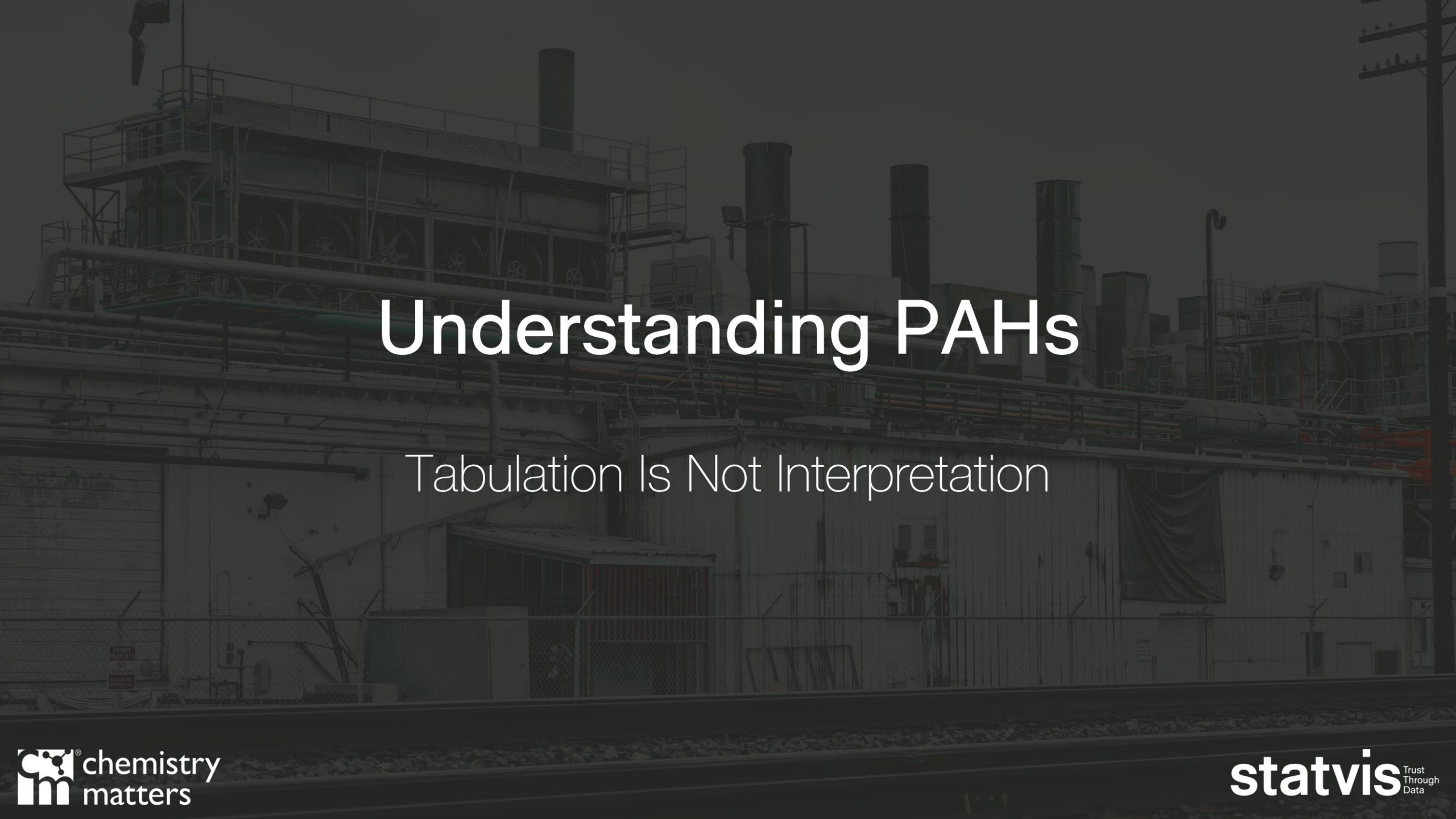


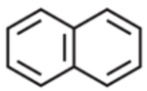
Understanding PAHs

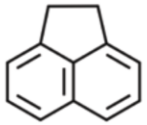
Tabulation Is Not Interpretation

chemistry matters

statvis Trust Through Data

US EPA 16 Priority Pollutants—PAH Compounds


naphthalene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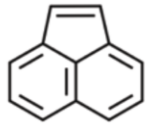
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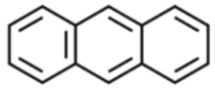
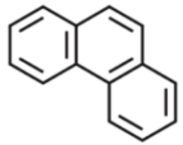

anthracene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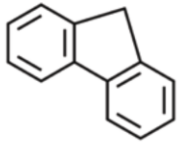
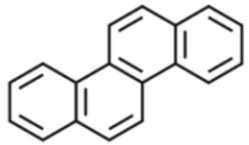

fluorene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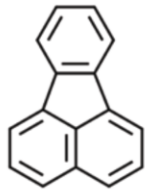
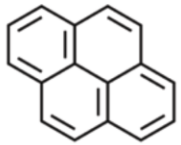
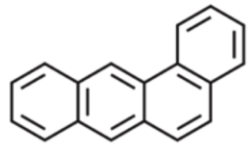
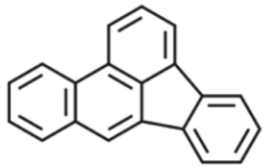
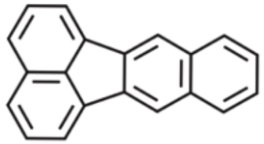
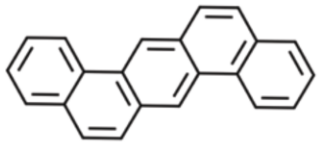

fluoranthene

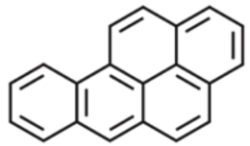

pyrene

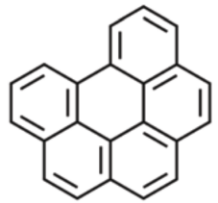

benz(a)anthracene

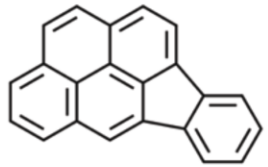

benzo(b)fluoranthene
benzo(b+j)fluoranthene


benzo[k]fluoranthene


dibenzo(a,h)anthracene


benzo(a)pyrene


benzo(ghi)perylene


Indeno(1,2,3-cd)pyrene

Tier 1—Carcinogenic Tier 1—Non-carcinogenic Tier 1—No guideline

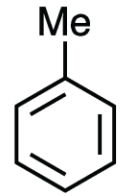
Chemical Patterns

- All contamination has a potential chemical signature
- If the chemical signature is unique to the contamination, then it can be used as a diagnostic fingerprint
- There are environmental weathering processes that can alter a fingerprint over time BUT…

  …weathering is predictable and is determined by the physical-chemical properties of the compounds
- Like chemicals – move together in the environment

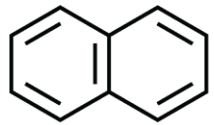
Behaviour of PAHs in the Environment

- Not very volatile
- Not soluble in water / bind to organic carbon
- Resist biodegradation
- Potential to bioaccumulate (very minimal), not biomagnify
- Known toxicity (mediated through Ah receptor)
- Percentage (<1-10%) quantities in crude oil
  - High enough concentrations to see in environment



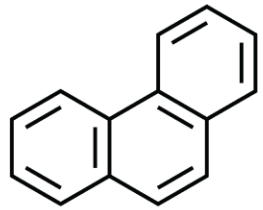
toluene

3800 Pa
470 mg/L
2.69



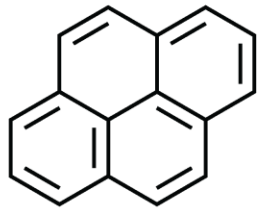
naphthalene

10.4 Pa
31 mg/L
3.37



phenanthrene

0.0161 Pa
1.1 mg/L
4.46

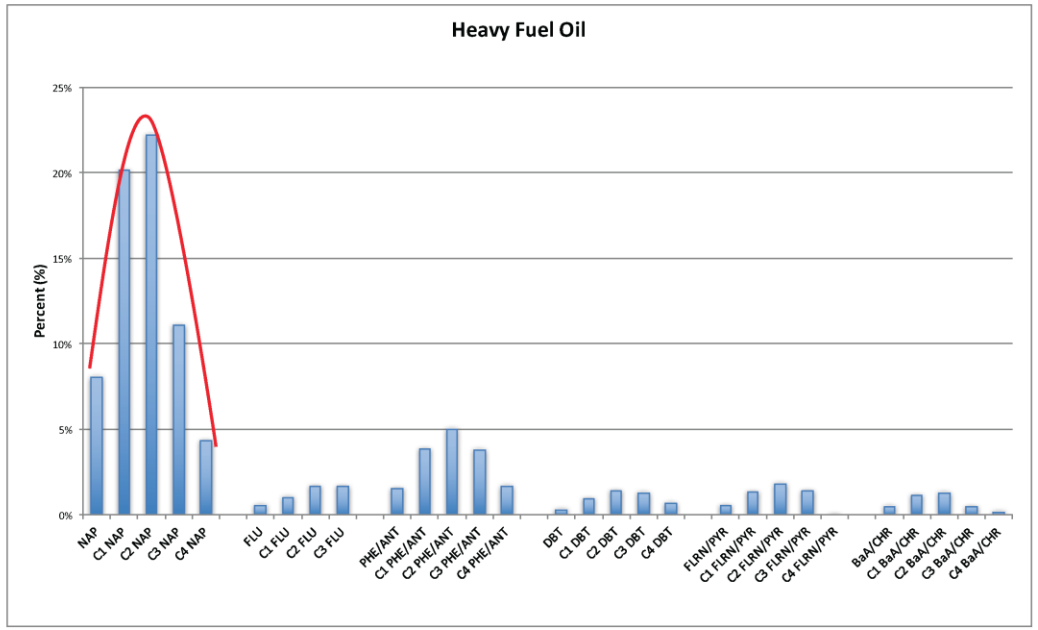


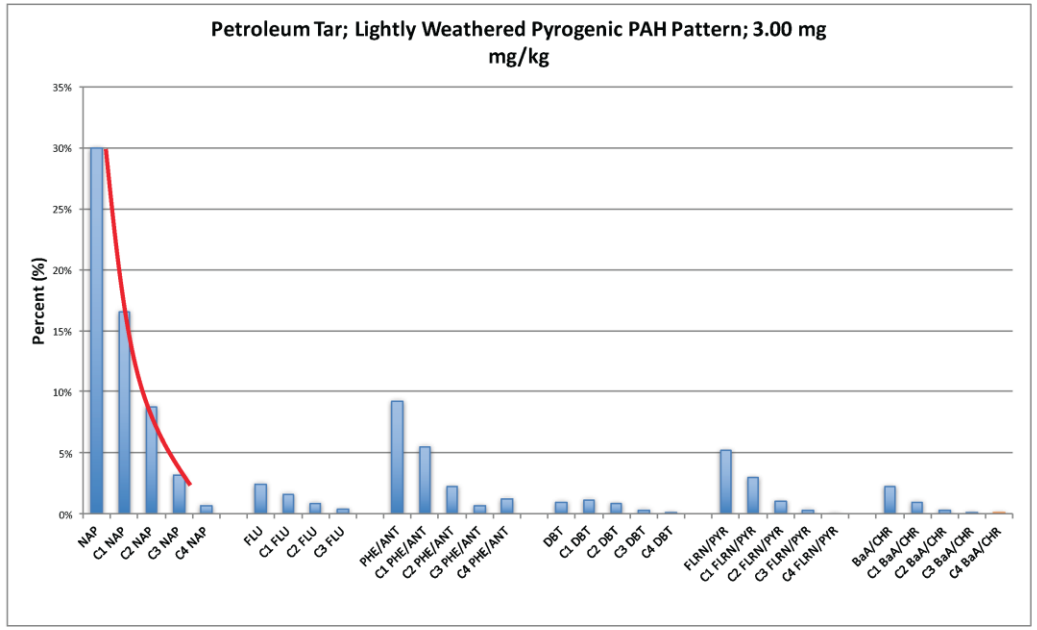
pyrene

0.0006 Pa
0.13 mg/L
8.8

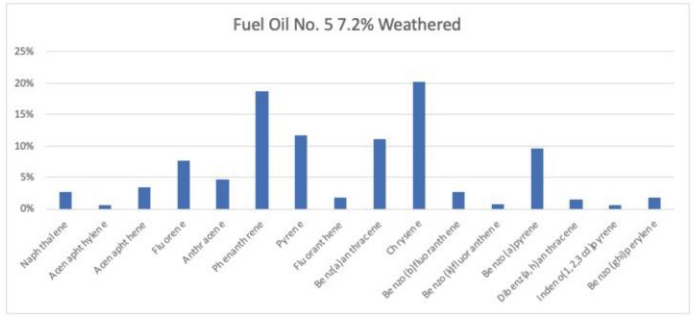
Volatility
Solubility
KOC

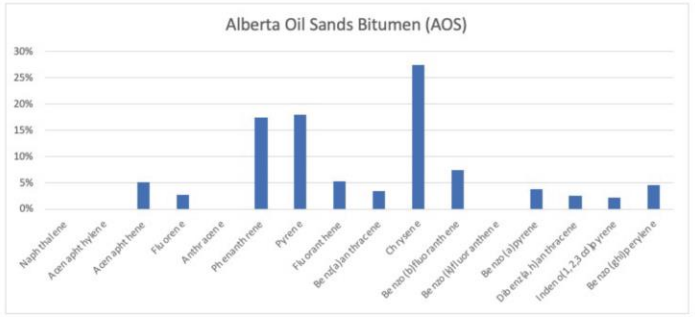
Pyrogenic vs. Petrogenic Patterns

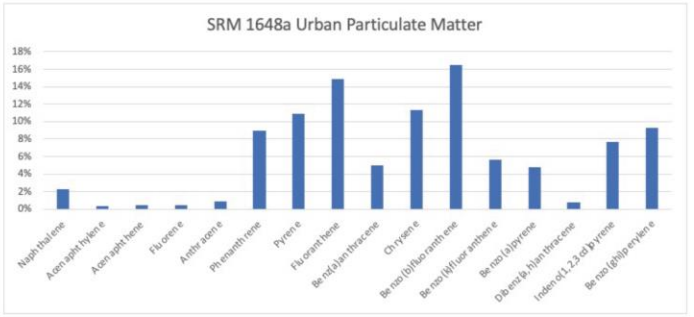


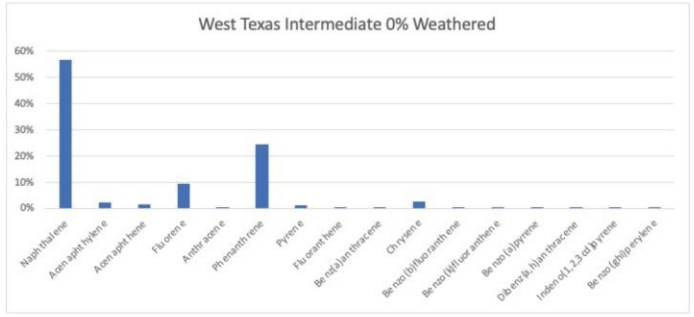


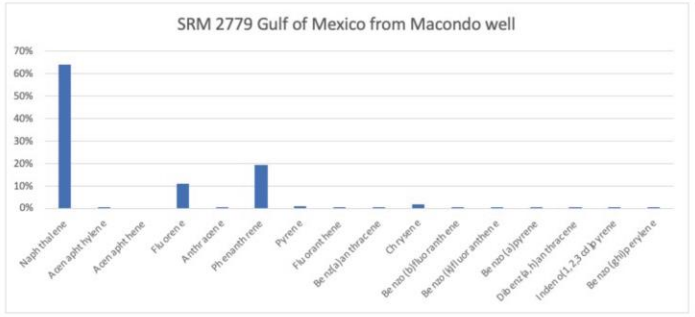
Various Product Patterns

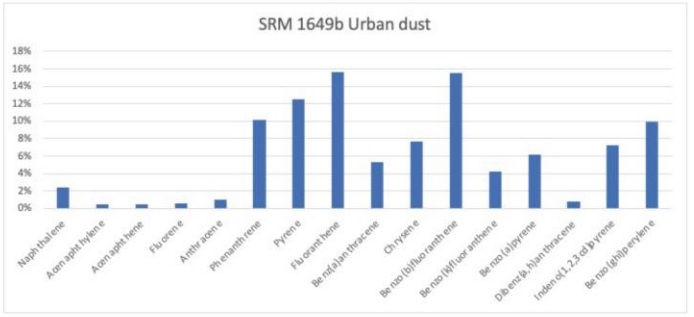


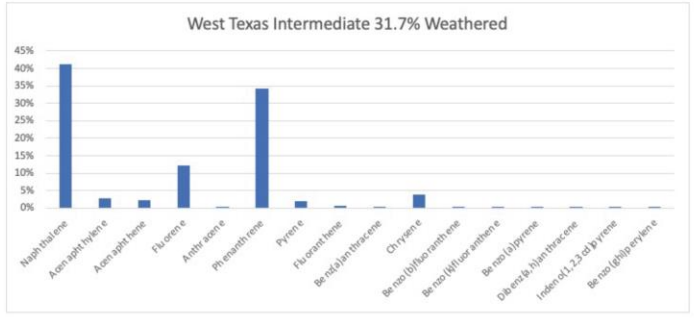


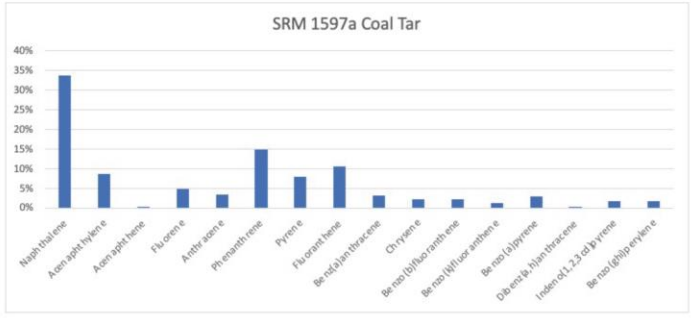






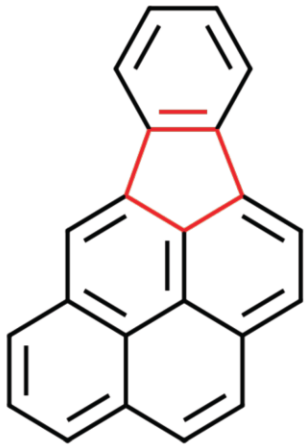






A Diagnostic Ratio

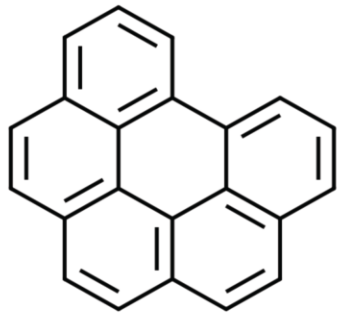
High Temperature Formation



Indeno[123,cd]pyrene

430 kJ/mol

Low Temperature Formation

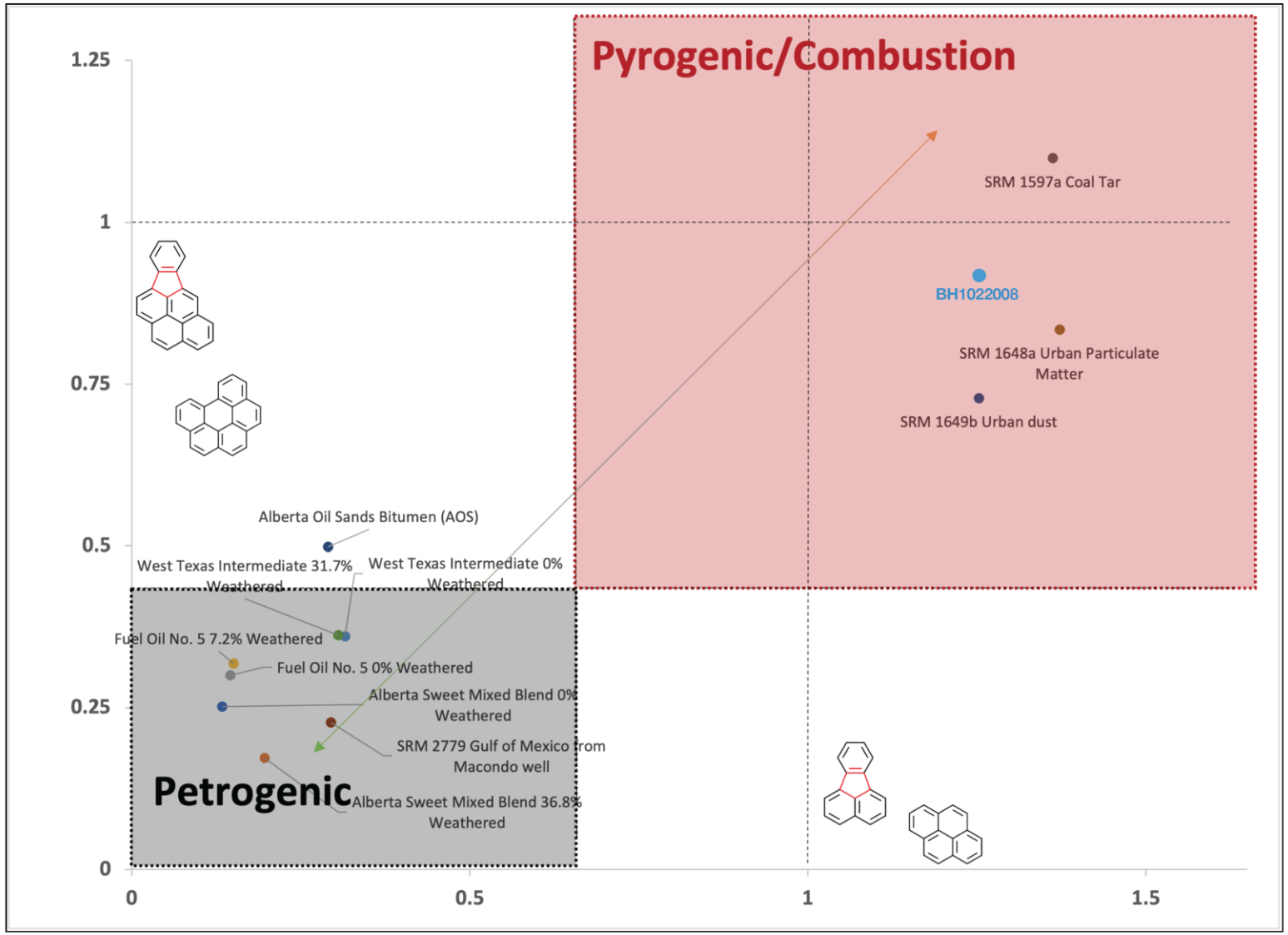


Benzo[ghi]perylene

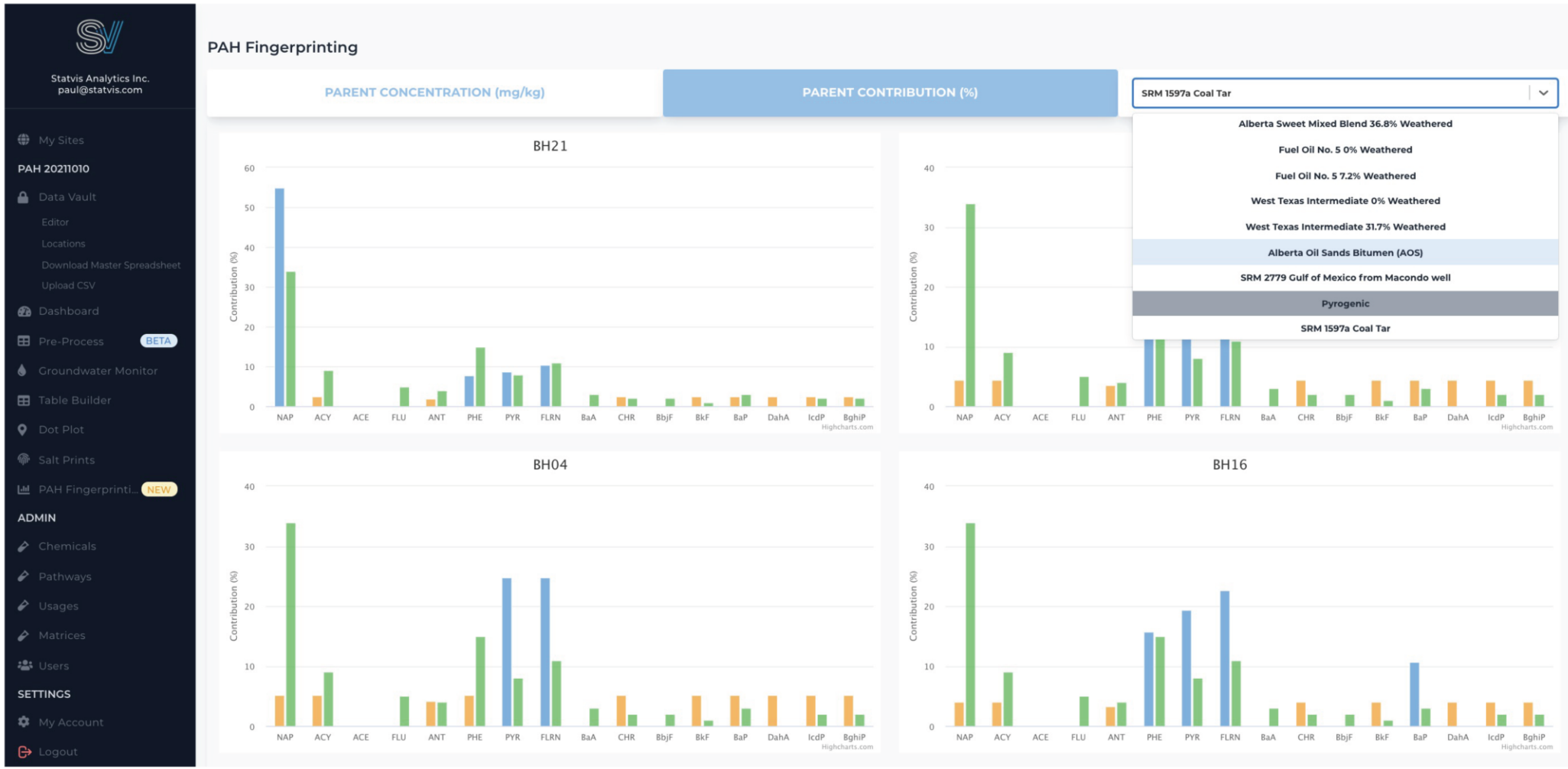
300 kJ/mol

- Uses fundamental chemistry properties (heats of formation) which drives their formation ($\Delta_f H°_m$)
- Uses similar size structures for ratio (behave the same in environment)

Diagnostic Double Ratio Plot

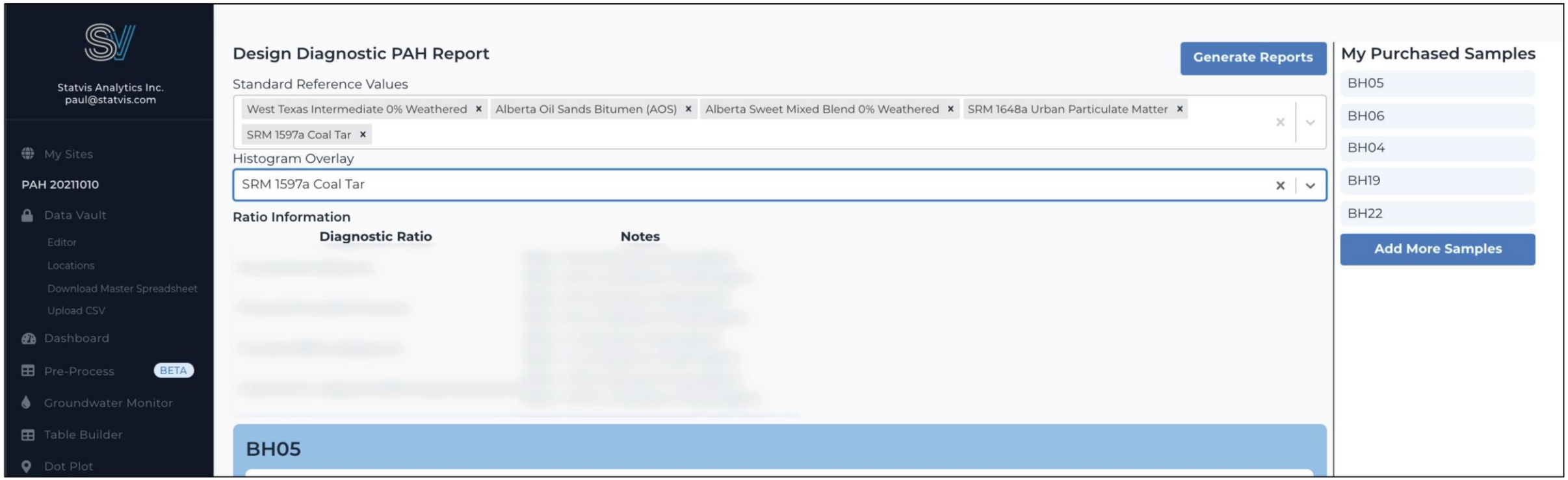


Compare Your Samples to Standards

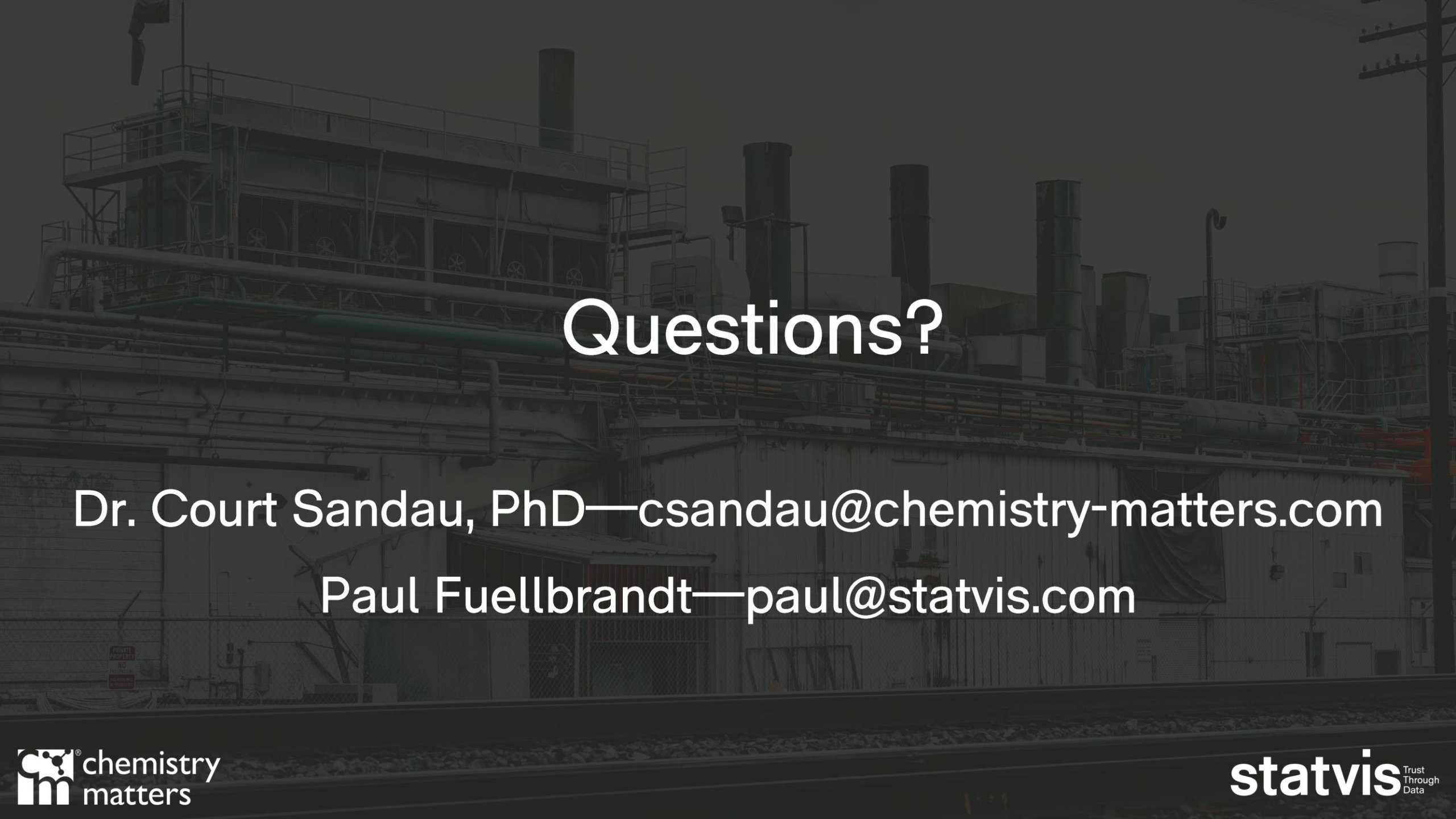


See Samples With Data for Fingerprinting

Design Diagnostic PAH Report



Output Diagnostic PAH Report



Questions?

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Paul Fuellbrandt—paul@statvis.com

chemistry matters

statvis Trust Through Data