Introduction to Data Validation

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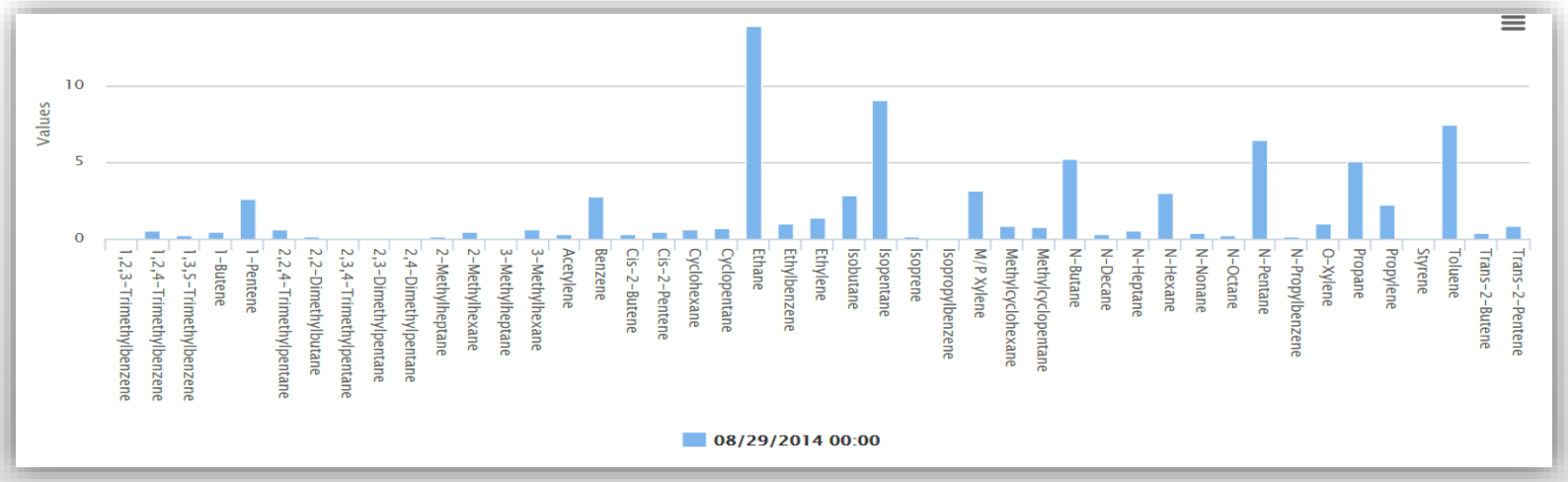
VOC and PM Speciation Data

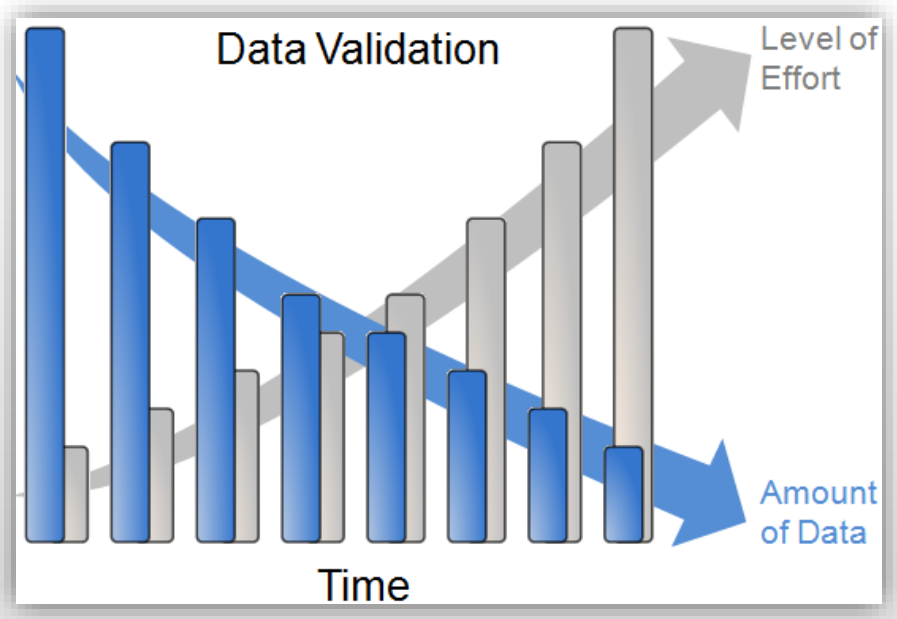
- Differences from one measurement (such as ozone or PM mass)
  - More complex instruments (more to go wrong?)
  - Many species per sample
  - Data overload
- Opportunity for intercomparison



Why You Should Validate Your Data (1)

- It is the monitoring agency's responsibility to prevent, identify, correct, and define the consequences of monitoring difficulties that might affect the precision and accuracy, and/or the validity, of the measurements.
- Serious errors in data analysis and modeling (and subsequent policy development) can be caused by erroneous data values.
- Accurate information helps you respond to community concerns.

Validate data as soon after collection as practical – it reduces effort and minimizes data loss



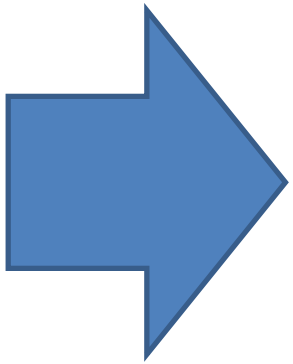
Why You Should Validate Your Data (2)

- Criteria pollutant data quality issues are important to national air quality management actions, including
  - Attainment/nonattainment designations
  - Clean data determinations
  - Petitions to EPA for reconsideration
- Air quality data are very closely reviewed by stakeholders
  - Do data collection efforts meet all CFR requirements?
  - Have procedures outlined in the QA handbook or project-specific QA plans been followed?
  - Are agency logbooks complete and up-to-date?
- Deviations are subject to potential litigation

From Weinstock L. (2014) Ambient Monitoring Update. Presented at the *National Ambient Air Monitoring Conference, Atlanta, GA, August 11-14*, by the U.S. Environmental Protection Agency Office of Air Quality Planning and Standards. Available at https://www3.epa.gov/ttnamti1/files/2014conference/tueweinstock.pdf.

Data Validation Process Changes

- More data being collected
- New instruments
- Better computing
- Better tools (e.g., visualization)
- Improved data handling and access allow for more frequent review



Provides ability to assemble data and metadata all in one place and allows a more efficient validation and review process.

Data Validation Levels

- Level 0 – Routine checks
  - Field and laboratory operations, data processing, reporting conducted in accordance with SOPs
  - Proper data file identification; review of unusual events, field data sheets, and result reports; instrument performance checks
- Level I – Internal consistency tests
  - Identify values that appear atypical when compared to values of the entire dataset
- Level II/III – External consistency tests
  - Identify values in the data that appear atypical when compared to other datasets
  - Continued evaluation of the data as part of the data interpretation process

From U.S. Environmental Protection Agency (1999) Particulate matter ($PM_{2.5}$) speciation guidance document. Available at http://www.epa.gov/ttnamti1/files/ambient/pm25/spec/specfinl.pdf

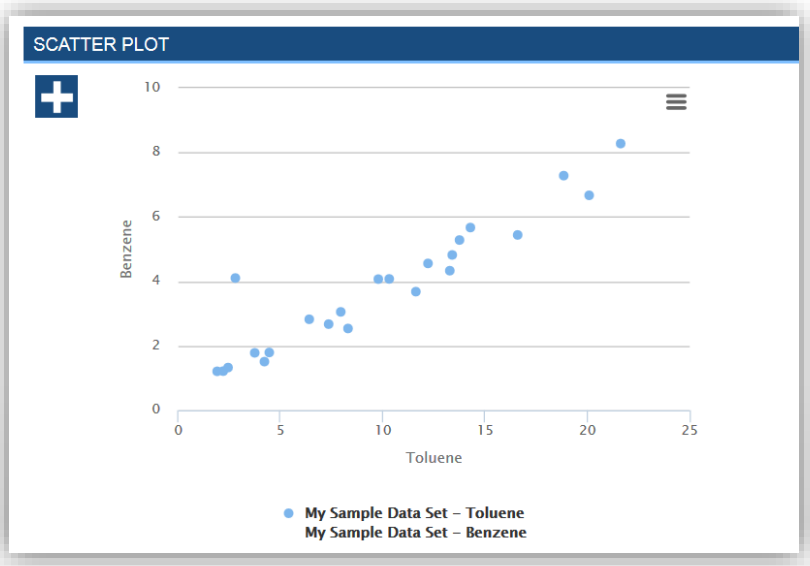
Sidebar: Outliers

- Definition: a value that lies outside most of the other values in a set of data.
- Identification: statistically, ideas include
  - >95th percentile (from exceptional event documentation)
  - 3 to 4 standard deviations above the mean
- Treatment: valid/suspect until proven invalid…

"The first assumption upon finding a measurement that is inconsistent with physical expectations is that the unusual value is due to a measurement error. If, upon tracing the path of the measurement, nothing unusual is found, the value can be assumed to be a valid result of an environmental cause."
Judy Chow, Desert Research Institute

General Approach to Data Validation

- Look at and manipulate your data—sort it, graph it, map it—so that it begins to tell a story.
- Examples
  - Scatter, time-series, and fingerprint plots
  - Summary statistics
  - Box-whisker plots
  - Wind, pollution roses



- Important issues or errors with data may become apparent only after someone begins to use the data for something

Approach/Tips

- Apply screening criteria to help focus validation efforts
- Inspect every species, even to confirm expectation that the species would normally be below the method detection limit
- Apply flags to data
- Document changes

Proceed from the big picture to the details

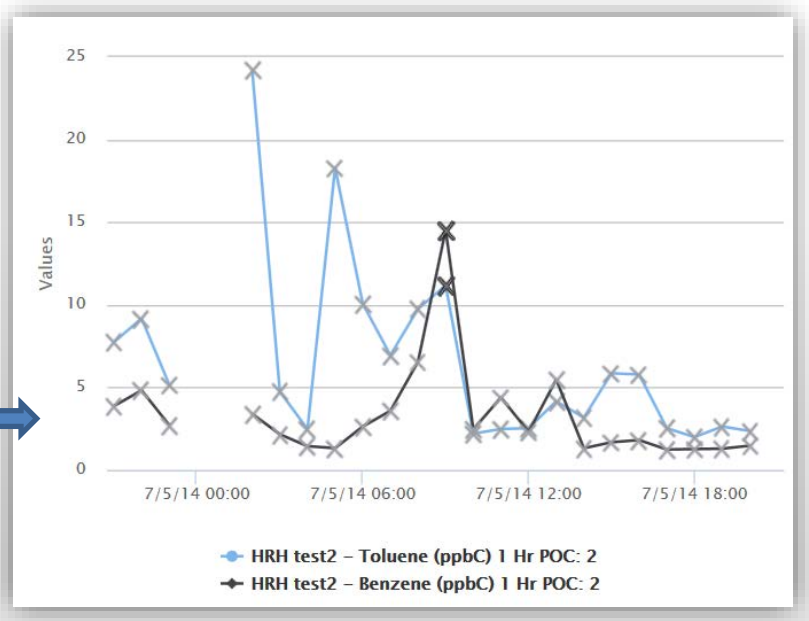
Considerations in Evaluating Your Data

- Levels of other pollutants
- Time of day/year
- Observations at other sites
- Audits and inter-laboratory comparisons
- Instrument performance history
- Calibration drift
- Site characteristics
- Meteorology
- Exceptional events

Screening Criteria

- Range
- Sticking
- Buddy site
- Temporal consistency
- Rate of change or spike
- Abundant species
- Chemical consistency
- Co-pollutants

Automated checks are helpful to focus efforts on the data that need the most attention.

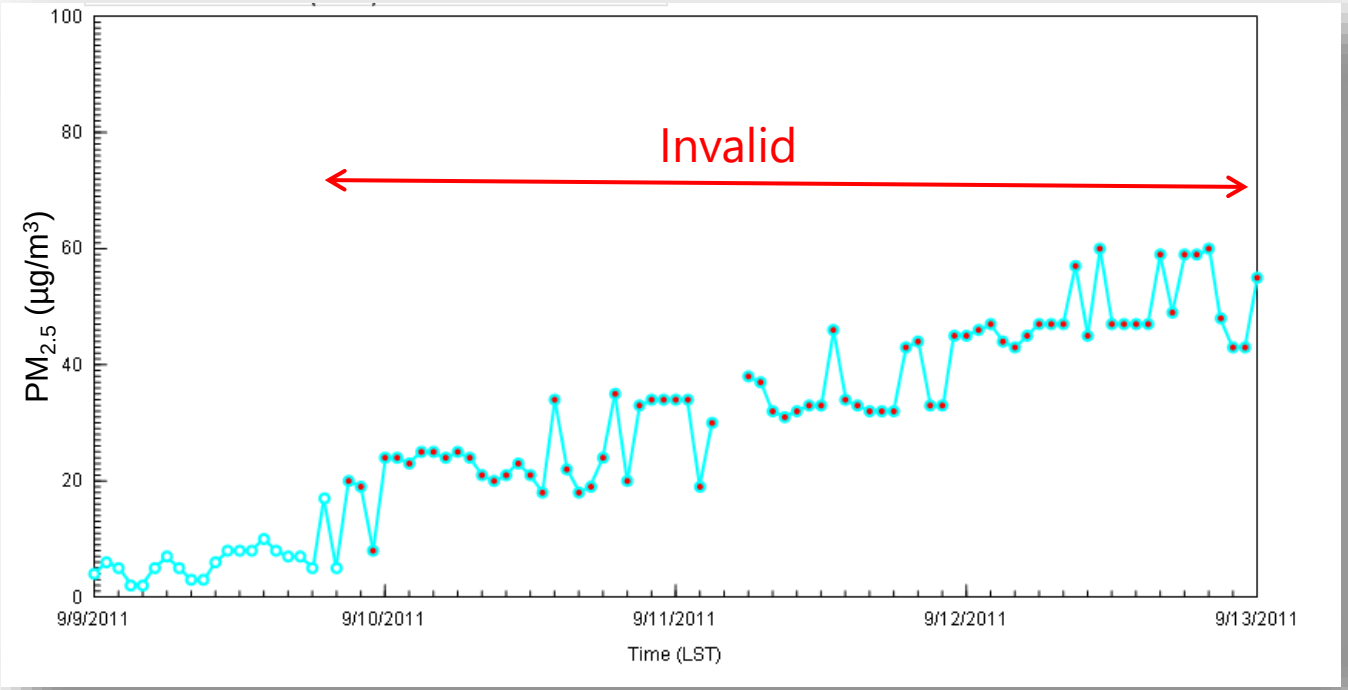


PAMS Auto-Validation: Screening

Check[a]	Fails If …	DART Smarts Action If Check Fails
Abundant Species	Any of Benzene, Propane, N-Butane, Isoprene, N-Hexane, Ethylbenzene are missing or 0	If two or more species missing or =0, flag sample with code "AQ"
TNMOC	-TNMOC is missing or 0; or -Unidentified exceeds 50% of TNMOC; or -Sum of PAMS exceeds TNMOC	-Flag TNMOC and unidentified with code "AN" -Flag Unidentified with code "DA" -Flag TNMOC and Sum of PAMS with code "DA"
Variability	Species concentration exceeds the mean + 4x standard deviation	None
Sticking	Species has same non-zero value for 3 or more consecutive samples	Flag species with code "DA"
Benzene : Toluene	Benzene exceeds 0.2 and exceeds Toluene	Flag Benzene and Toluene with code "DA"
Ethylene : Ethane	Ethylene exceeds 0.5 and exceeds Ethane	Flag Ethylene and Ethane with code "DA"
Propylene : Propane	Propylene exceeds 0.5 and exceeds Propane	Flag Propylene and Propane with code "DA"

[A] *All checks done in ppbC. AQ = collection error; AN = machine malfunction; DA = aberrant data; TNMOC* = total nonmethane organic compounds

Data Review: Human Eyes Needed!

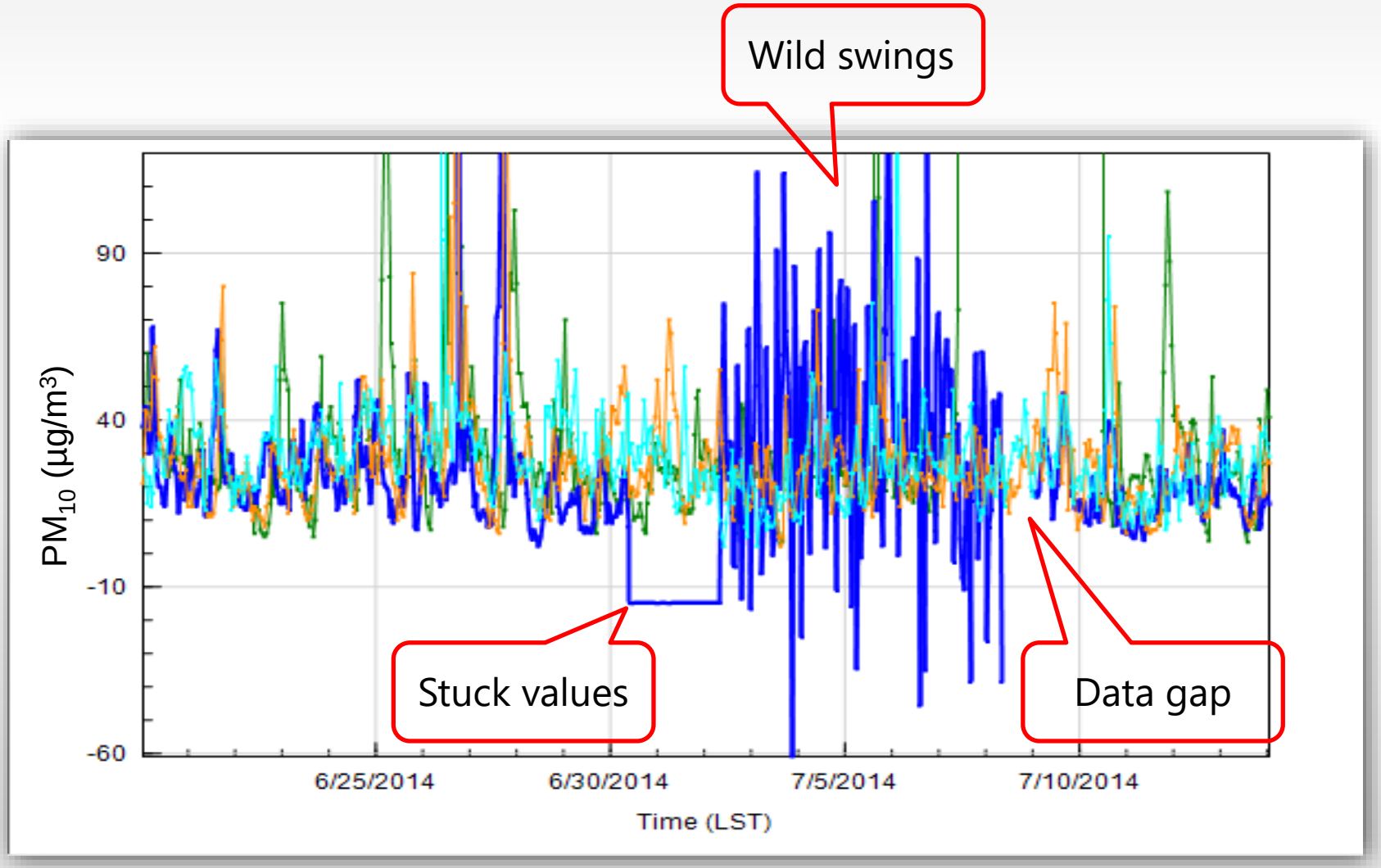


$PM_{2.5}$ concentrations (µg/m^3) gradually increased over a period of days, but there were no known local major PM sources or regional build-up expected to affect the site. PM concentrations were not high enough to trigger auto-QC checks. The agency responsible for the monitor noted "a communication error between [the monitor] and the data logger."

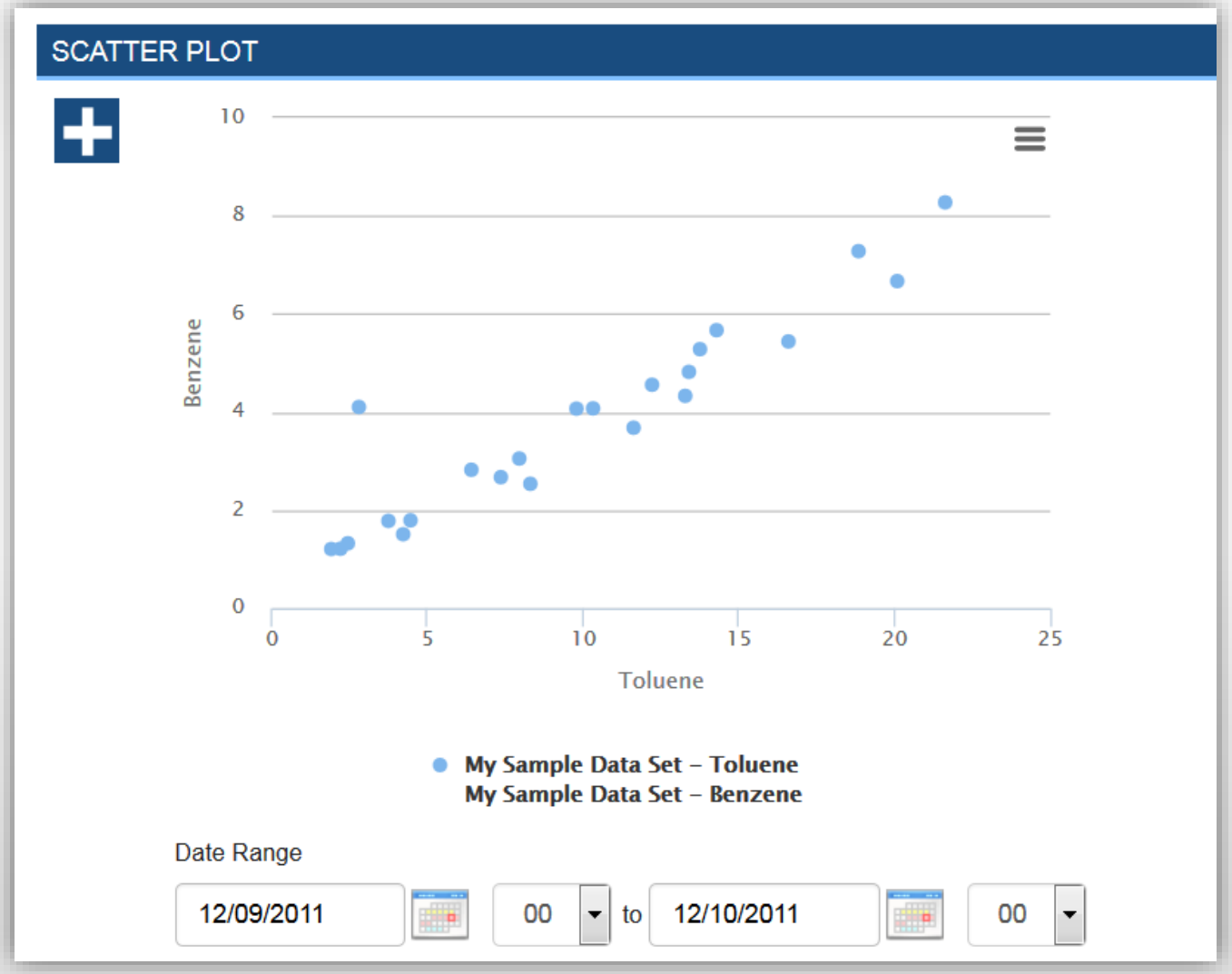
Visual Data Review: Time Series

- Look for
  - Jumps, dips
  - Periodicity of peaks
  - Calibration gas, carryover
  - Expected diurnal pattern
  - Expected relationships
  - High concentrations of less abundant species or low concentrations of more abundant species

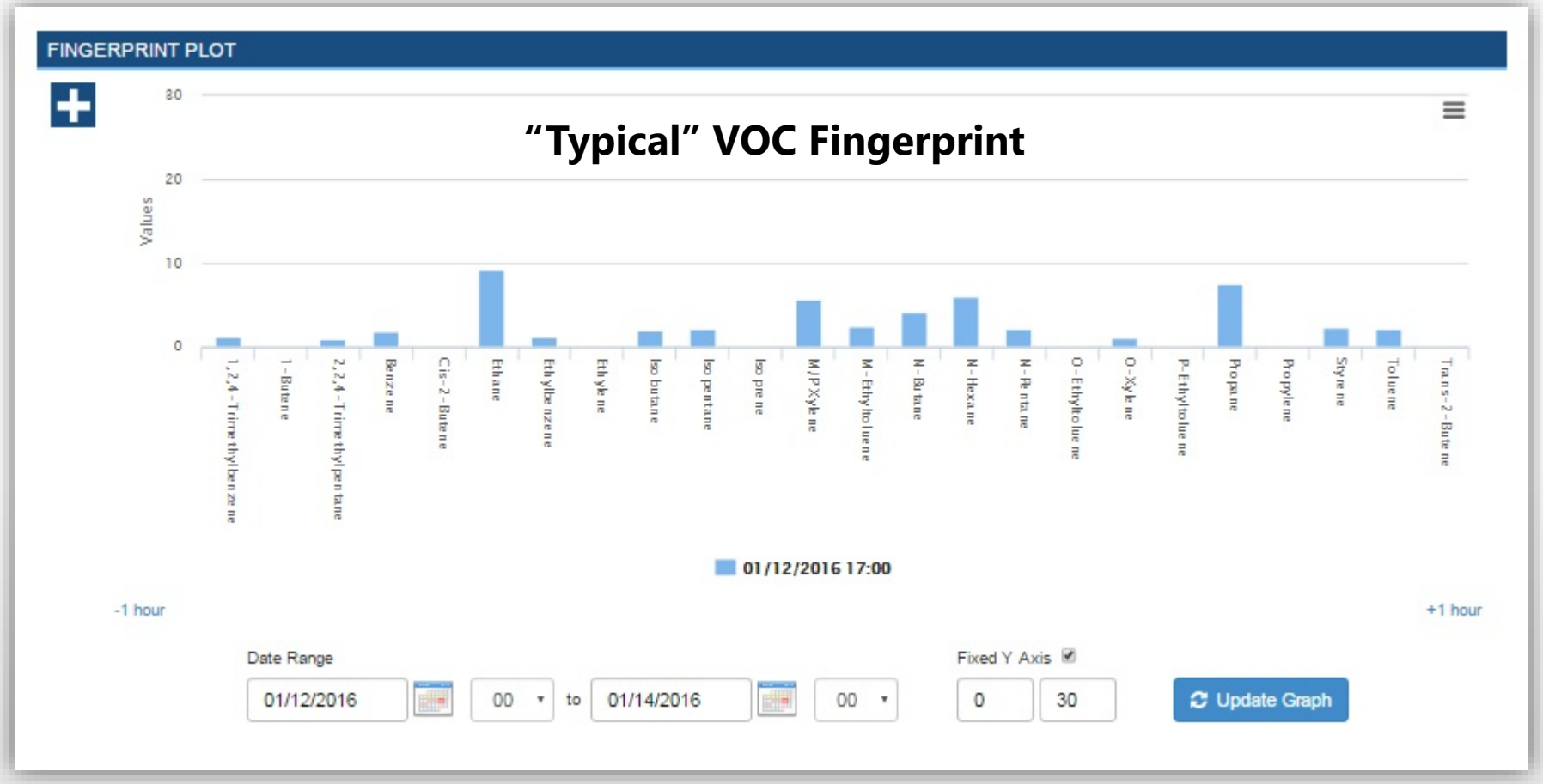
Visual Data Review: Time Series



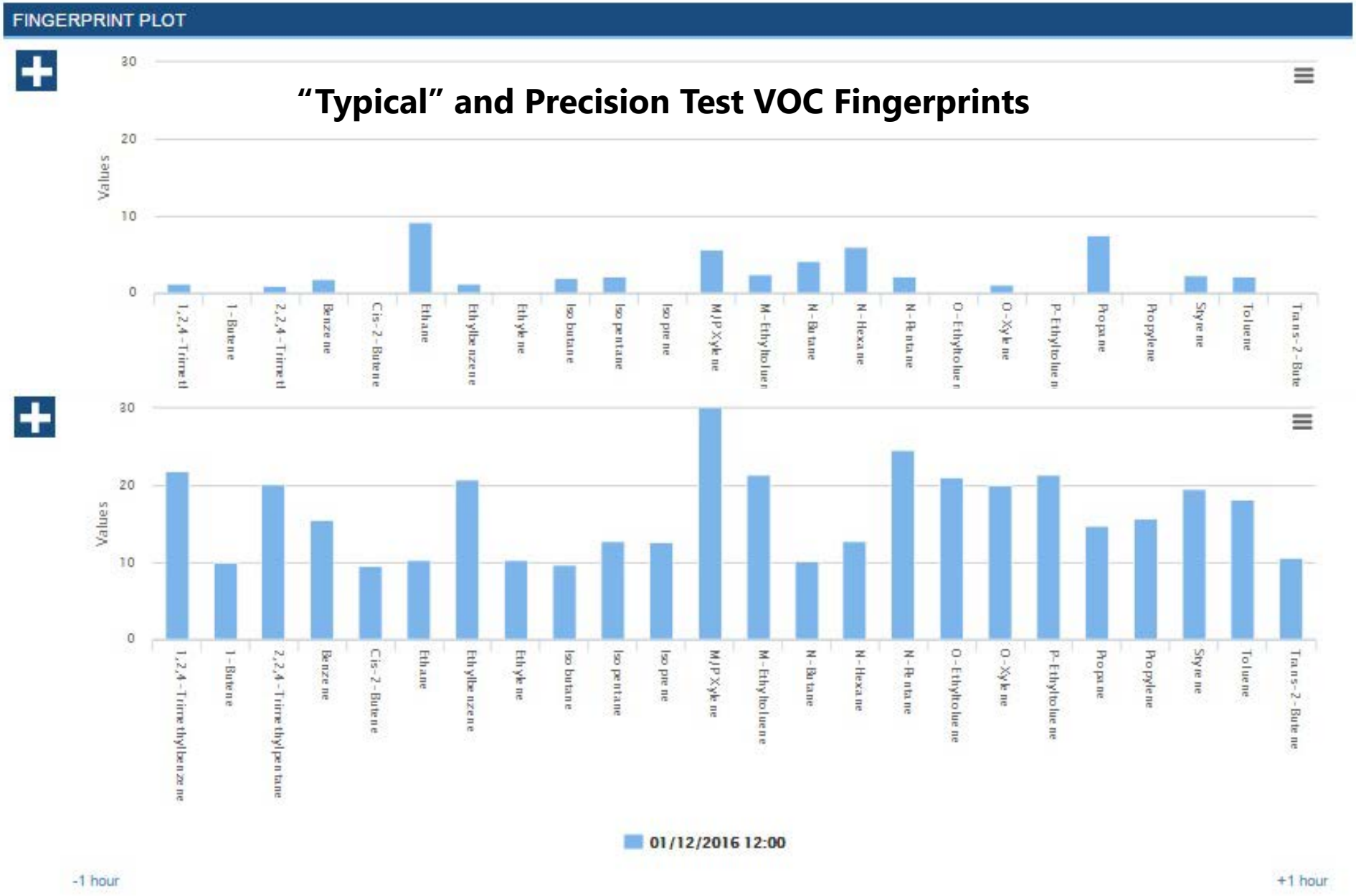
Visual Data Review: Scatter Plots



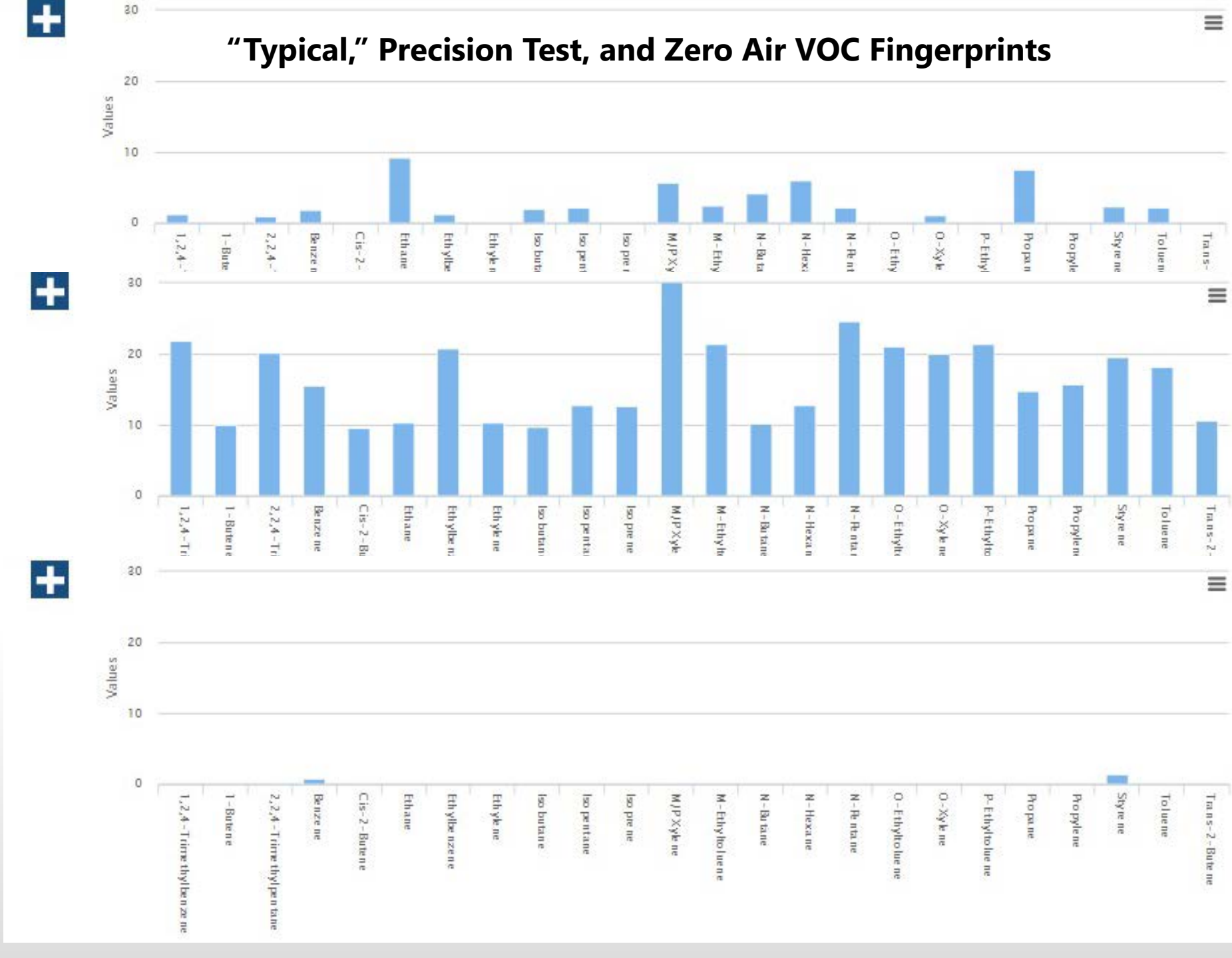
Visual Data Review: Fingerprint Plots



“Typical” and Precision Test VOC Fingerprints

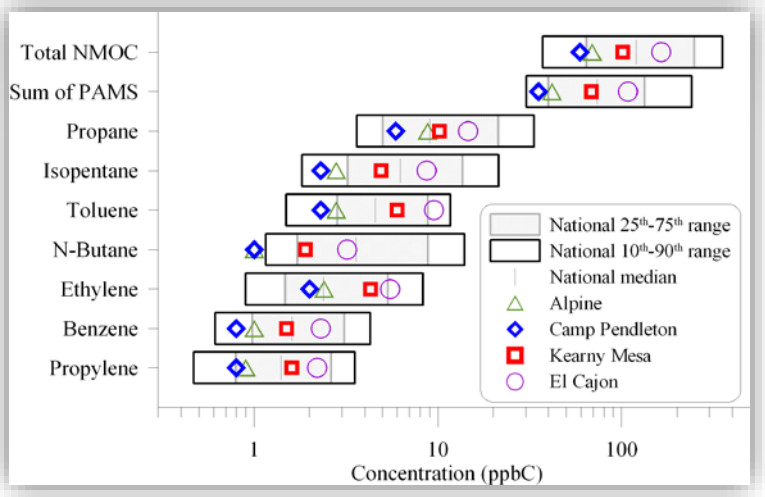


“Typical,” Precision Test, and Zero Air VOC Fingerprints

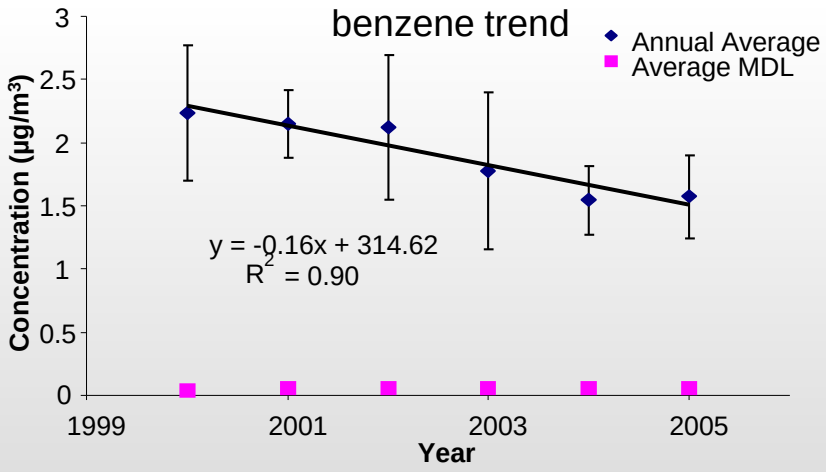


Putting Your Data in Perspective

- National averages
- Trends over time
- Comparison to nearby sites, similar areas
- Detection limits



A statistically significant decreasing benzene trend



Using the Validated Data

- Health effects research
- Model validation
- Emissions inventory evaluation
- Trends analysis
- Control strategy development and effectiveness
- Supporting other programs (e.g., air toxics)
- Comparisons to other similar cities/areas

What's Coming Up Next?

- This session
  - UC Davis Data Validation Procedures
  - DART for CSN and PAMS Data Validation

- Wednesday
  - PAMS Session

Contact

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