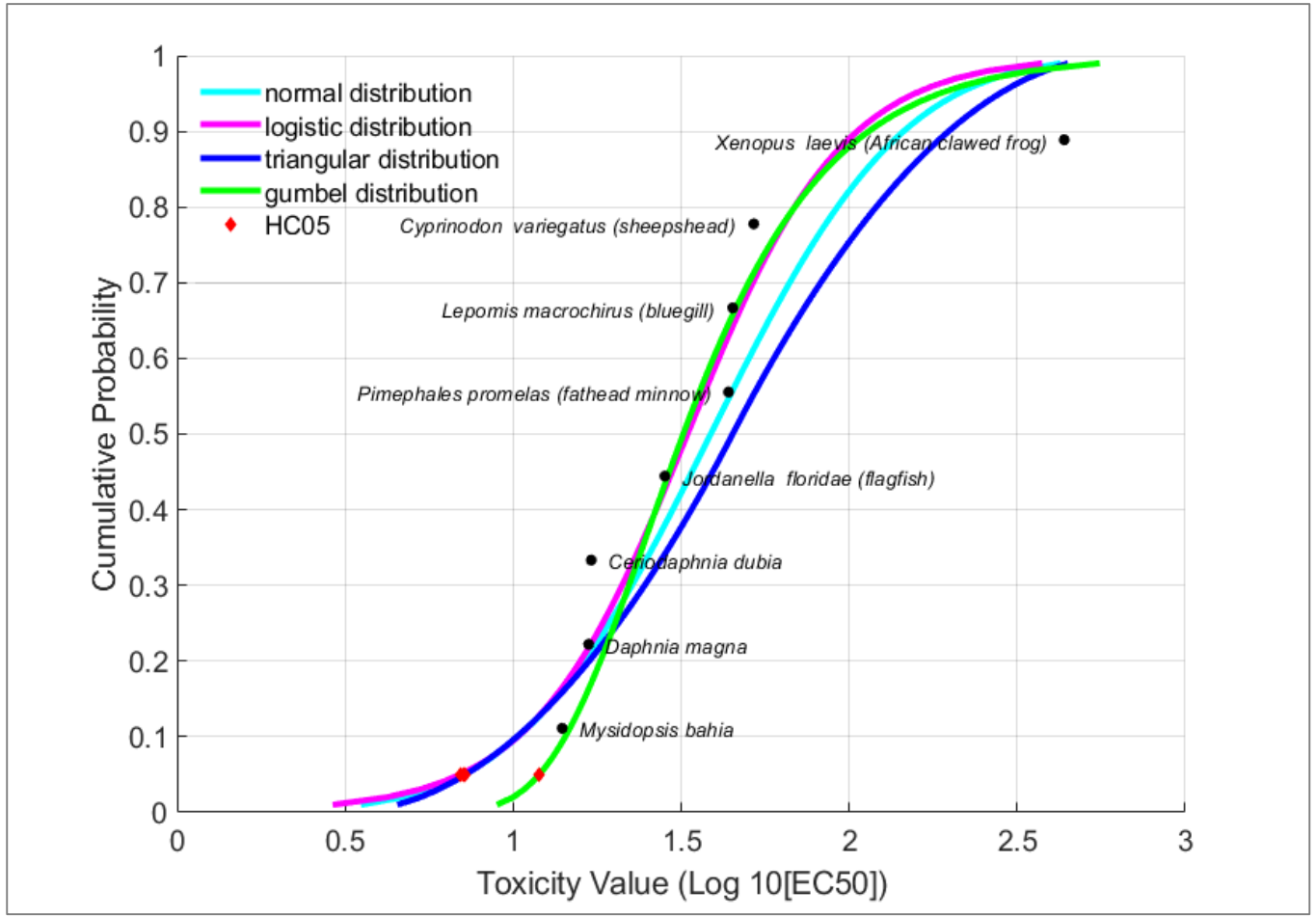
Fig 1. SSD using EC_{50} algae data for TCE (triangular)



Acute aquatic toxicity data for TCE

- SSD was also used as a line of evidence for interpreting acute toxicity data for other aquatic organisms.
- The model-averaged HC_{05} from all four distributions was 9.9 mg/L or 9,900 µg/L.
- The SSDs showed aquatic invertebrates were the most sensitive species.

Fig 2. SSDs using acute data for TCE (Gumbel, logistic, triangular, normal)

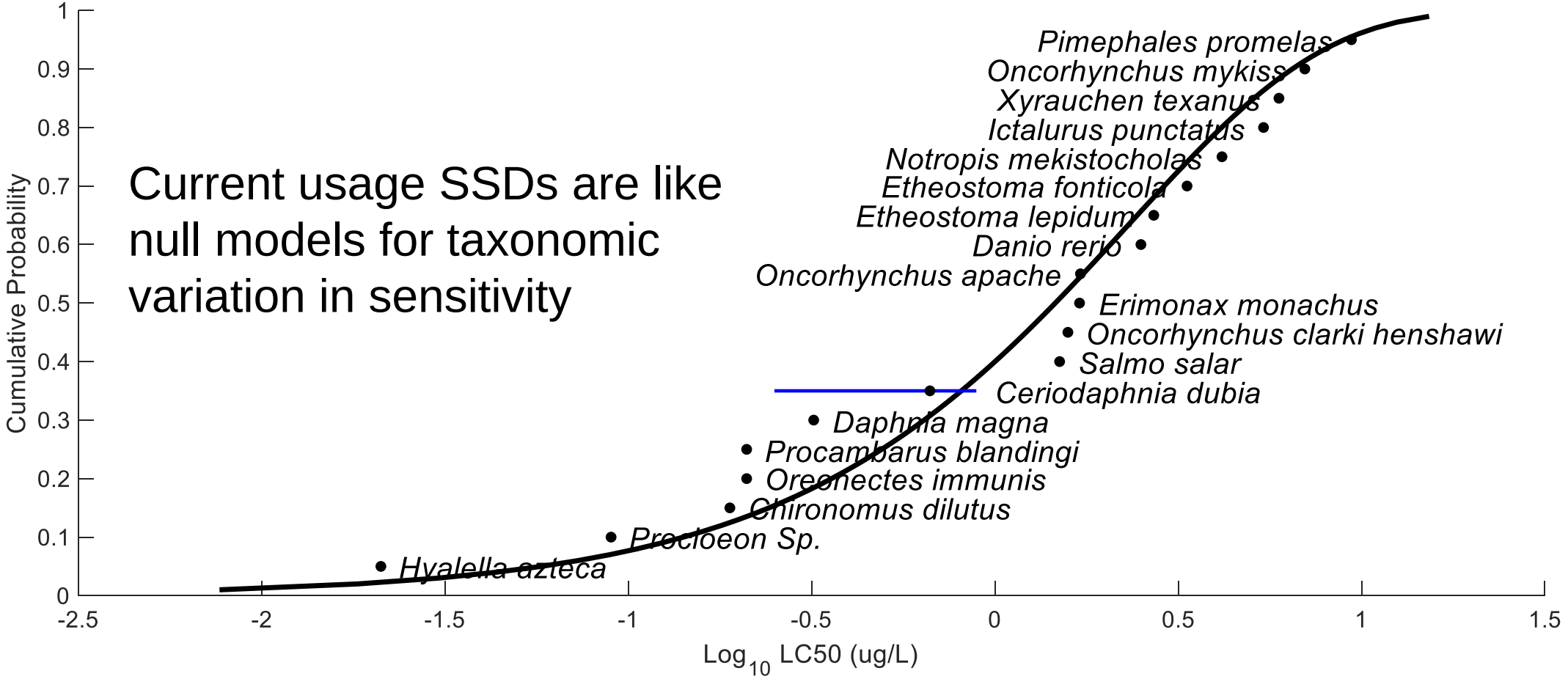


The Future of SSD: Systematic Variation

$\text{Log}_{10}(\text{LC50}) \sim \mu + \varepsilon$

- $\varepsilon \sim N(0,\sigma)$

Data from Fojut et al. 2012. Rev. Env. Contam. & Tox.

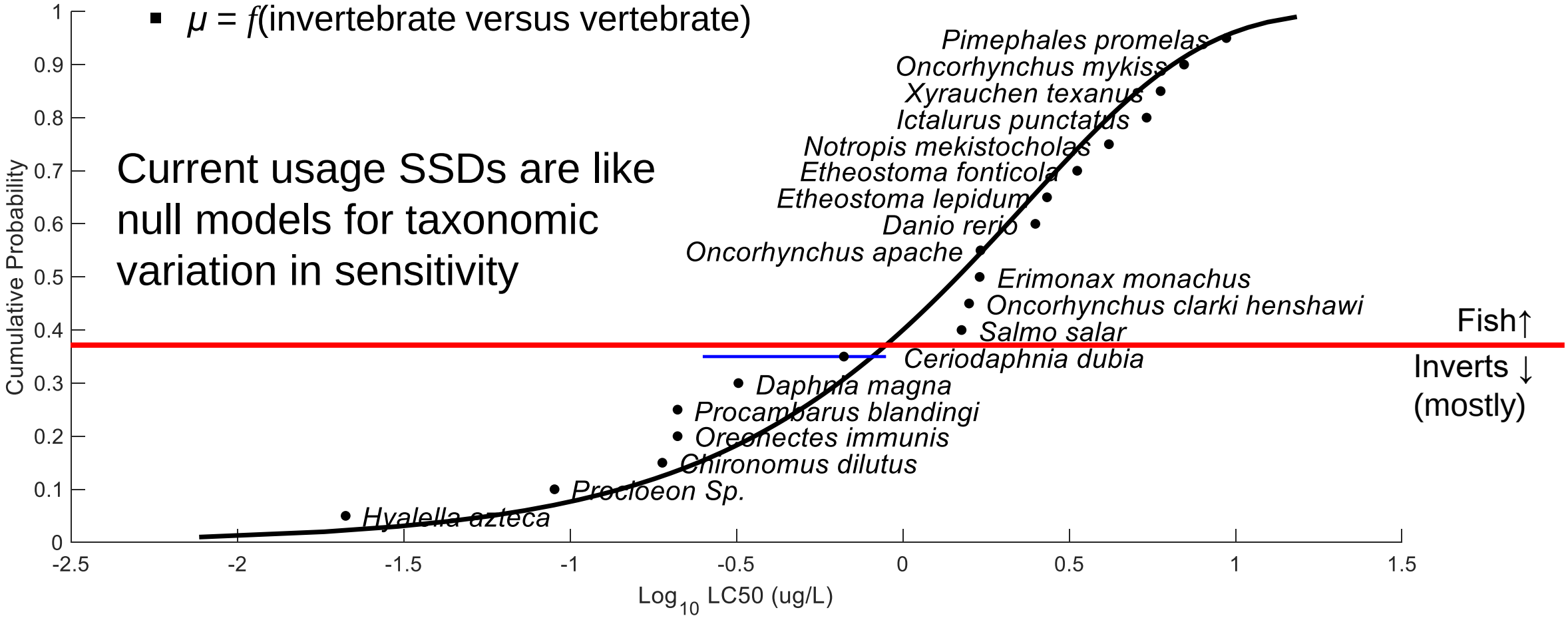


The Future of SSD: Systematic Variation

$\text{Log}_{10}(\text{LC50}) \sim \mu + \varepsilon$

- $\varepsilon \sim N(0,\sigma)$
- $\mu = f$(invertebrate versus vertebrate)

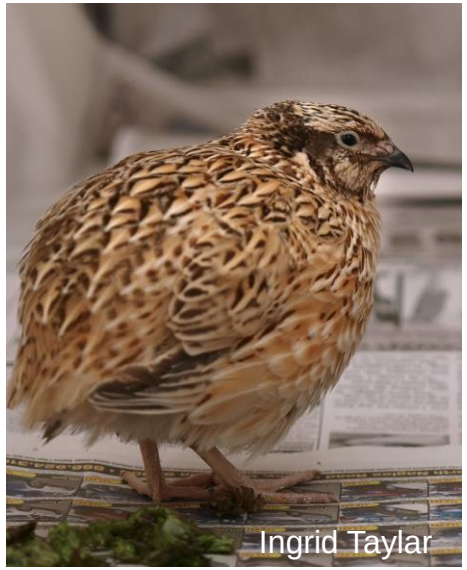
Data from Fojut et al. 2012. Rev. Env. Contam. & Tox.

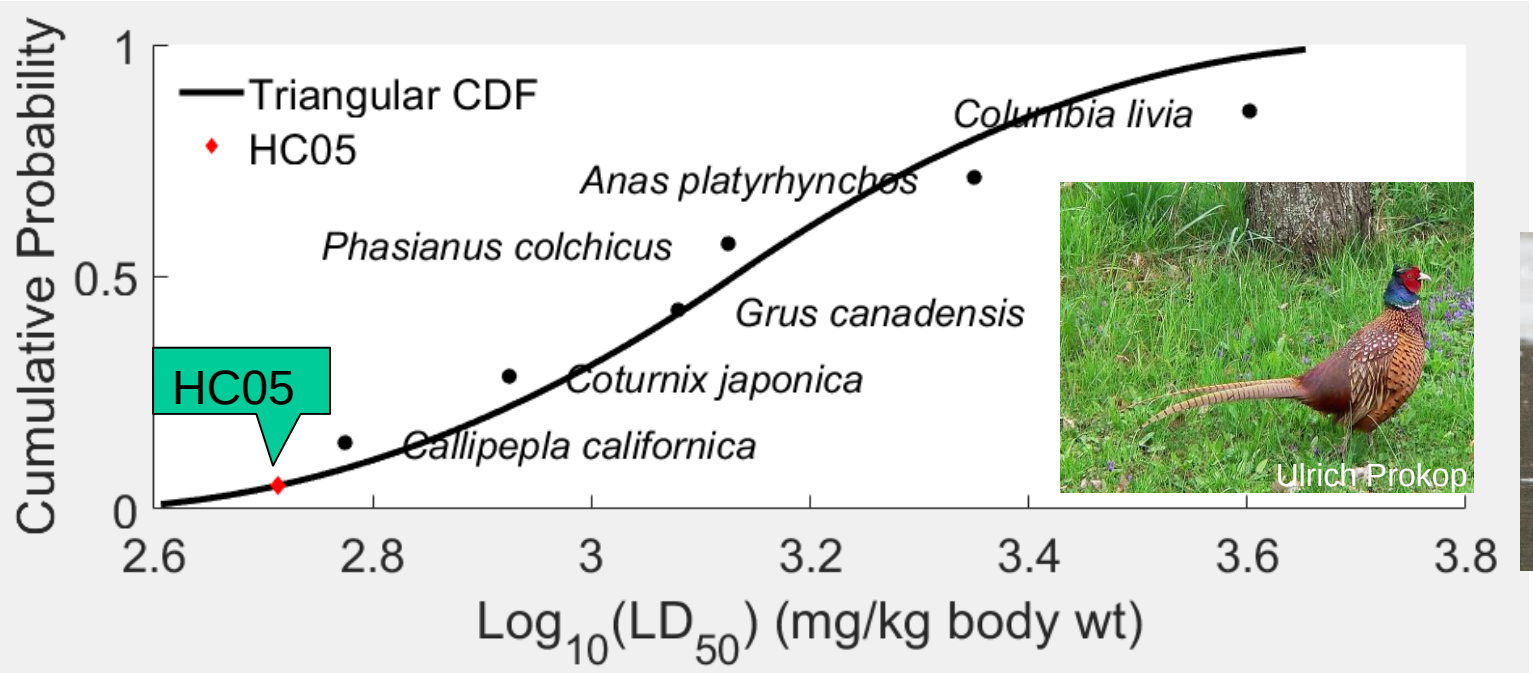


The Future of SSD: Systematic Variation

$\text{Log}_{10}(\text{LC50}) \sim \mu + \varepsilon$

- $\varepsilon \sim N(0,\sigma)$
- $\mu = ?$

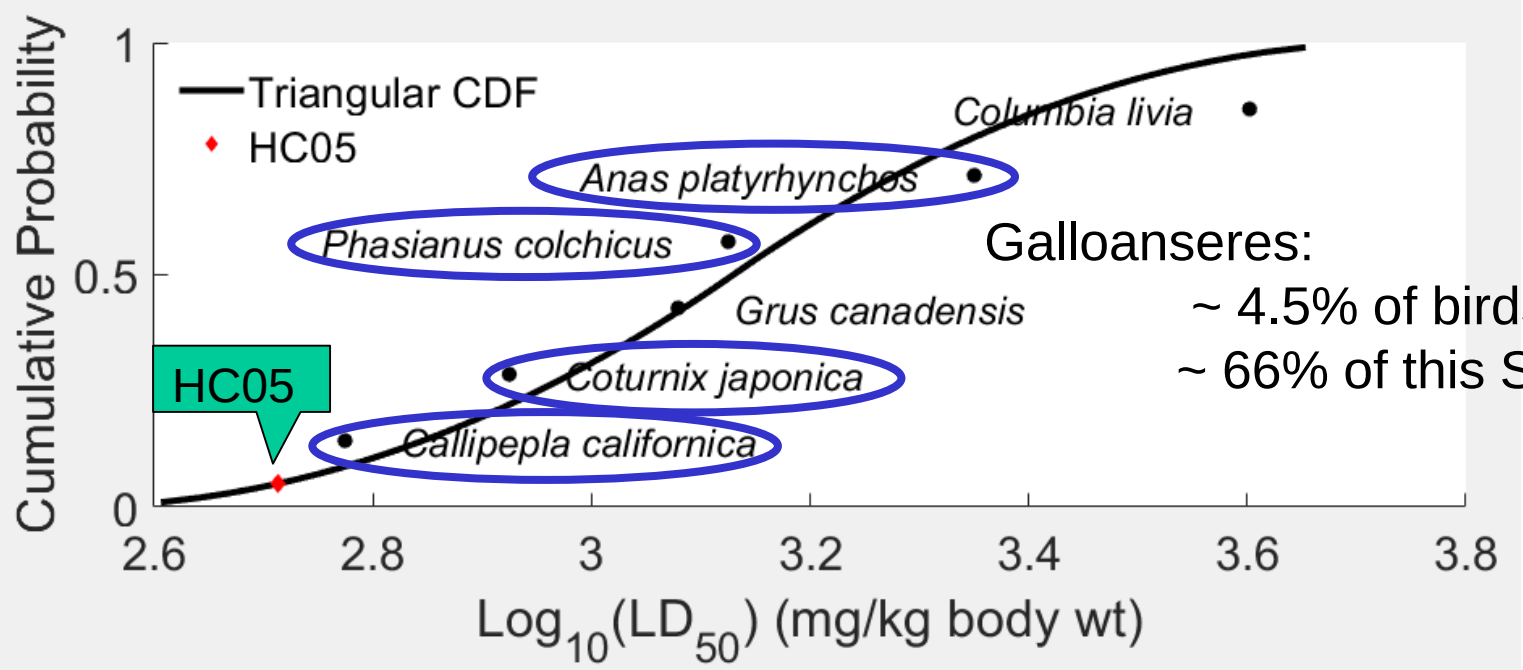




The Future of SSD

$\text{Log}_{10}(\text{LC50}) \sim \mu + \varepsilon$

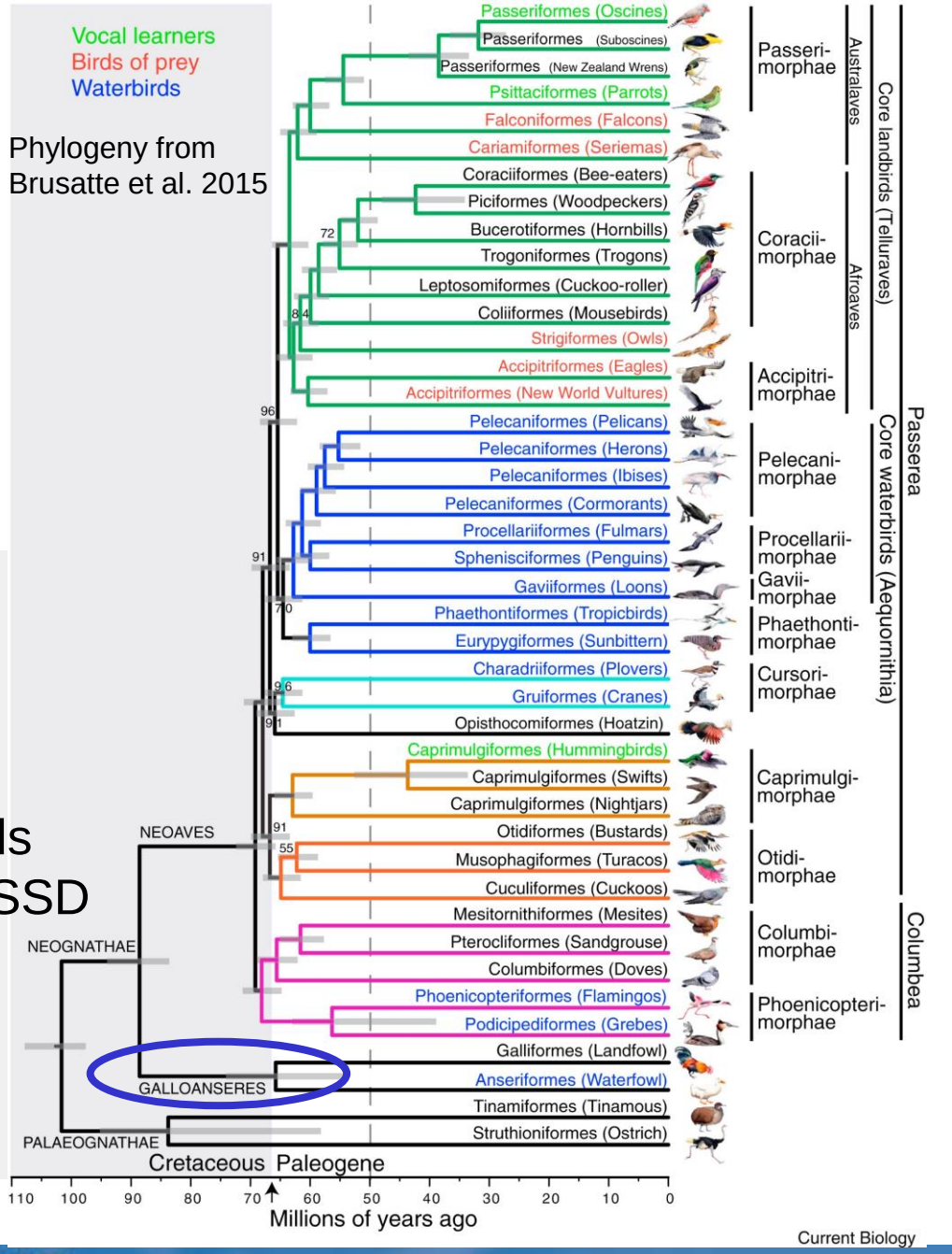
- $\varepsilon \sim N(0,\sigma)$
- $\mu = f$(phylogeny + natural history + AOP + …?)



Galloanseres:

~ 4.5% of birds

~ 66% of this SSD



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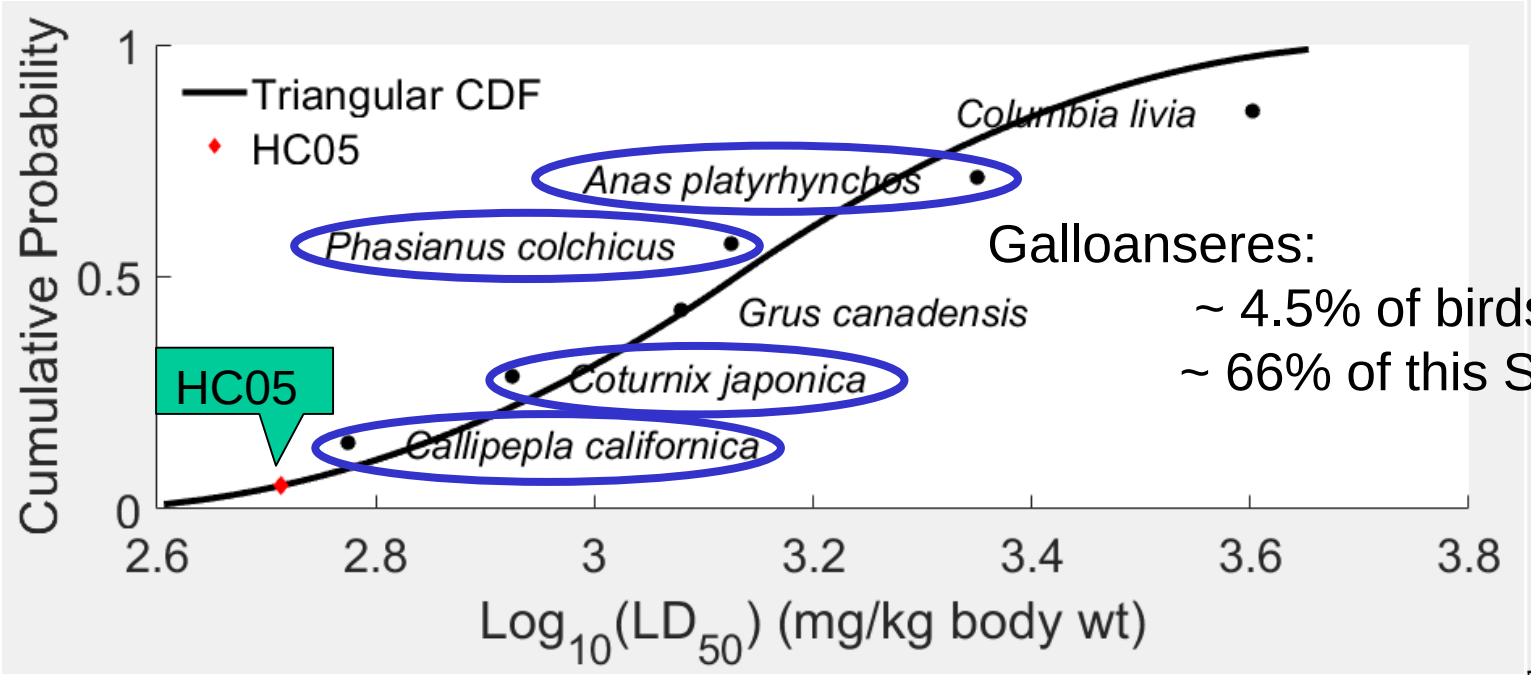

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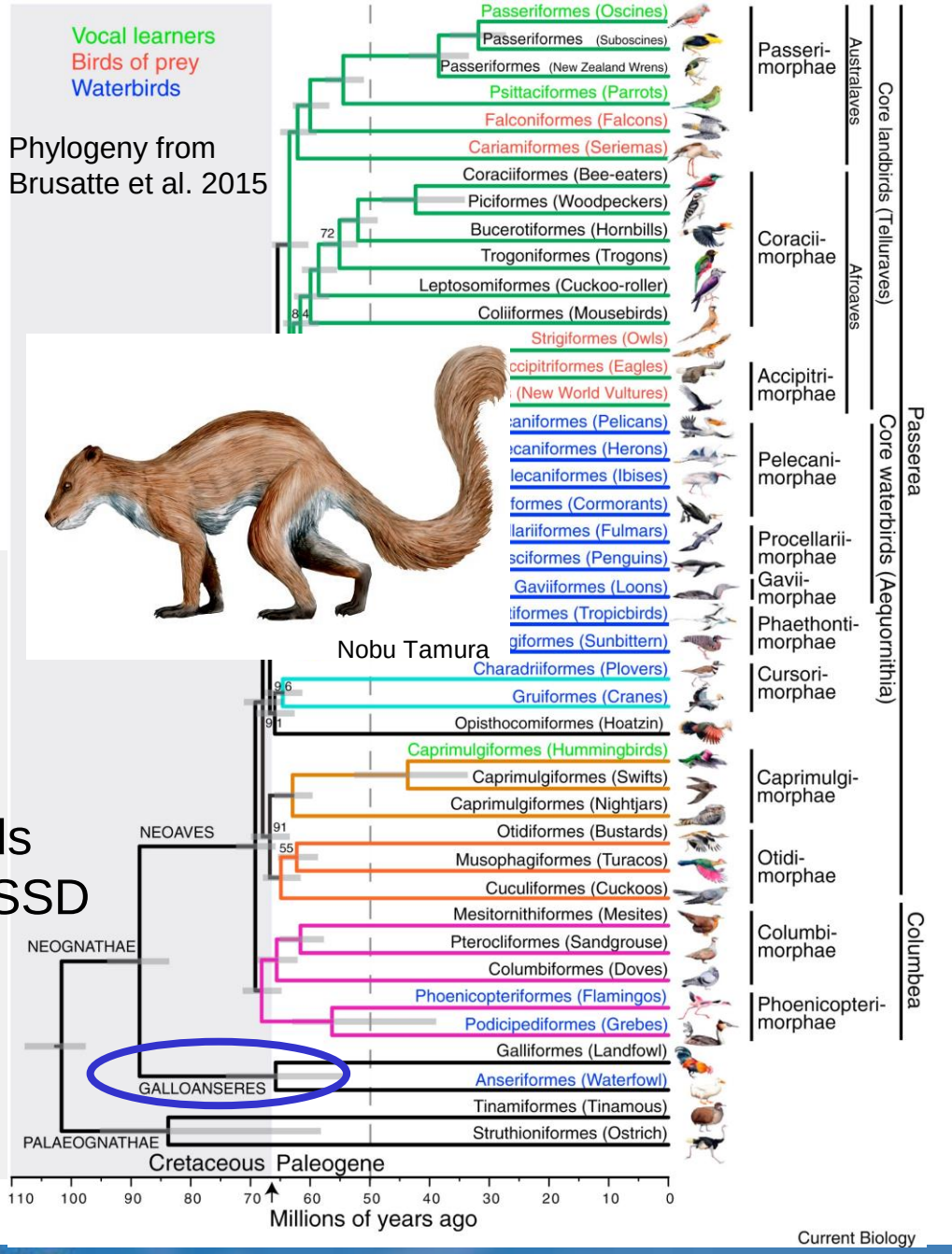

Future of the SSD Toolbox?

- www.epa.gov/chemical-research/species-sensitivity-distribution-toolbox ←**Going live soon!**
- Further enhancement of visualization tools
- Increased model-fitting capacity using MCMC sampler