

THE IMPORTANCE OF VALIDATING SOURCE IDENTIFICATION RESULTS AND EVALUATING ALTERNATIVE HYPOTHESES IN A FORENSIC EVALUATION

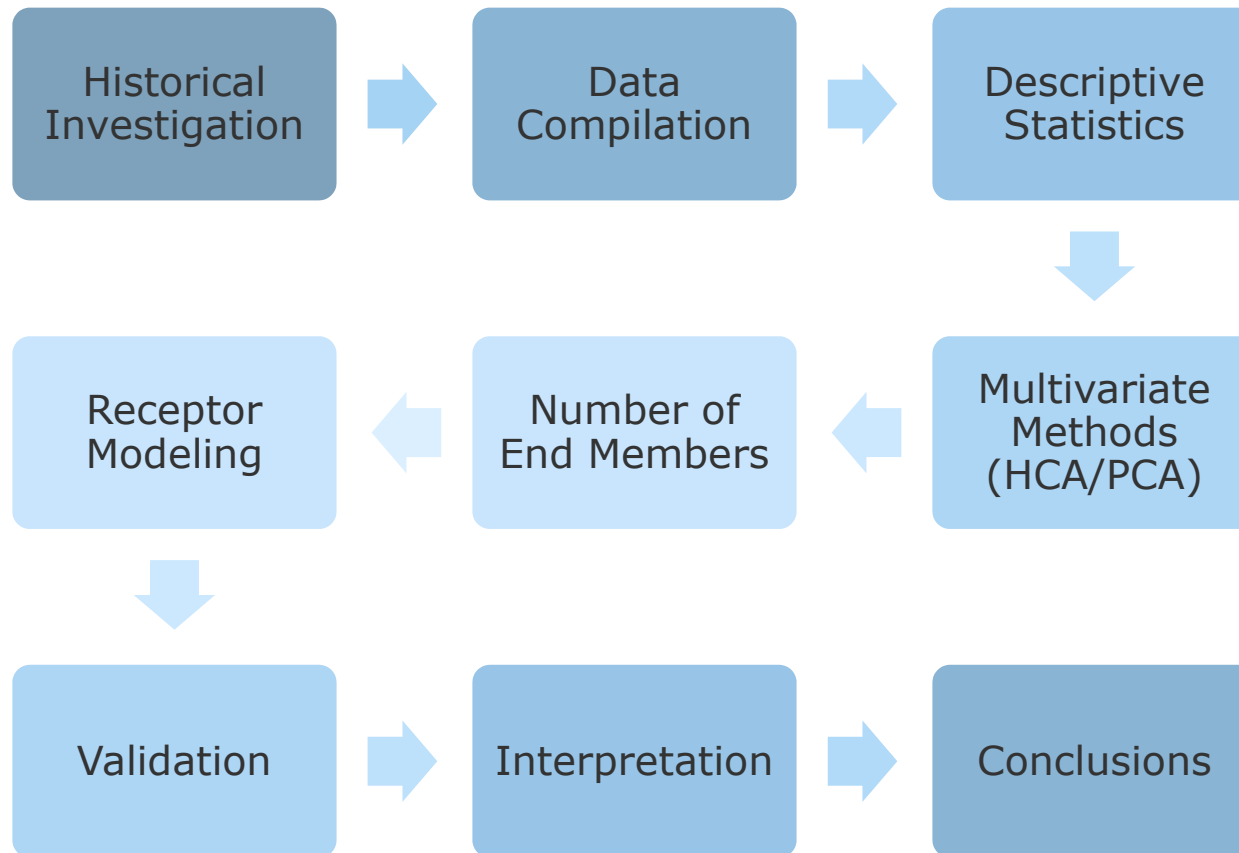
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OVERVIEW

- The use of statistical methods for source identification have gained wide acceptance
- Because of the complexity of the methods, their validity and accuracy are often not questioned
- Model testing and validation is often skipped or incomplete
- Formal hypotheses are either unstated or not developed
- When these steps are not rigorously followed and documented, incorrect conclusions are likely

TYPICAL WORKFLOW



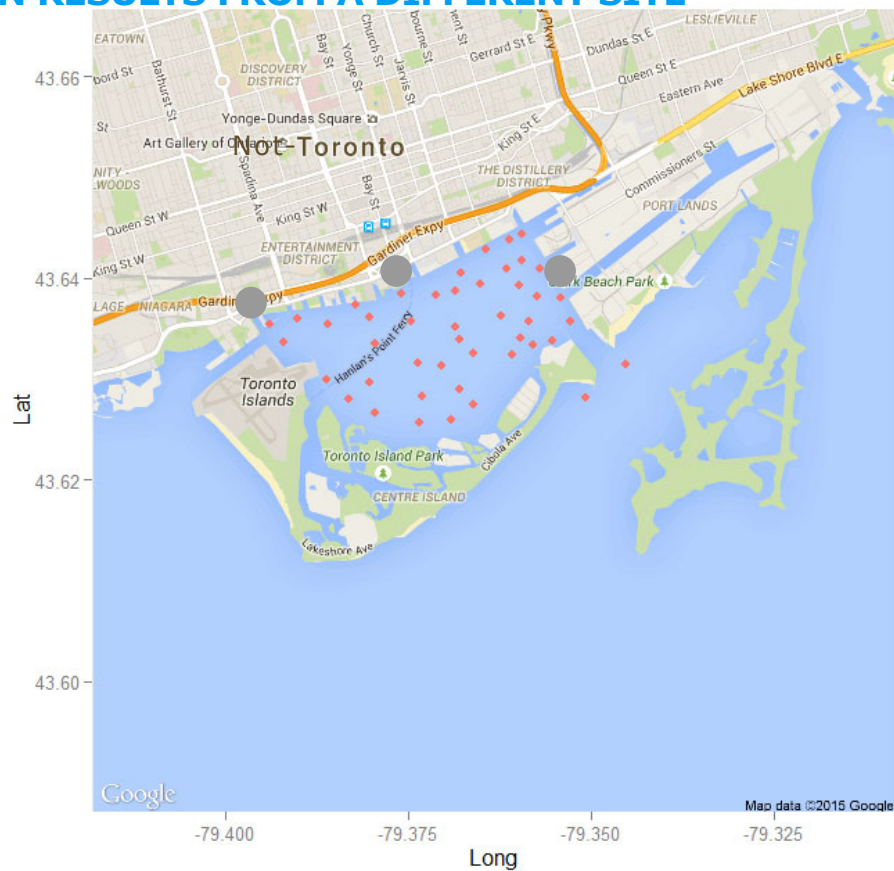
SIMULATED CASE STUDY

- Inspired by a dioxin site
- Setting changed to a different harbor complex
- Chemicals of concern changed to PCBs
- Simulated PCB profiles based on Frame Aroclor data plus random variation

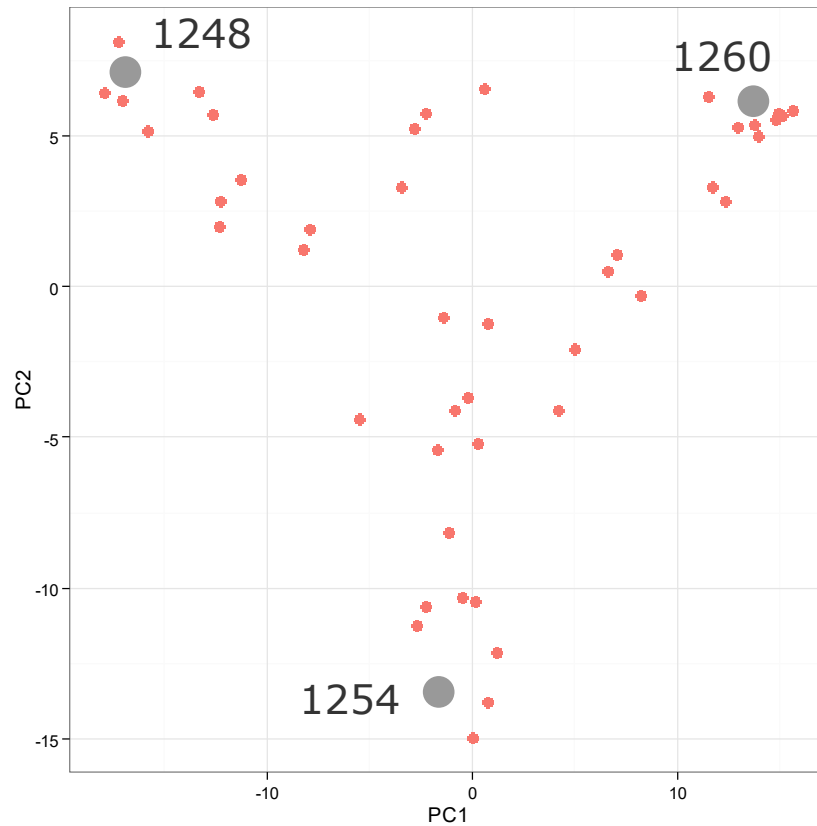
Any resemblance to a real site is purely coincidental

SIMULATED PCB EXAMPLE

ADAPTED FROM DIOXIN RESULTS FROM A DIFFERENT SITE



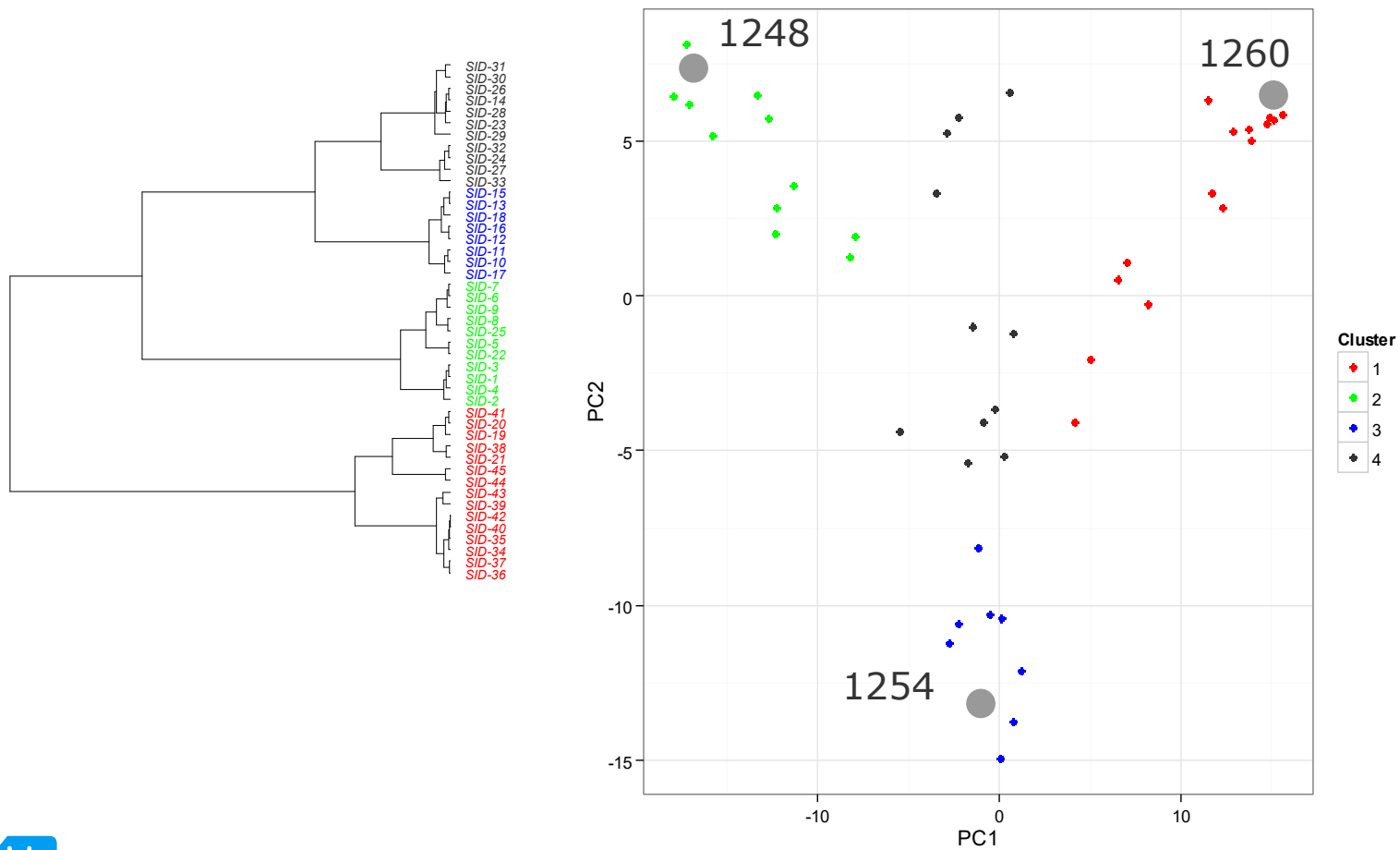
TYPICAL SIMPLE PCB PCA ANALYSIS



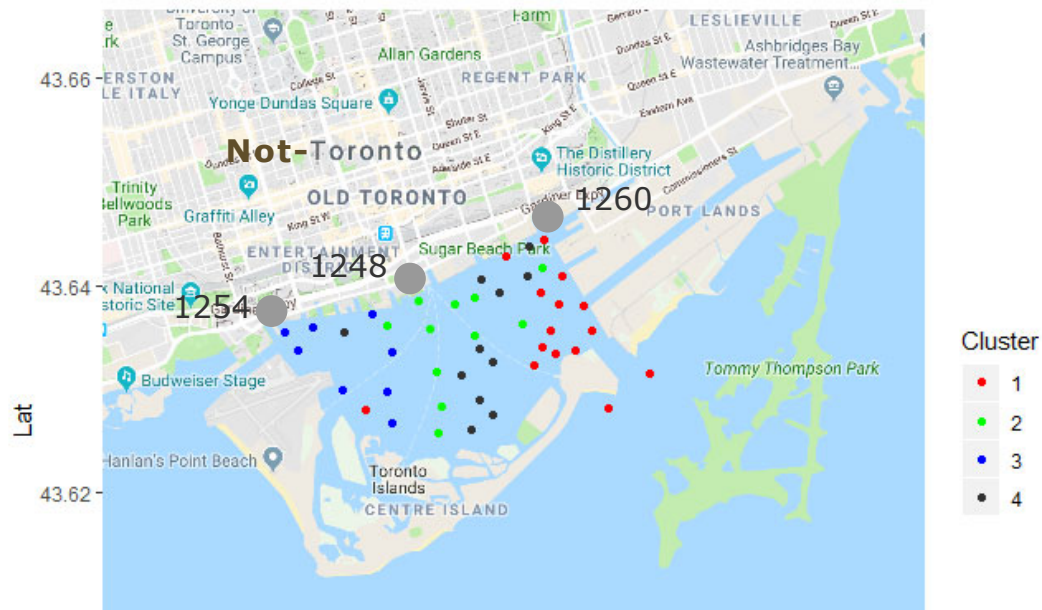
Asked to review previous assessment

- PCA analysis of normalized data
- Consistent with three sources
 - 1248
 - 1254
 - 1260
- No formal assessment of end members
- No formal assessment of individual profiles
- Limited historical investigation, assumed background provided by regulators was correct

SAMPLES ASSIGNED TO GROUPS BASED ON HCA



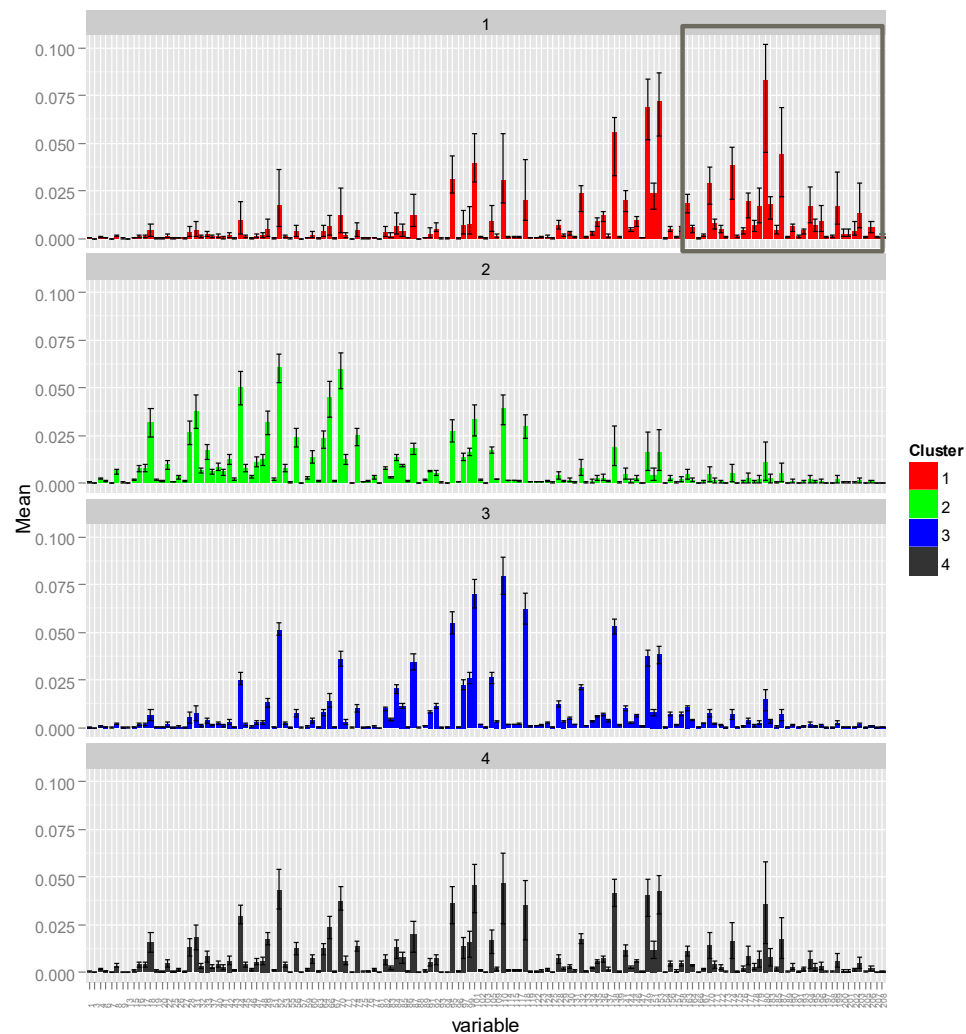
INITIAL CONCLUSIONS



- Three known PCB sources: (1) 1248 (2) 1254 and (3) 1260 sites
- Impacts from the 1260 source have migrated outside of the harbour
- Addition investigation outside of the harbour recommended to delineate the 1260 source
- Validated the calculations of the other expert, but is this an accurate assessment of sources?

CLUSTER VARIABILITY

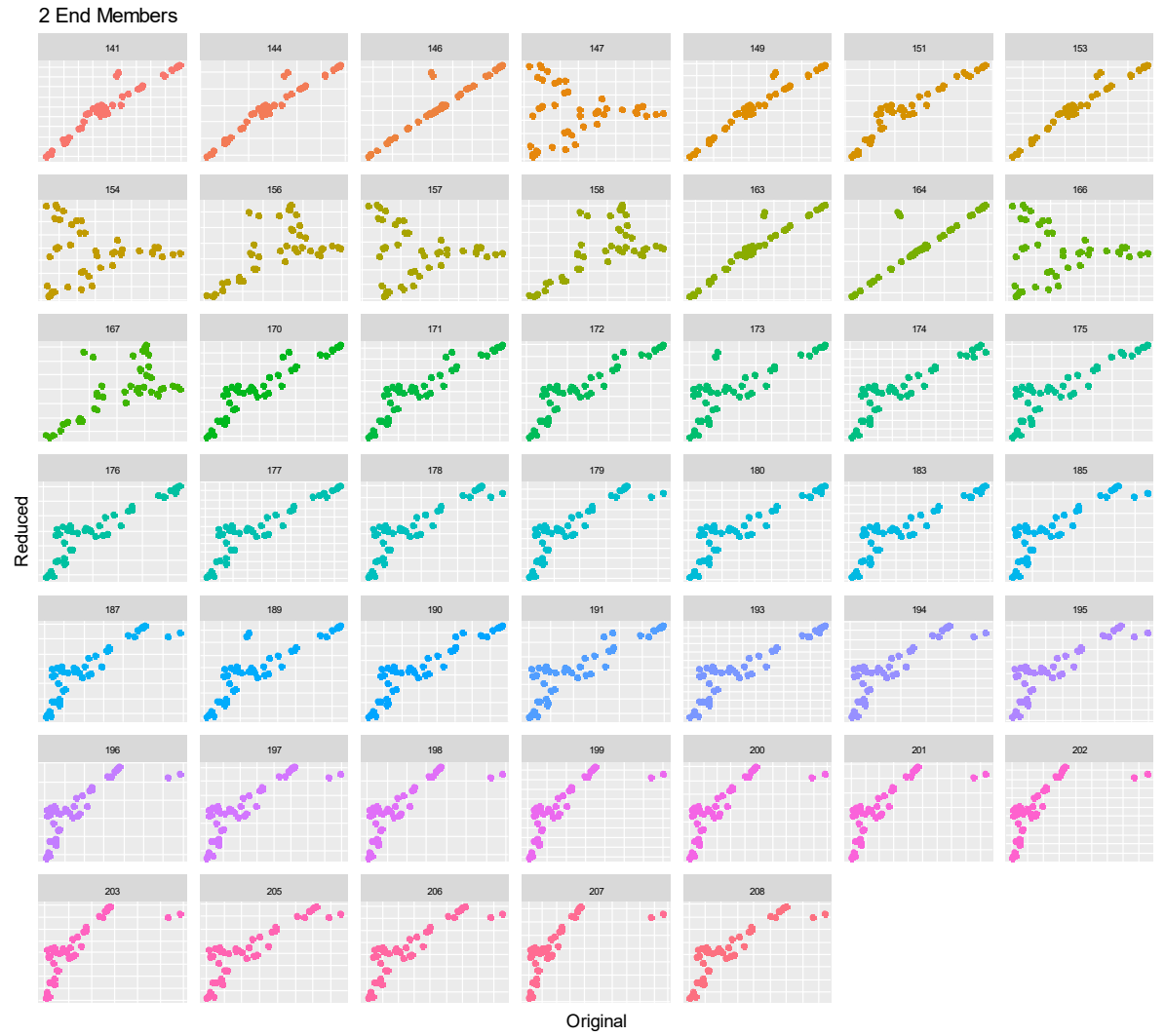
- Variability in Cluster 1 is higher than Clusters 2, 3, and 4
 - Congeners 180, 187, 199, and 203 show more variability than most of the others
- Initial suggestion that the conceptual model and the statistical model may both be wrong



DETERMINATION OF NUMBER OF END MEMBERS

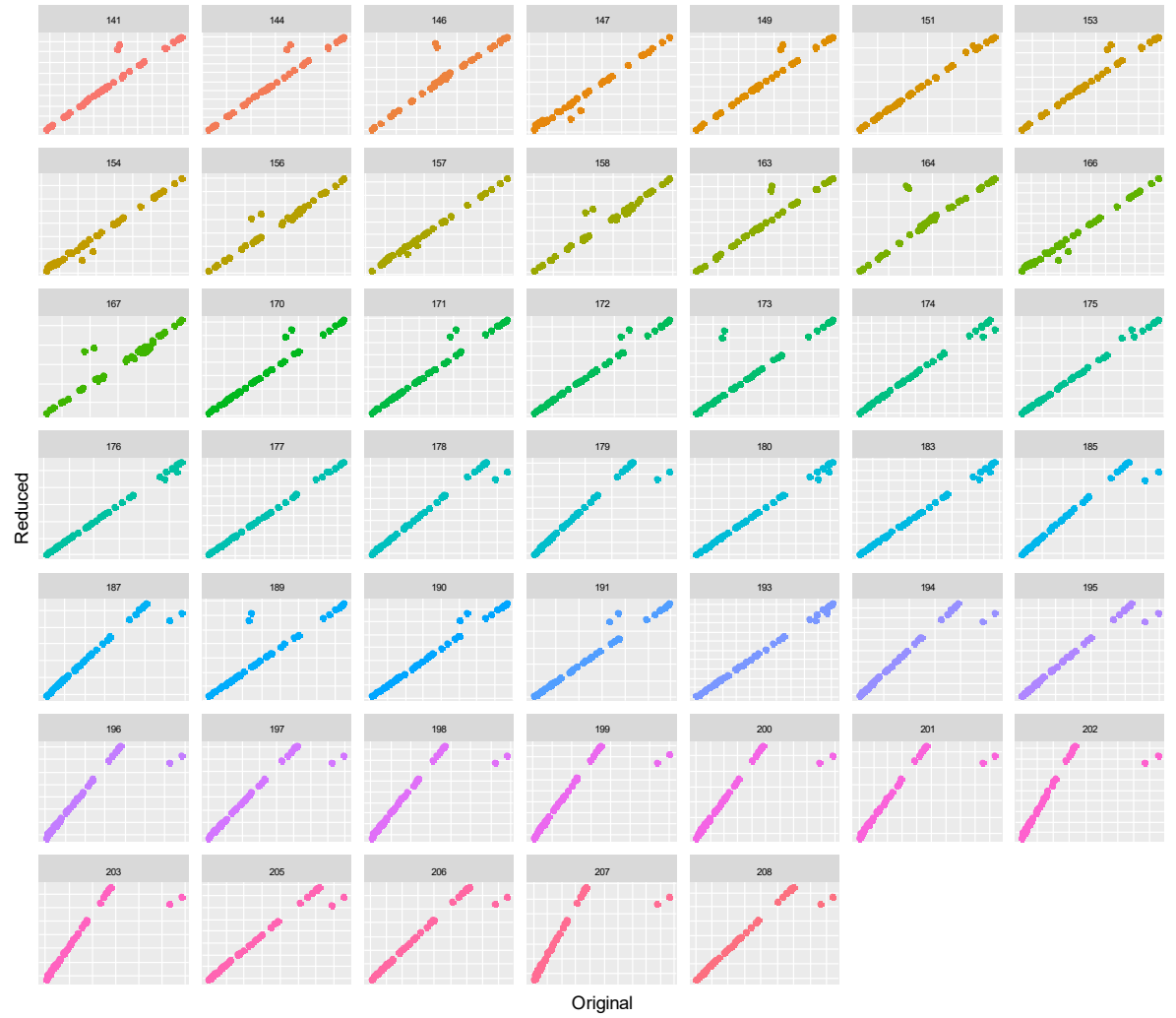
- Use PCA analysis to reduce the dimensionality of the dataset
 - Retain the 1st 2-4 principal components
 - Recalculate the original values
 - Test GOF
- Confirm number of end members and confirm fit

TWO END MEMBERS

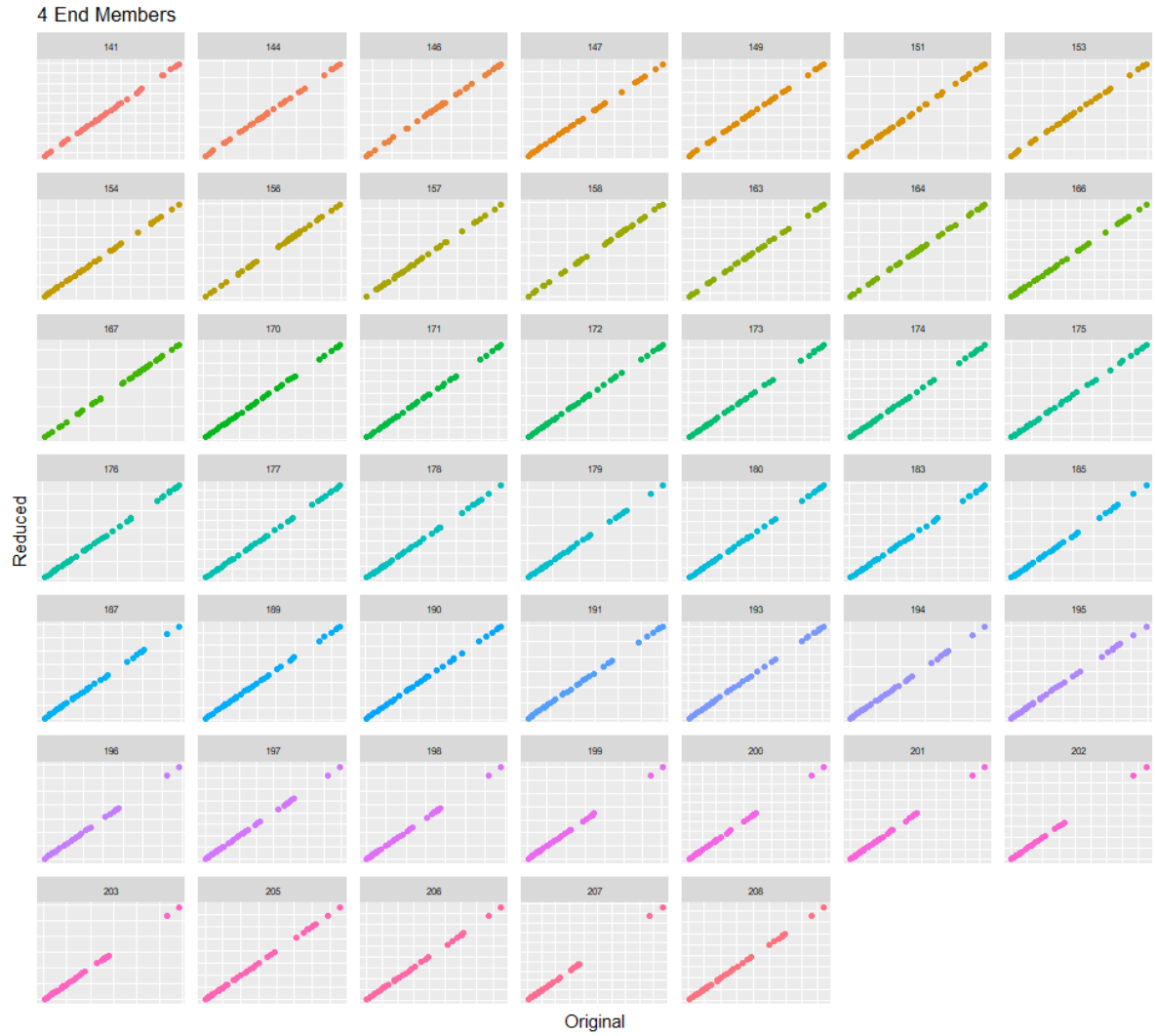


THREE END MEMBERS

3 End Members



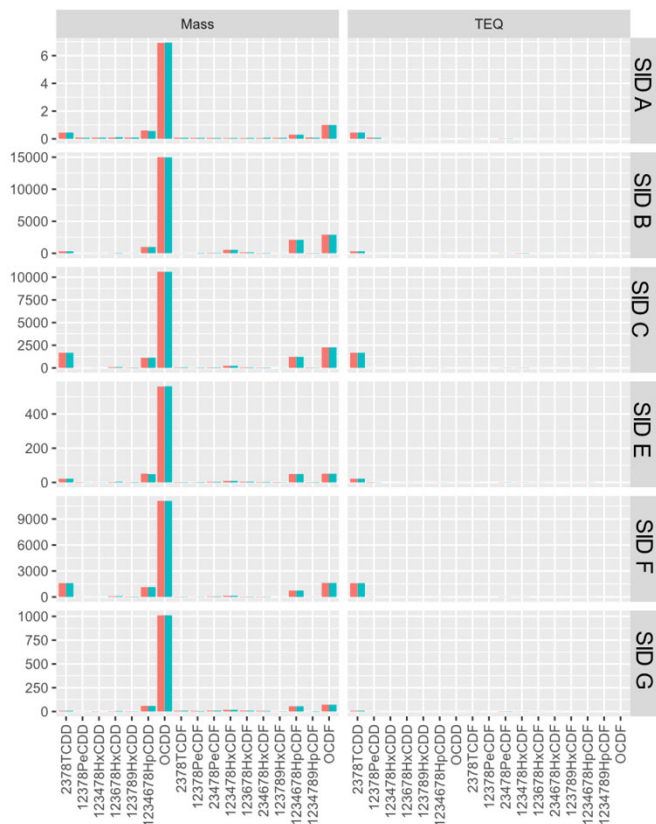
FOUR END MEMBERS



UNMIXING MODELING AND VALIDATION

- Begin with PCA/HCA
 - Variability within clusters
 - Frequency of detection
- Number of end members for receptor modeling
 - Model versus measured fit by analyte
- 'Remix' the sample and calculate goodness of fit
 - Model versus measured by analyte
 - Model versus measured by sample (RMSE and by sample plots)
- Try to find flaws in the statistical model
 - Revise/update model
 - Retest

COMPARISON OF MODELED AND MEASURED PROFILES

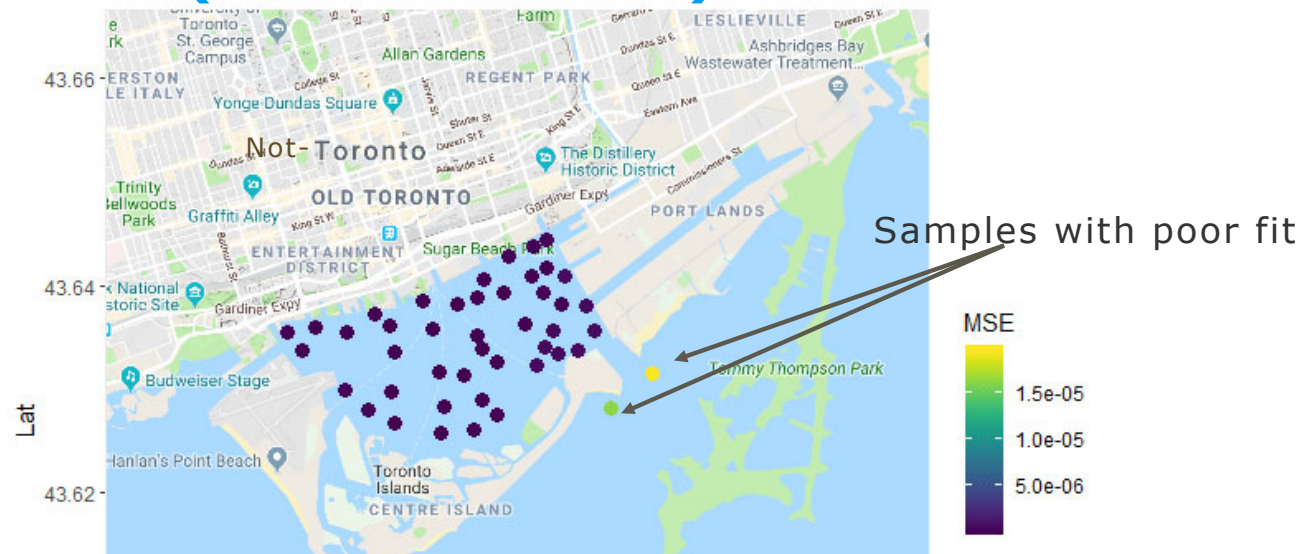


“Remixing” the samples

- Use modeled source profiles and source contributions to recalculate profiles
- Compare measured and modeled profiles

Type ■ Measured ■ Modeled

GOODNESS OF FIT (3 END MEMBERS)



- Calculated the mean squared error for the 3 end member model
- Poor fit for the samples collected outside of the harbour
- Laboratory and data validation reports obtained and reviewed
- New historical records search initiated

SOURCE ATTRIBUTION VALIDATION

- Compare the modeled end member profiles to each other
- Compare the modeled end member profiles to a source library
 - Source profiles from the literature
 - Source profiles based on upland data
- Interpretation of end members and source profiles
 - Are the modeled end members represented in the source library?
 - Can the unusual end members be simply explained?
 - Revise and update the model if flaws are apparent?
- Source attribution
 - Endmembers <> sources

HYPOTHESIS TESTING

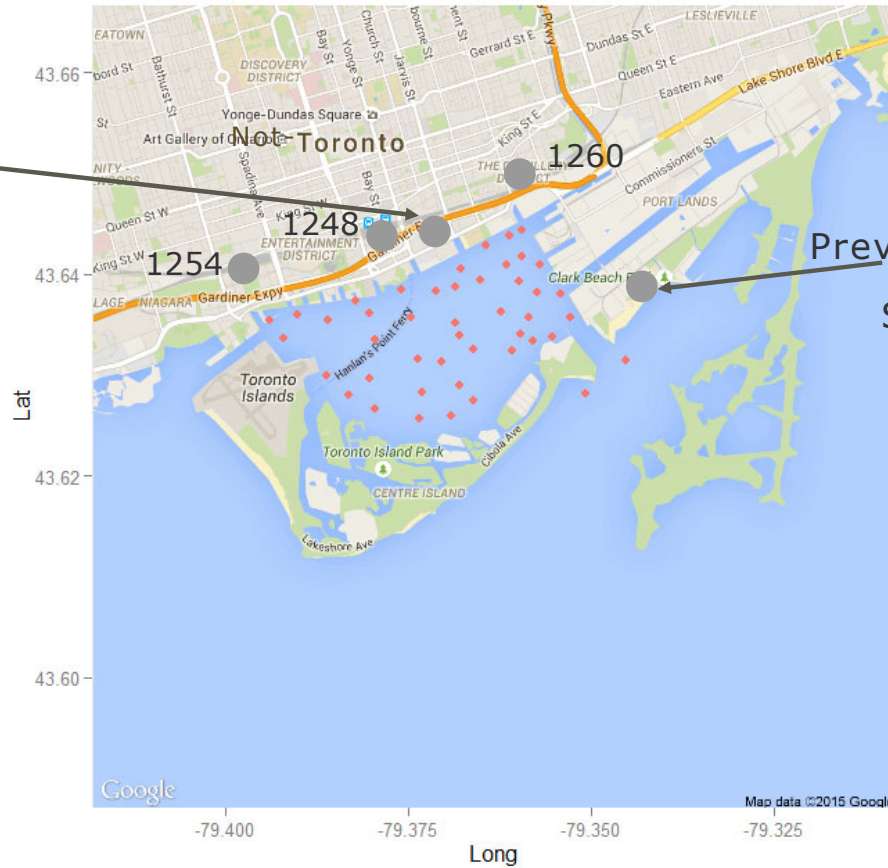
- Formal hypothesis
 - H0: Site A is not a significant contributor to an end member
 - HA: Site A cannot be ruled out as a significant contributor to an end member
- Receptor modeling cannot differentiate between similar source types, for example:
 - The same PCB Aroclor could have been used at multiple sites
 - Multiple waste incinerators could have released dioxins
 - Nearby herbicide manufactures could have used the same dioxin production process or ingredients
- The first site you find that matches the end member is often not the only potential source
 - Comprehensive historical record search is required
 - Chemical processes and quantities
 - Waste handling and discharge pathways
 - The lack of records regarding usage and discharges is a data gap and not exculpatory

ADDITIONAL SOURCE INVESTIGATION

NEW PCBS SOURCES LOCATED: 1248 AND 1262 WERE USED AT TWO NEW SITES

Previously Unknown

Source: 1248



Previously Unknown

Source: 1262

CONCLUSIONS

- Formal validation of the statistical model must be complete
- Developing the model should be an iterative process: refine -> test -> refine
- Hypotheses should be formally stated and tested
- A complete background investigation is needed
- Weight of evidence evaluation can be used to evaluate multiple lines of evidence
- Uncertainties and data gaps should be formally acknowledged
- Unforced errors can be avoided with careful analysis

