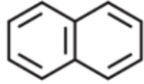


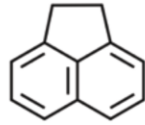
Understanding PAHs

Tabulation Is Not Interpretation

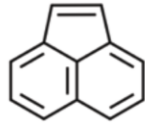
US EPA 16 Priority Pollutants—PAH Compounds



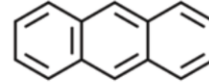
naphthalene



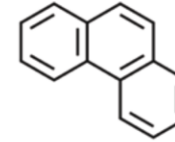
acenaphthene



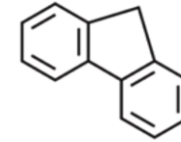
acenaphthylene



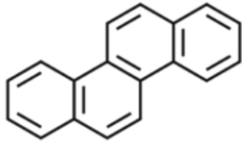
anthracene



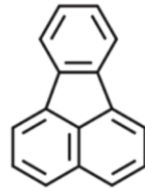
phenanthrene



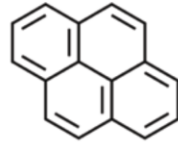
fluorene



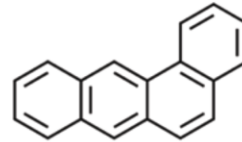
chrysene



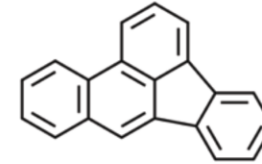
fluoranthene



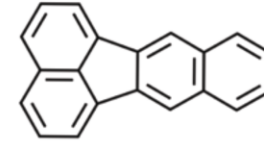
pyrene



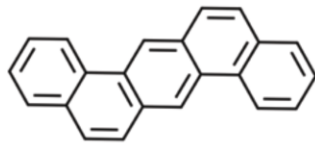
benz(a)anthracene



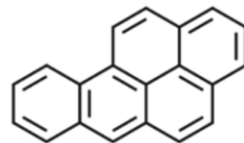
benzo(b)fluoranthene
benzo(b+j)fluoranthene



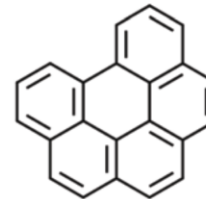
benzo(k)fluoranthene



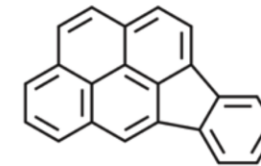
dibenzo(a,h)anthracene



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...**

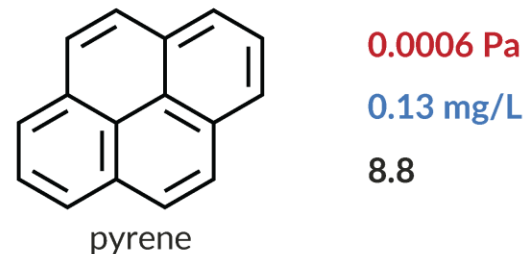
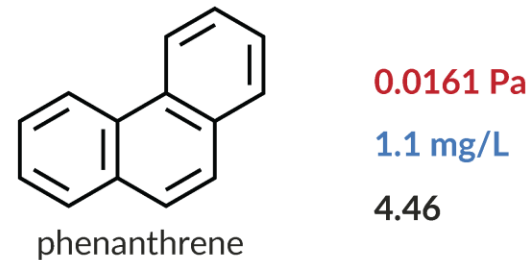
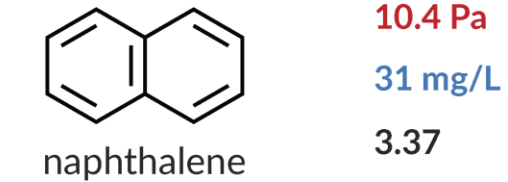
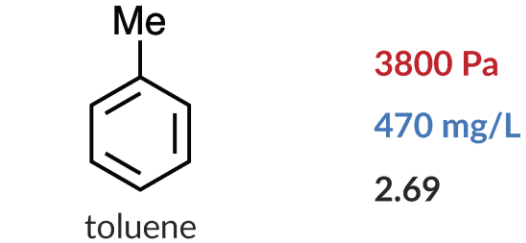
...weathering is predictable and is determined by the physical-chemical properties of the compounds
- Like chemicals – move together in the environment





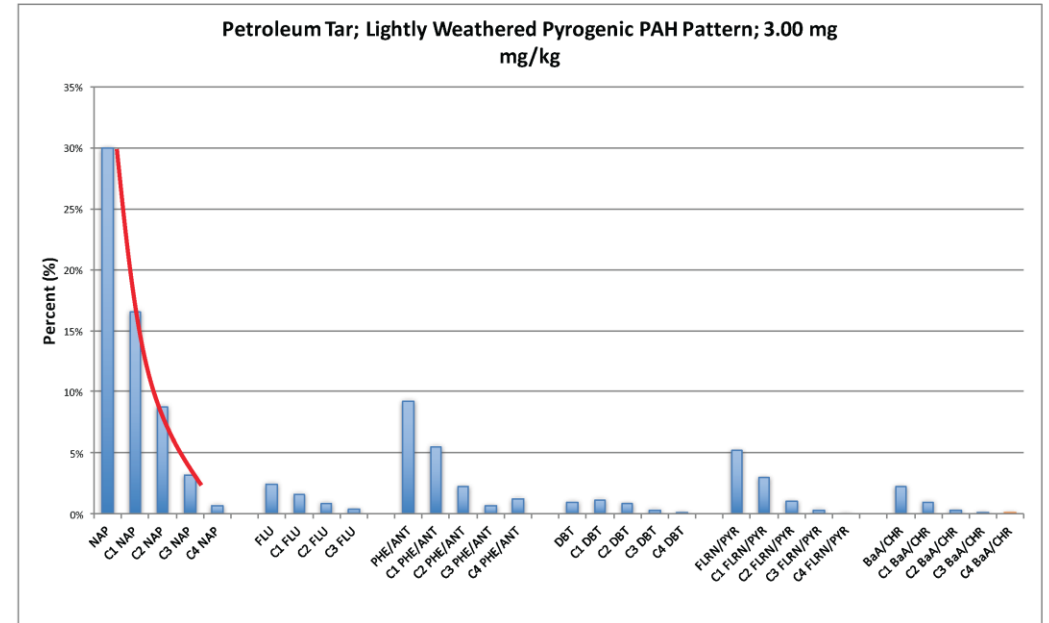
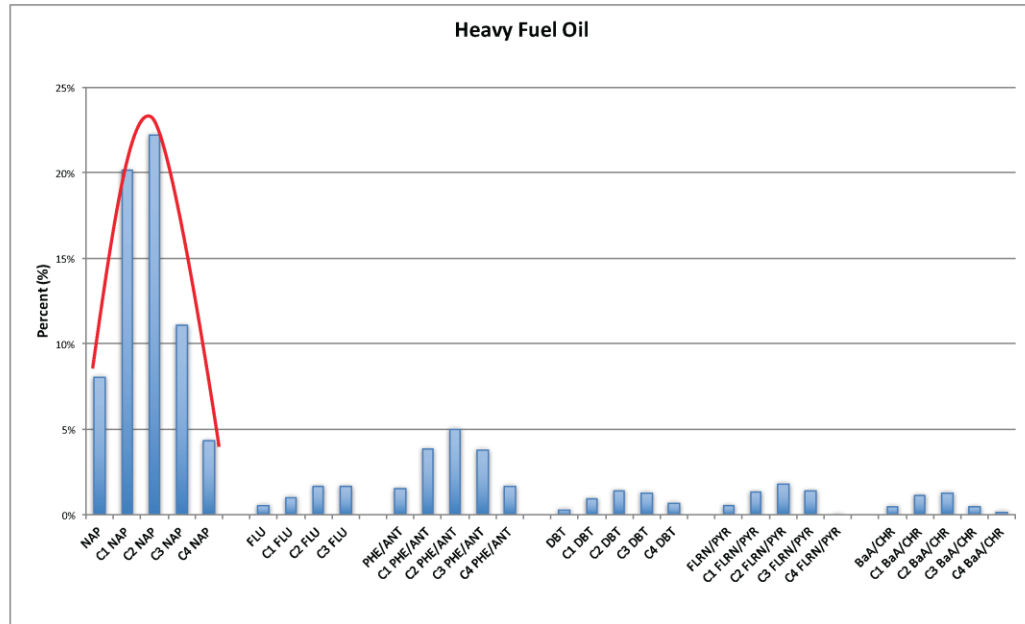
Behaviour of PAHs in the Environment

- 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



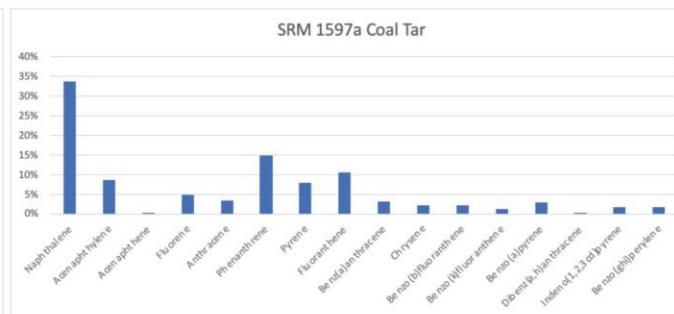
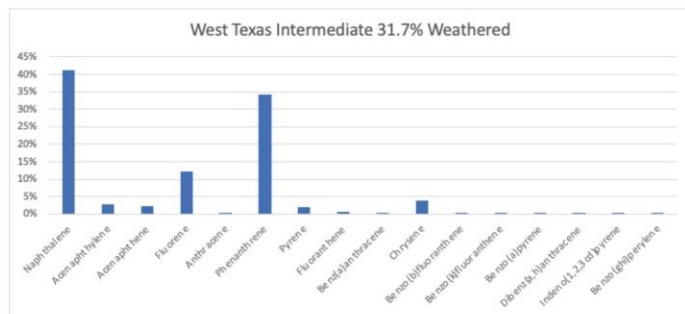
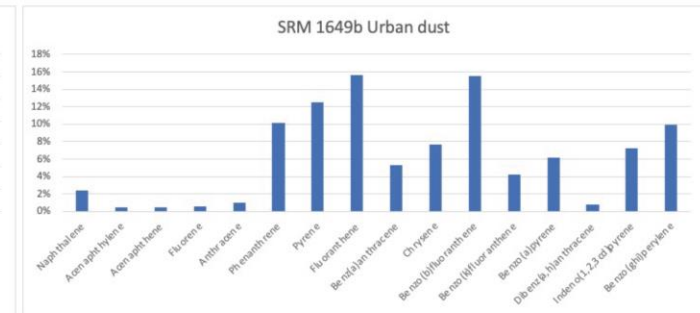
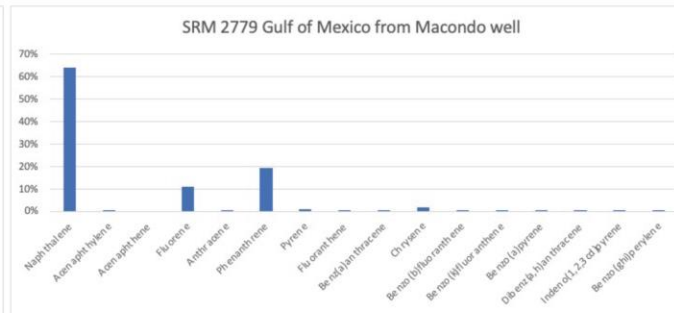
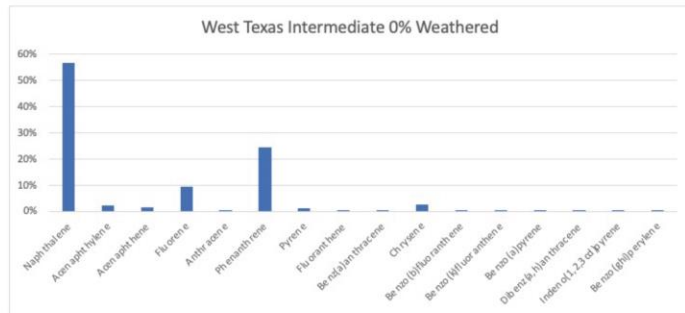
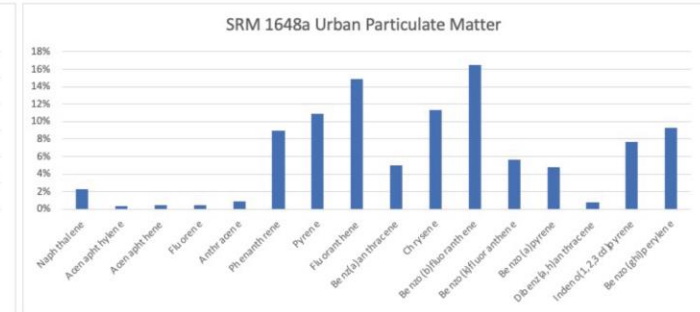
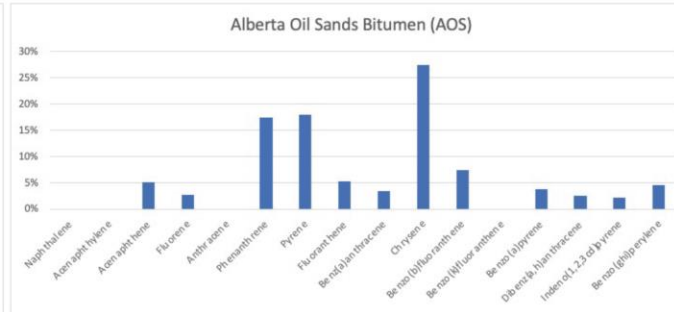
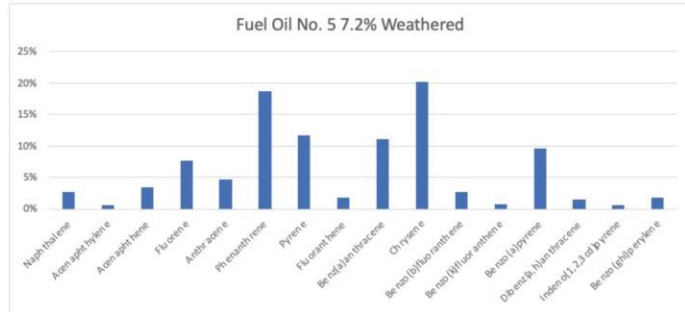
Volatility
Solubility
KOC

Pyrogenic vs. Petrogenic Patterns





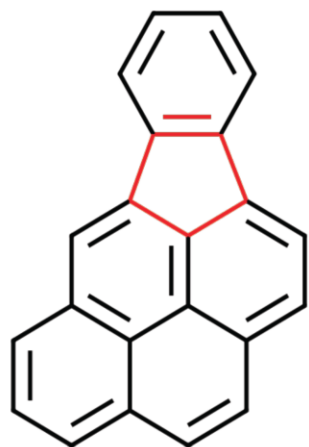
Various Product Patterns



A Diagnostic Ratio

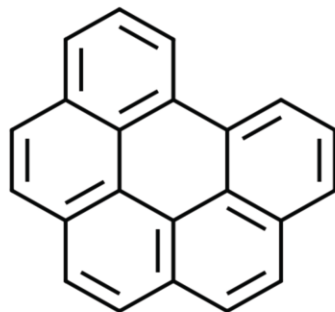
High Temperature Formation

Low Temperature Formation



Indeno[123,cd]pyrene

430 kJ/mol



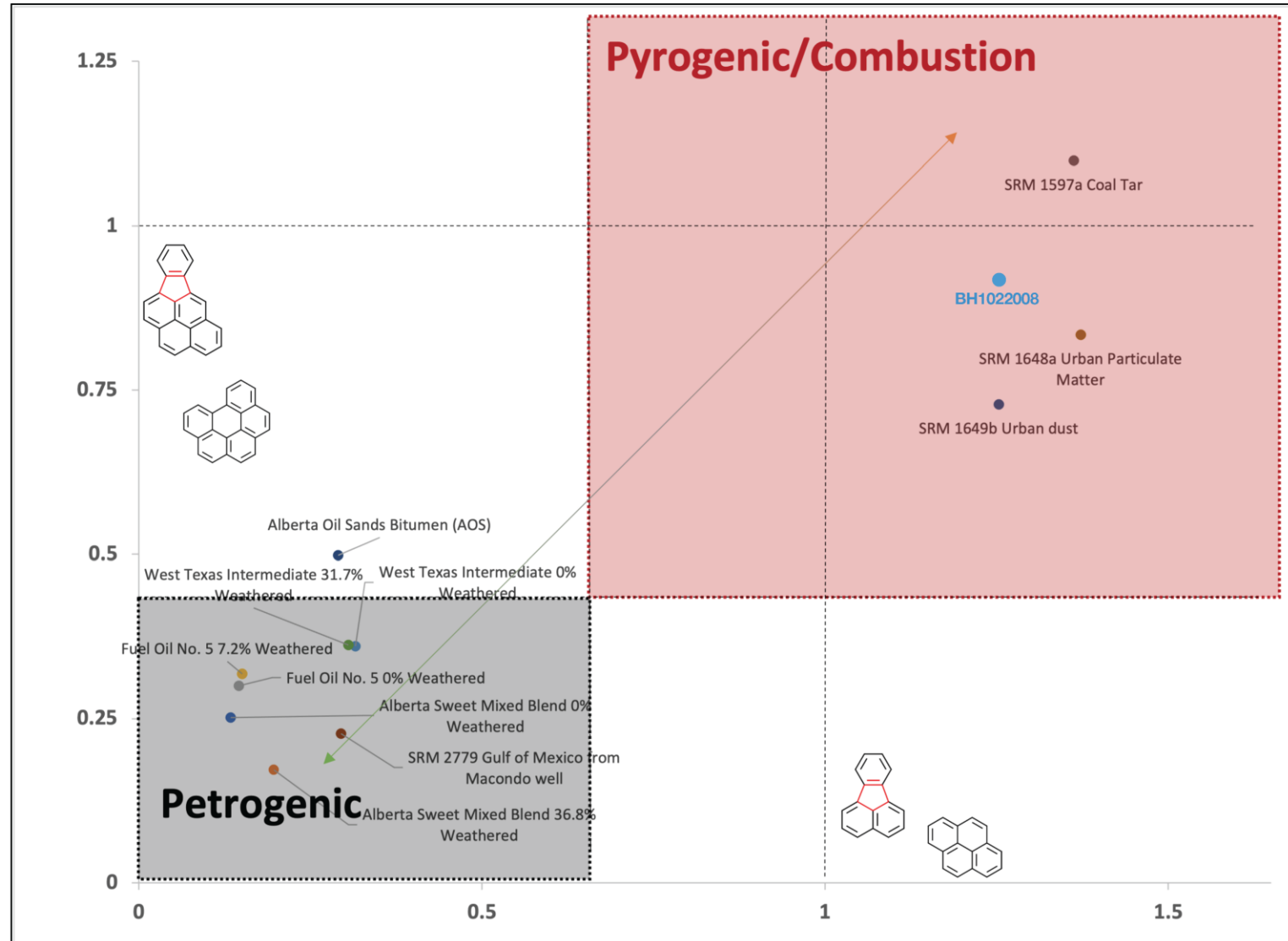
Benzo[ghi]perylene

300 kJ/mol

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



Diagnostic Double Ratio Plot





Compare Your Samples to Standards

SV
Statvis Analytics Inc.
paul@statvis.com

My Sites

PAH 20211010

- Data Vault
- Editor
- Locations
- Download Master Spreadsheet
- Upload CSV

Dashboard

Pre-Process **BETA**

Groundwater Monitor

Table Builder

Dot Plot

Salt Prints

PAH Fingerprinting **NEW**

ADMIN

- Chemicals
- Pathways
- Usages
- Matrices
- Users

SETTINGS

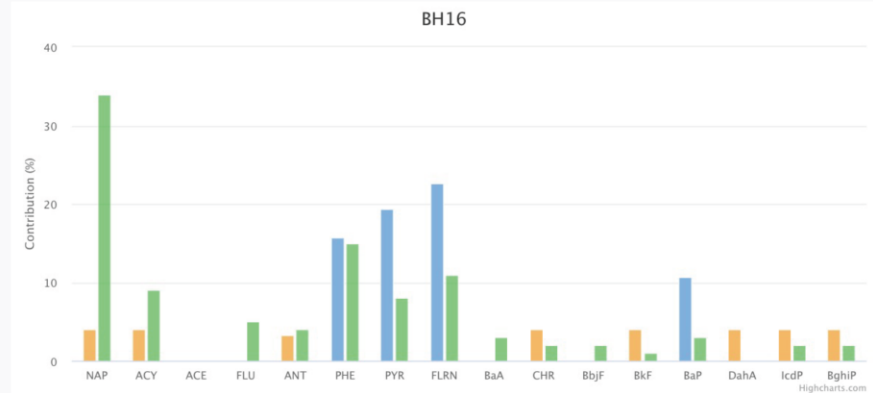
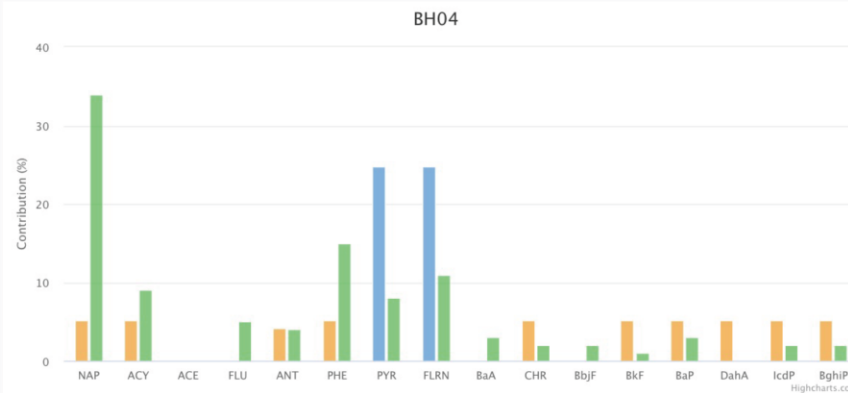
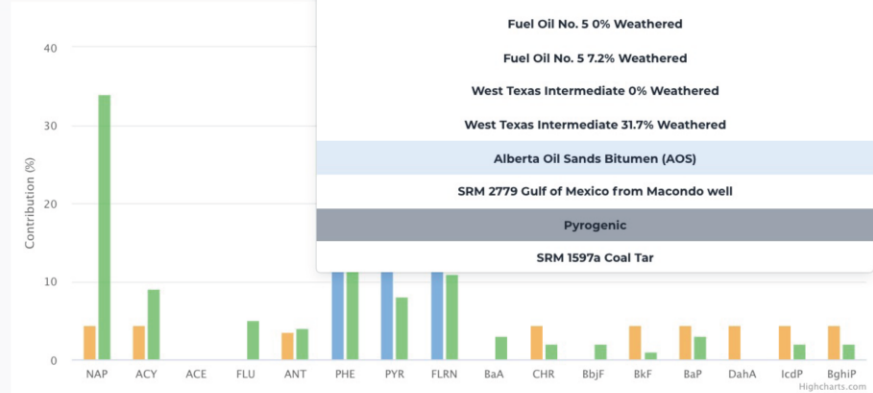
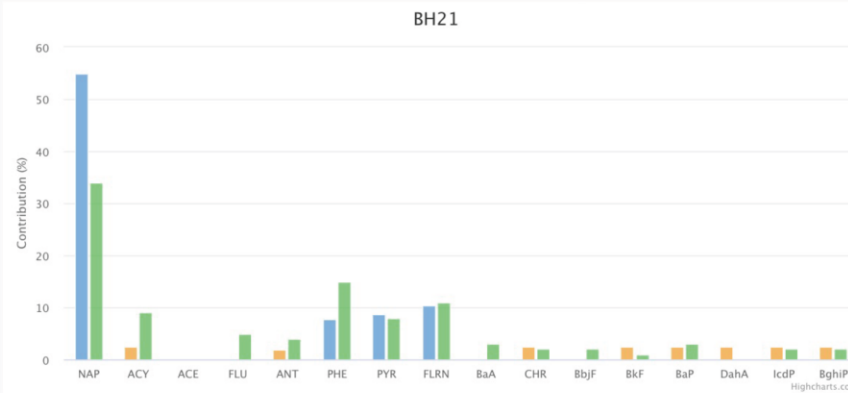
- My Account
- Logout

PAH Fingerprinting

PARENT CONCENTRATION (mg/kg)

PARENT CONTRIBUTION (%)

SRM 1597a Coal Tar






See Samples With Data for Fingerprinting





Design Diagnostic PAH Report



Statvis Analytics Inc.
paul@statvis.com

- My Sites
- PAH 20211010**
- Data Vault
 - Editor
 - Locations
 - Download Master Spreadsheet
 - Upload CSV
- Dashboard
- Pre-Process BETA
- Groundwater Monitor
- Table Builder
- Dot Plot

Design Diagnostic PAH Report

[Generate Reports](#)

Standard Reference Values

West Texas Intermediate 0% Weathered x Alberta Oil Sands Bitumen (AOS) x Alberta Sweet Mixed Blend 0% Weathered x SRM 1648a Urban Particulate Matter x

SRM 1597a Coal Tar x

Histogram Overlay

SRM 1597a Coal Tar x

Ratio Information

Diagnostic Ratio	Notes

BH05

My Purchased Samples

- BH05
- BH06
- BH04
- BH19
- BH22

[Add More Samples](#)





Output Diagnostic PAH Report



Questions?

Dr. Court Sandau, PhD—csandau@chemistry-matters.com

Paul Fuellbrandt—paul@statvis.com