

ExpoCast: High Throughput Exposure Prediction

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Introduction

Goal: There are thousands of chemicals, many without enough data for evaluation – working to provide a high-throughput exposure approach to use with the ToxCast chemical hazard identification.

TSCA21: Prioritization of ~500 Toxic Substances Control Act (TSCA) chemicals

EDSP21: Prioritization of ~2000 Endocrine Disruptors Screening Program (EDSP) chemicals

OW21: Development of next chemical contaminants list (CCL)

Using fate and transport models to predict the contribution from manufacture and industrial use to overall exposure rapidly and efficiently

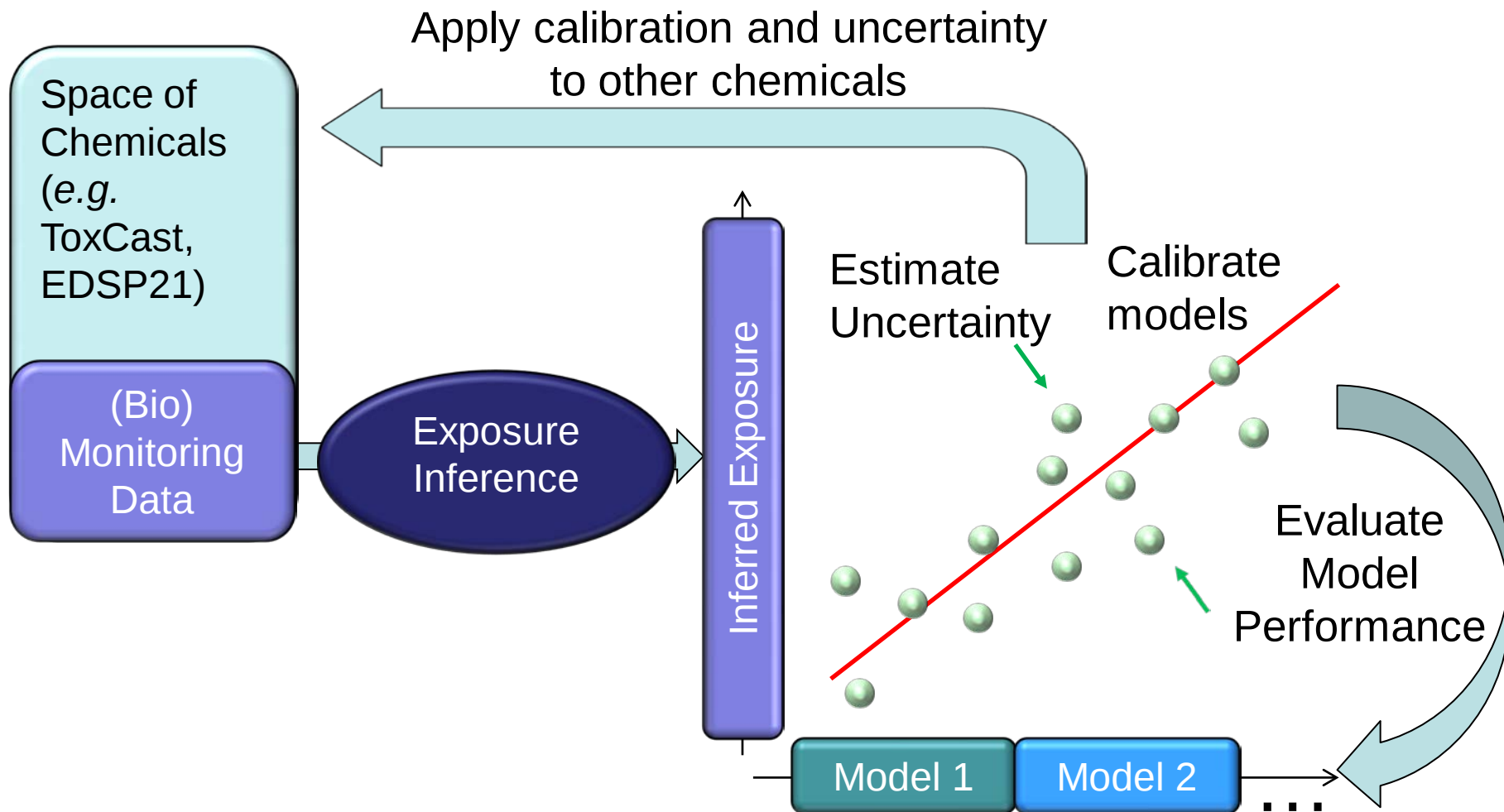
Applying and developing new high throughput models of consumer use and indoor exposure

Environmental Fate and Transport



Consumer Use and Indoor Exposure

Framework for High Throughput Exposure Models



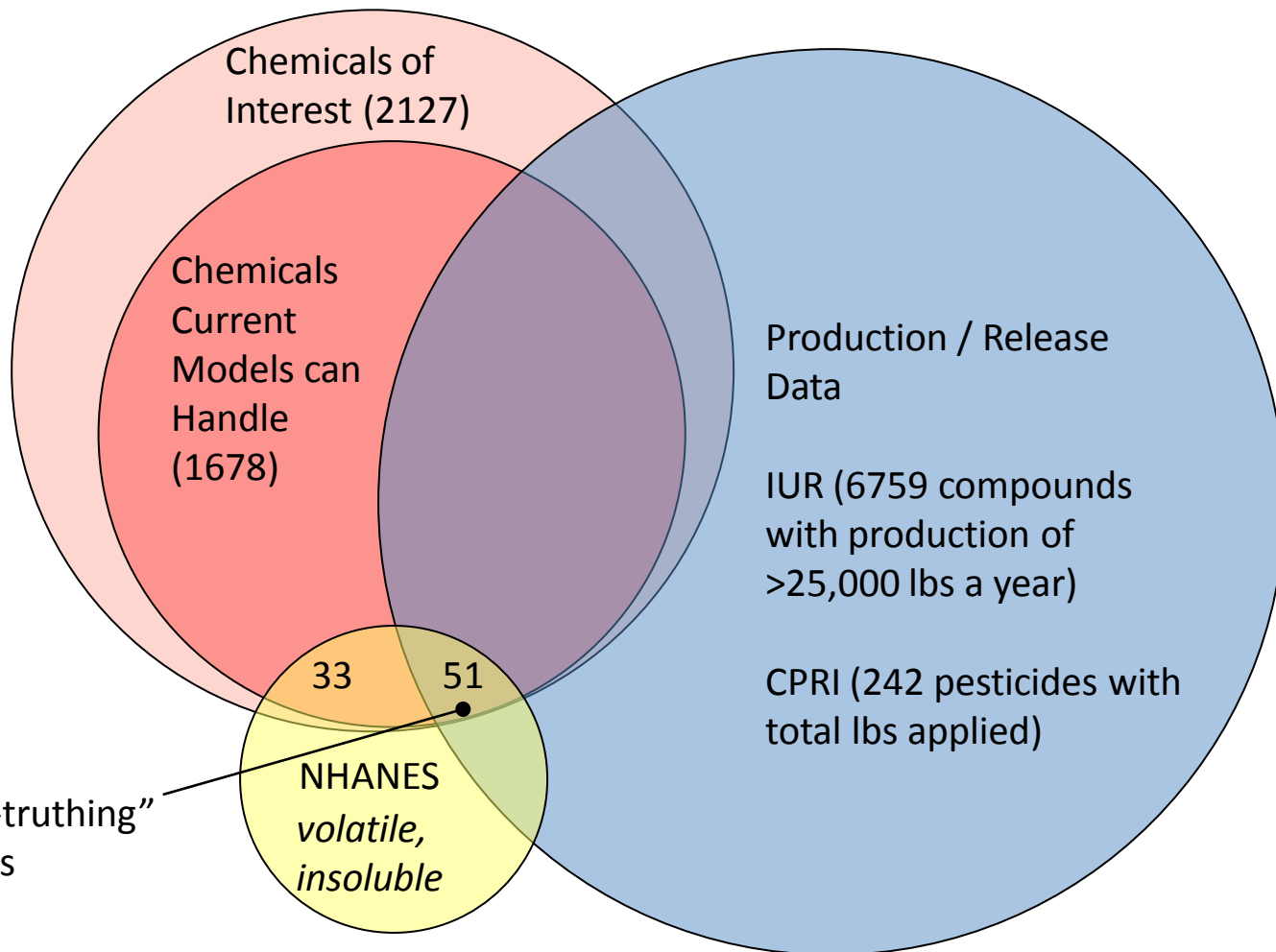
Data Availability for Model Predictions and Ground-truthing

Ground—truth
with CDC NHANES
urine data

Focusing on U.S.
median initially

Capable of adding
population
variability, but will
need consumer
use models

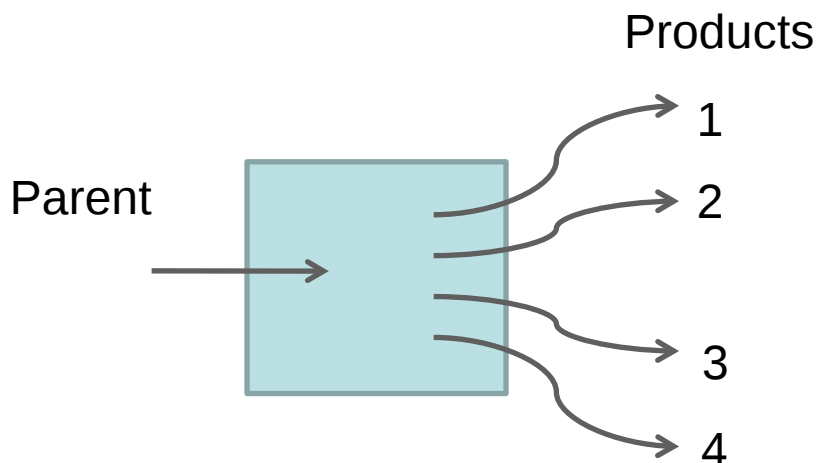
“Ground-truthing”
Chemicals



Linking NHANES Urine Data and Exposure

Steady-state assumption

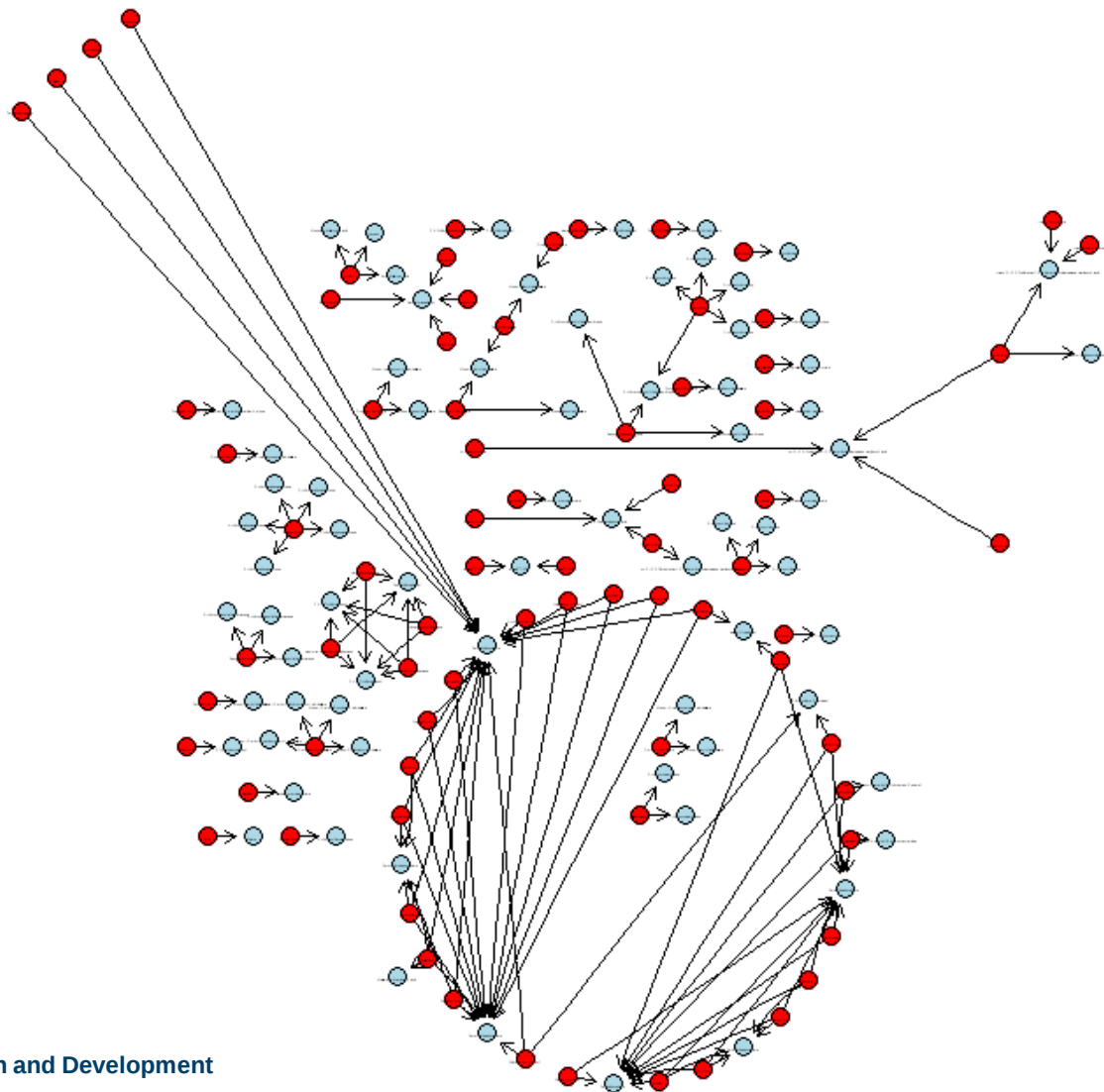
$$(\text{mg/kg/day})_i = \frac{1}{70 \text{ kg}} \frac{\text{mg}_i}{g_{\text{creatinine}}} * \frac{g_{\text{creatinine}}}{\text{day}}$$



$$(\text{mg/kg/day})_0 = \text{MW}_0 \sum_i \phi_{0i} \frac{(\text{mg/kg/day})_i}{\text{MW}_i}$$

Lakind and Naiman (2008)

Stoichiometry of NHANES Parents and Metabolites

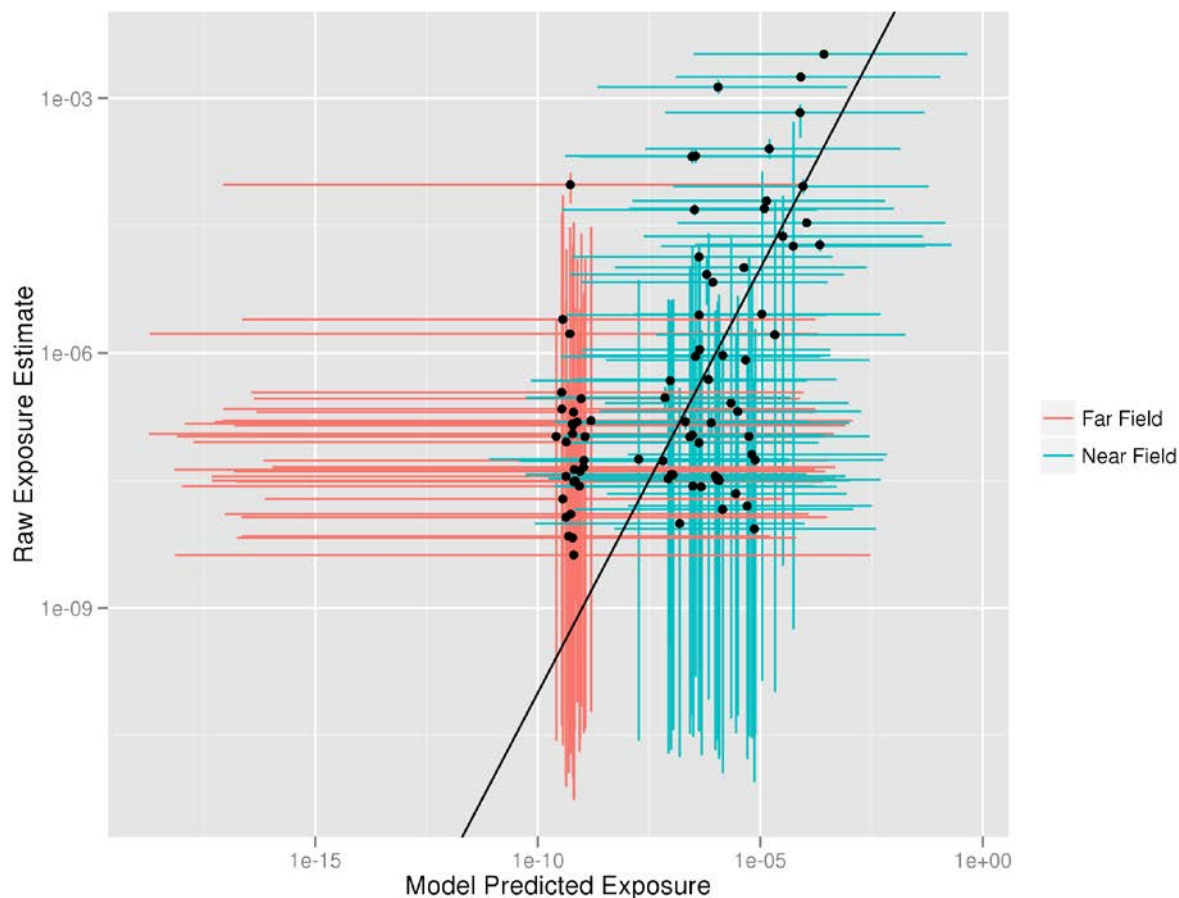


Calibrate ExpoCast Predictions to CDC NHANES Data

$$Y \sim b_1 + b_2 * N + m_2 \log(vu) + m_3 \log(vr)$$

Comparison between
model predictions and
biomonitoring data
indicates correlation

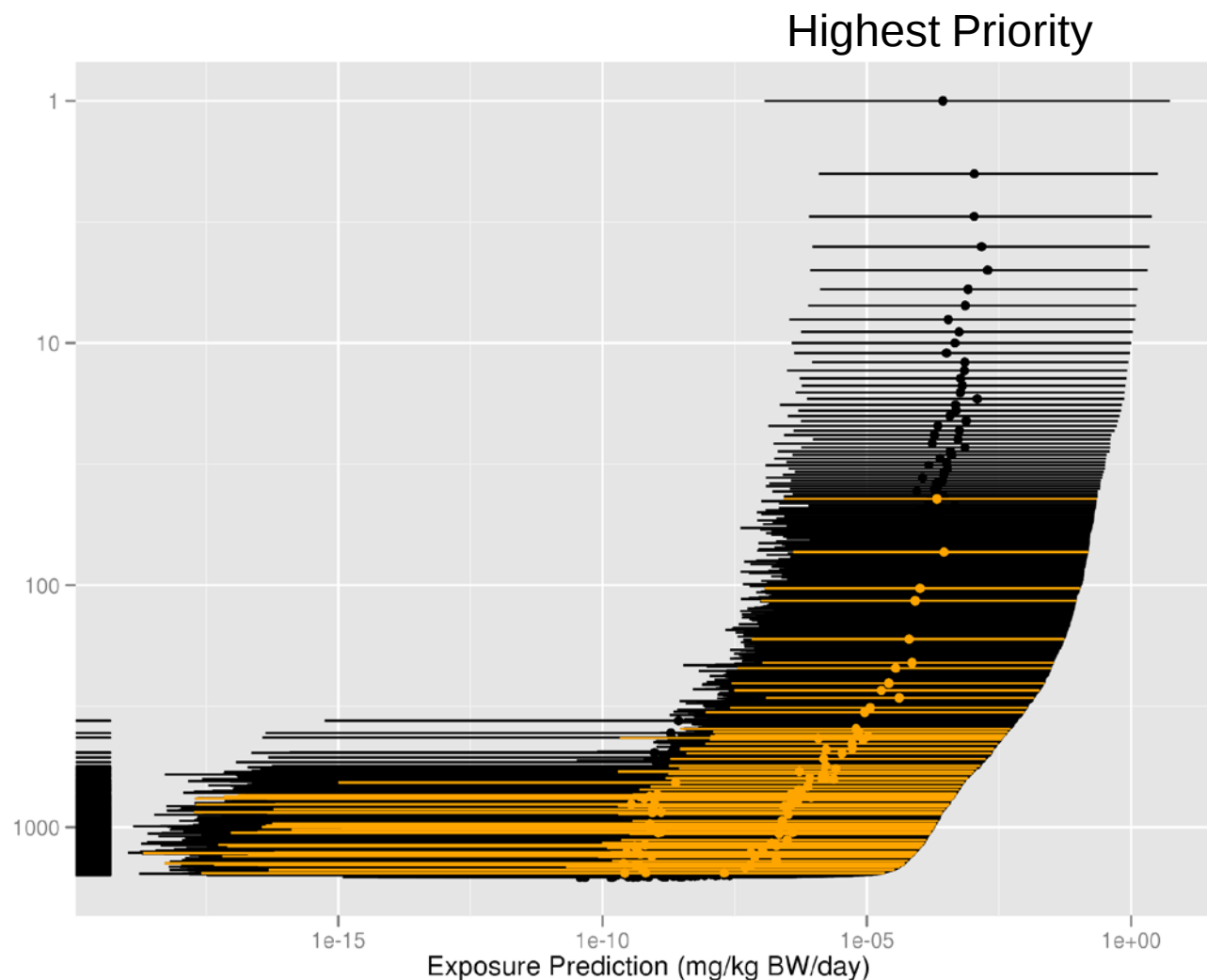
Indoor/consumer use is
critical:
Compounds with near-
field applications more
than 100x greater



Exposure Prioritization from ExpoCast

Uncertainty of prediction indicated by the horizontal confidence interval from the empirical calibration to the NHANES data

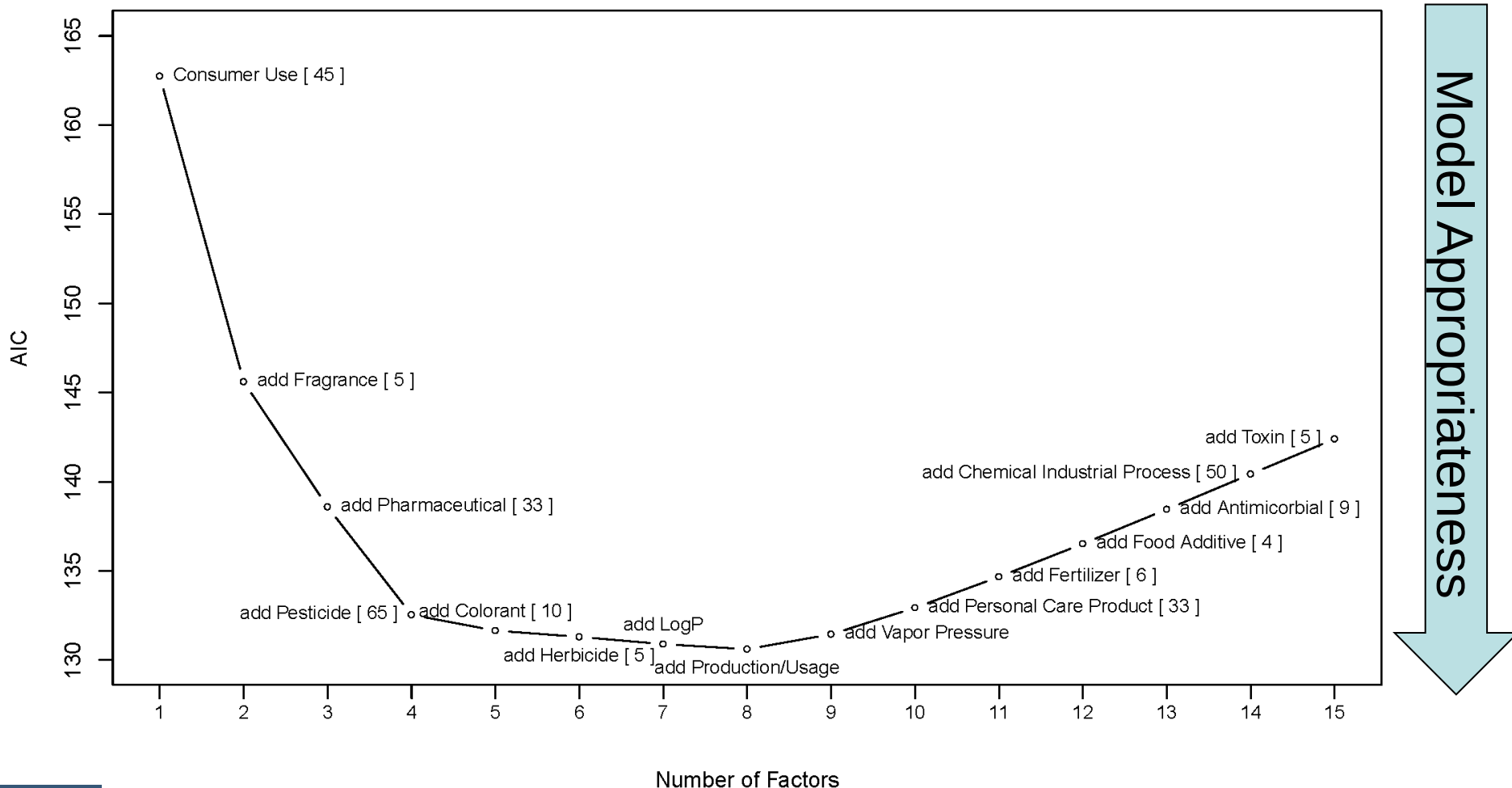
Horizontal dotted line indicates the fiftieth percentile rank and the vertical dotted line indicates the cutoff between overlapping top-half and lower half confidence intervals





Statistical Near Field Model

Analysis by Amber Wang (EPA/NCSU) of Alicia Frame's HT use descriptors



Conclusions

- ExpoCast can use environmental fate and transport models to make high-throughput exposure predictions
 - These prioritizations have been ground-truthed with CDC NHANES data
 - This biomonitoring data gives empirical calibration and estimate of uncertainty
- Indoor/consumer use is a primary determinant
- Next steps:
 - HT models for exposure from consumer use and indoor environment
 - Use and evaluate these models as additional HT exposure assays



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