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Making chemistry data meaningful



PAHs – Families and Fingerprints

Phil Richards and Court Sandau



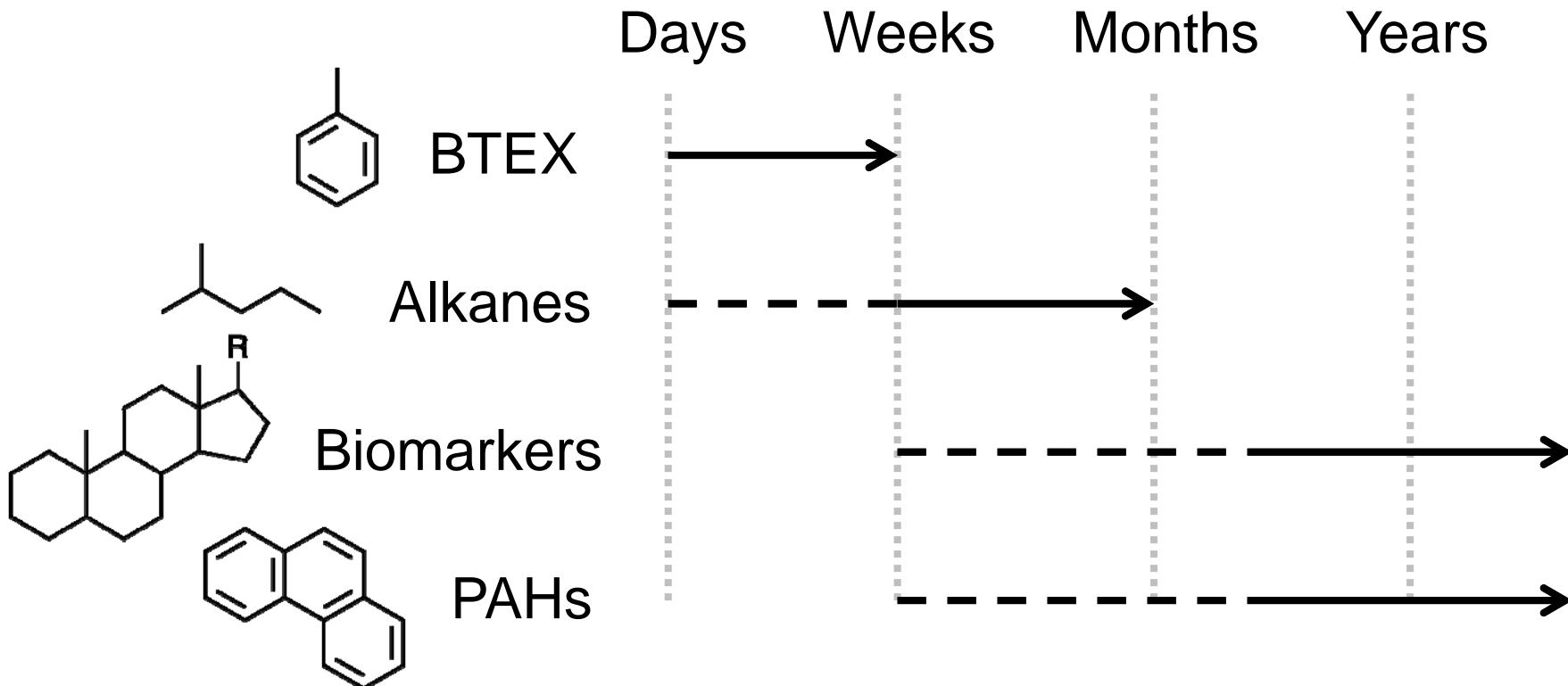
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Overview

- PAHs are a focus of delineation and remediation.
- PAHs are everywhere, take care with the data!
- Natural exceedances are likely in many types of area.
- Advanced analysis techniques are very useful.
 - Fingerprints
 - Diagnostic ratios
 - Statistical analysis

Recognizing that PAHs move together as a family means they can be fingerprinted!

Surficial Impact Residues

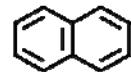


PAH Analysis

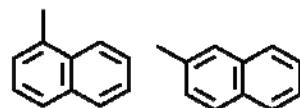
Parent PAHs
20 typical

Extended PAHs
50+

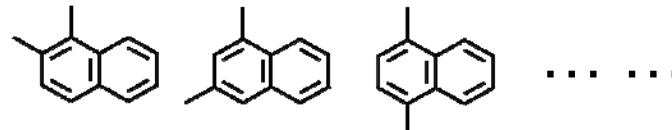
Naphthalene



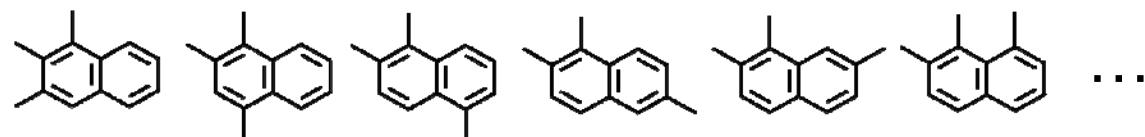
C1-Naphthalenes



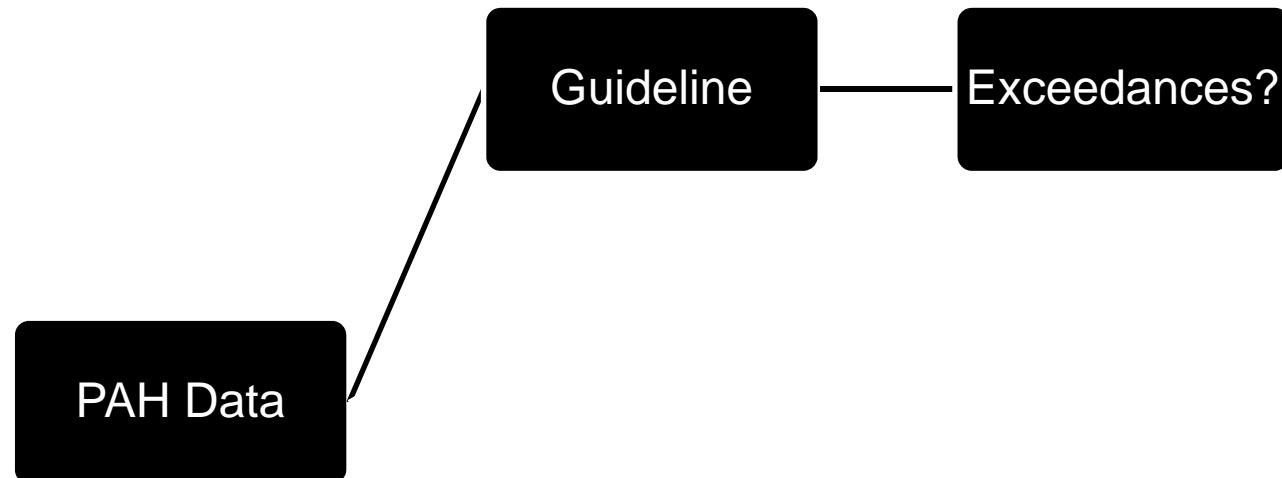
C2-Naphthalenes



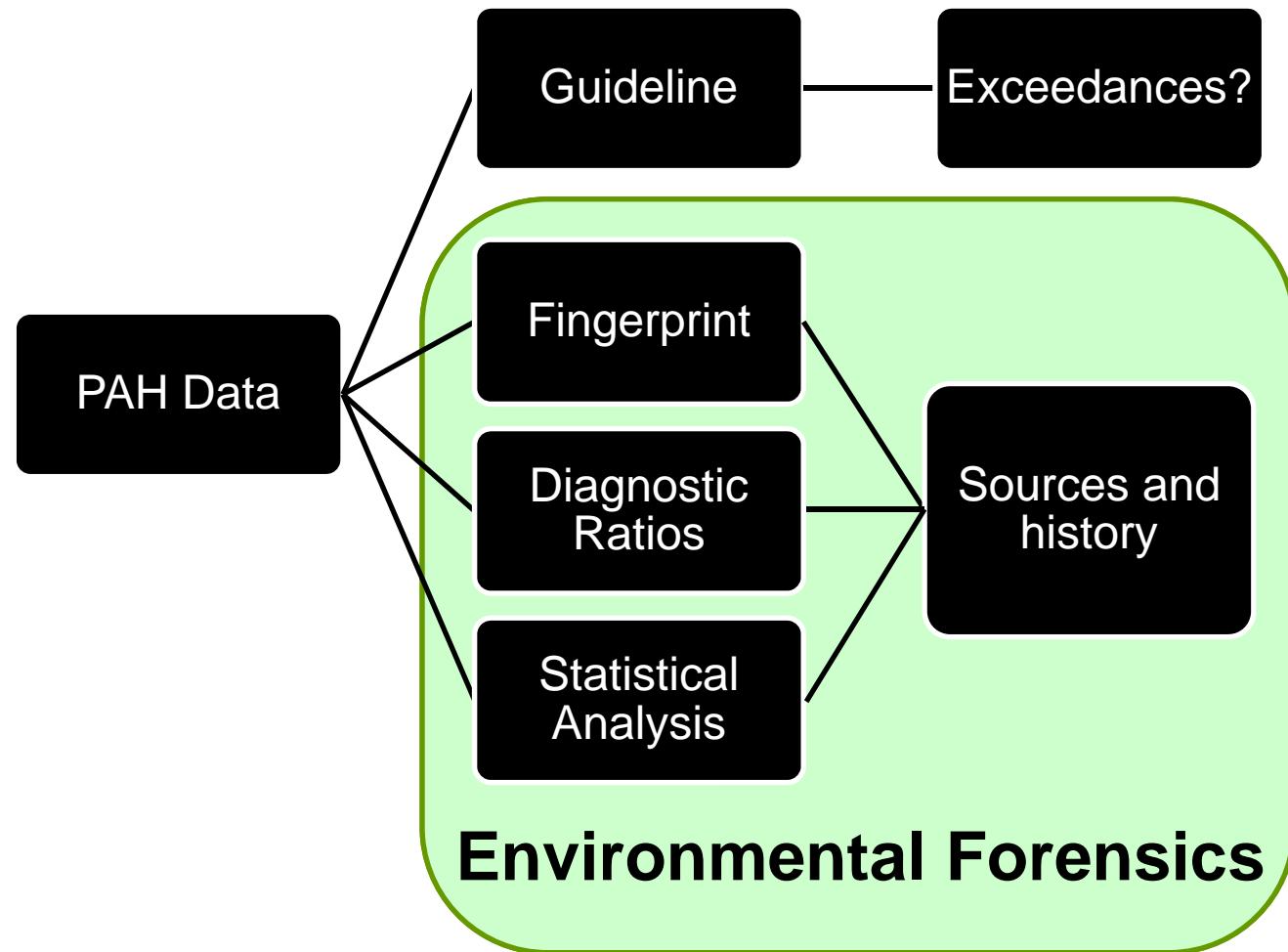
C3-Naphthalenes



Interpretation of Parent PAHs Data



Interpretation of Extended PAHs Data



Environmental Forensics

Fingerprint

Visual comparison of PAH data

Diagnostic Ratios

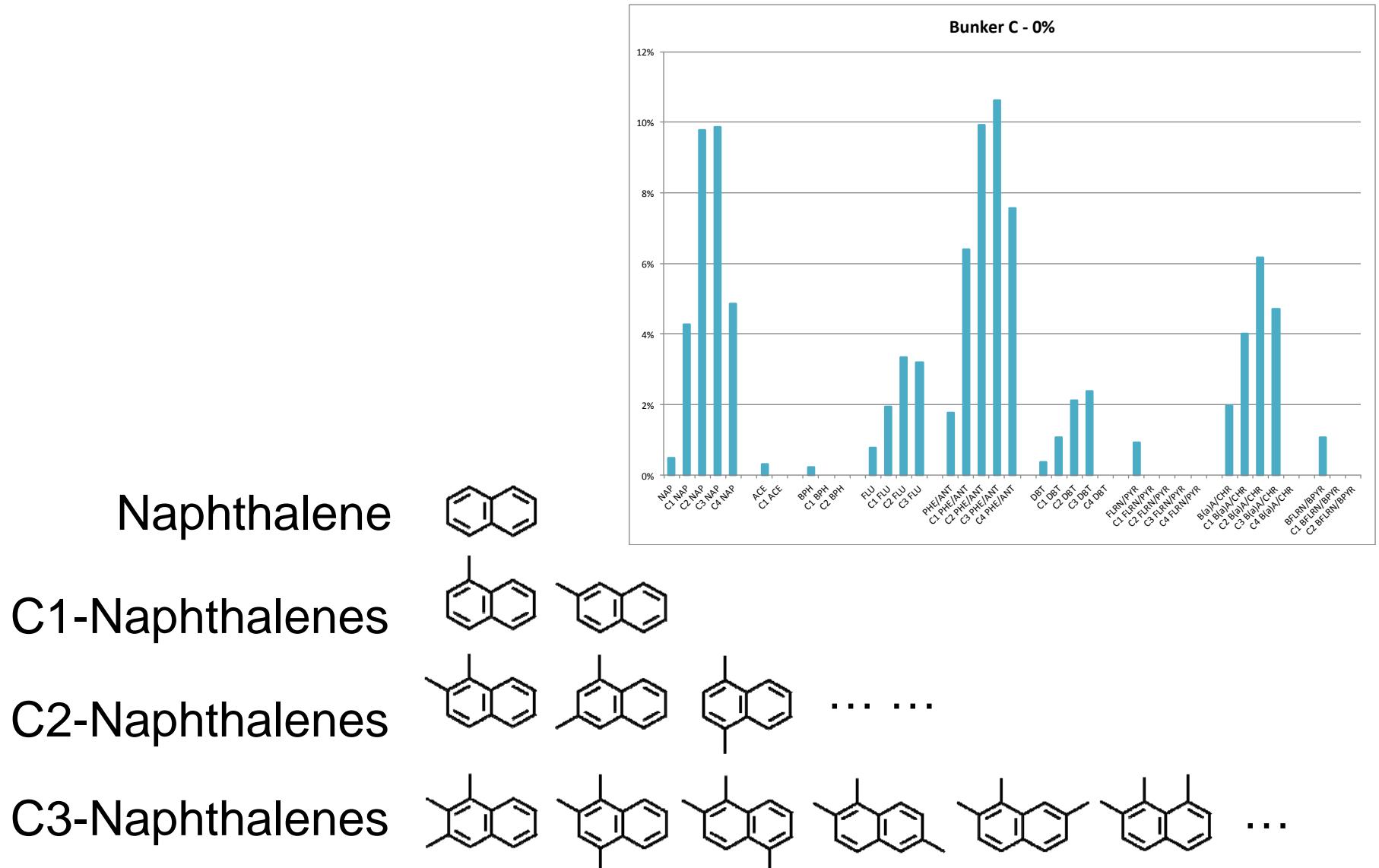
Relative concentration of key PAHs

Statistical Analysis

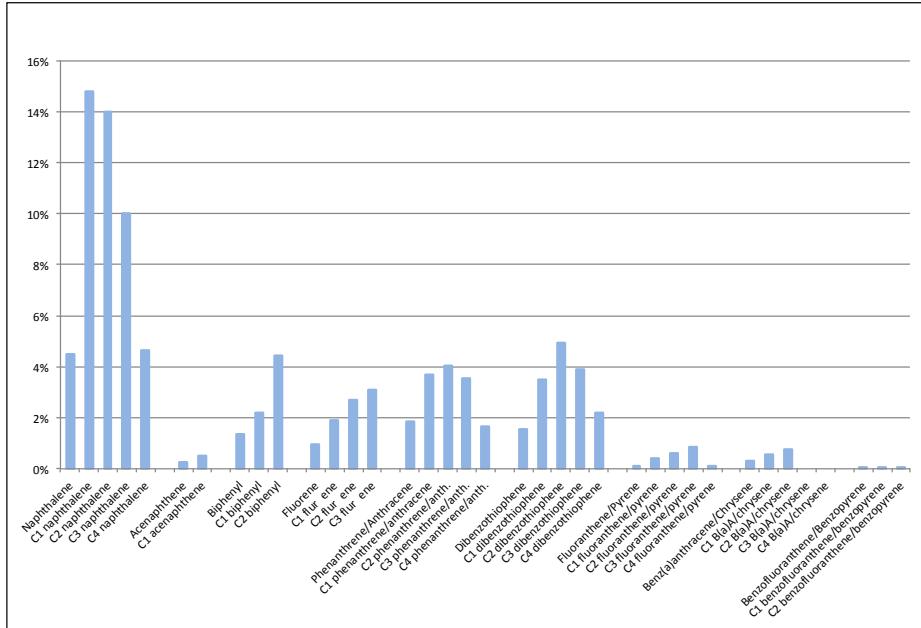
Comprehensive analysis of all PAH data



Fingerprint Graphs

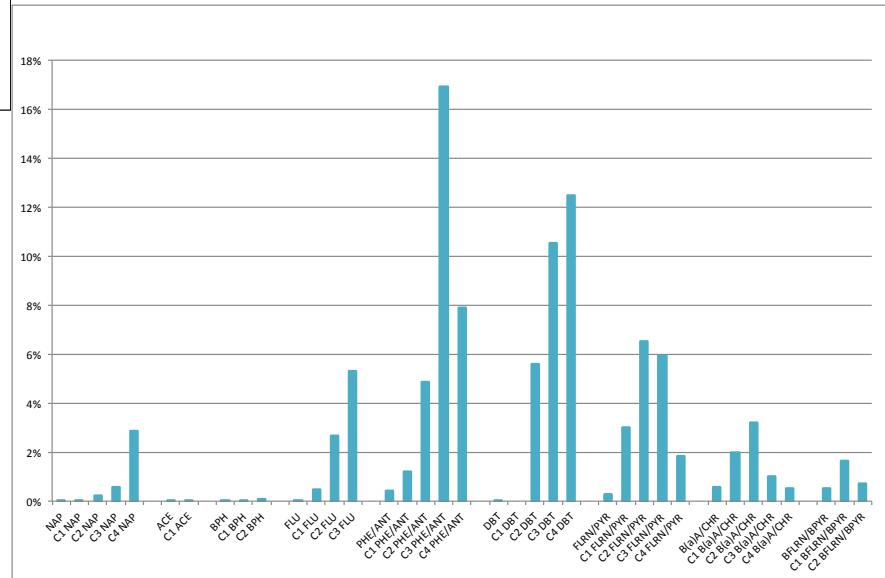


Oil Types



Light Crude

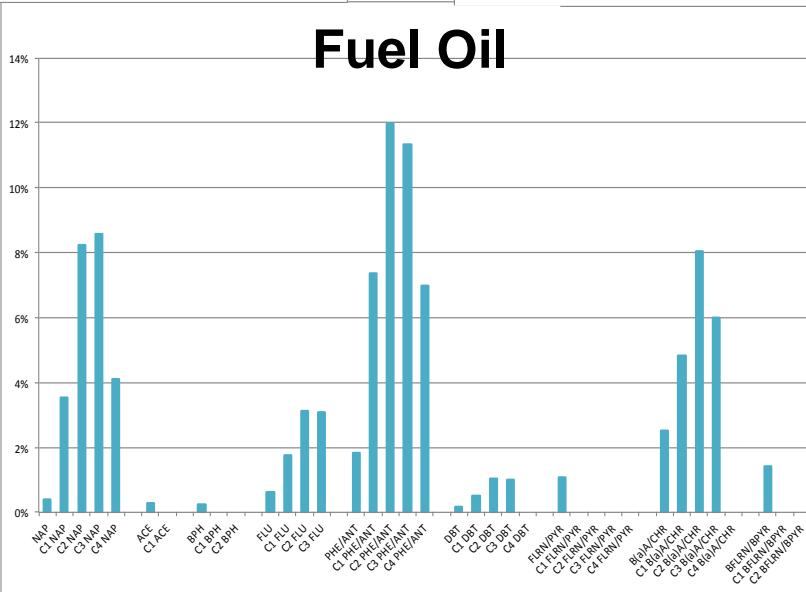
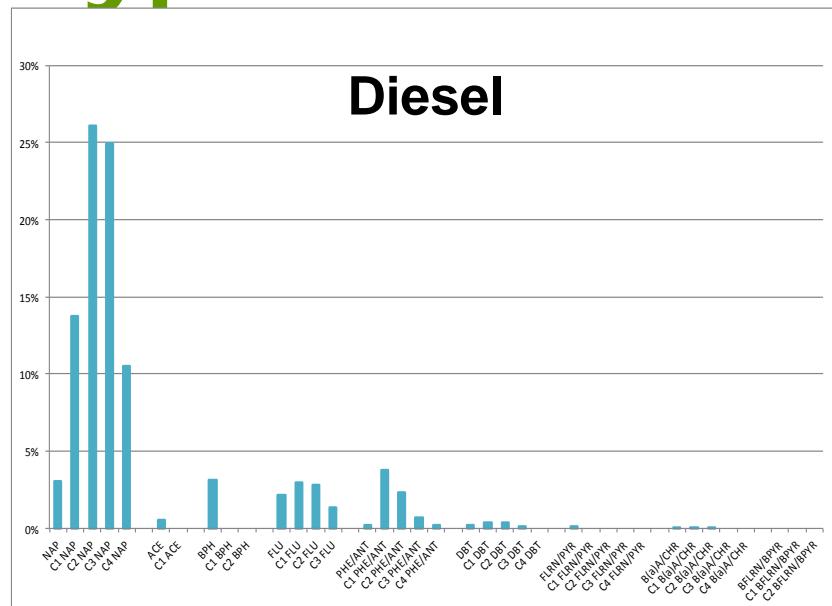
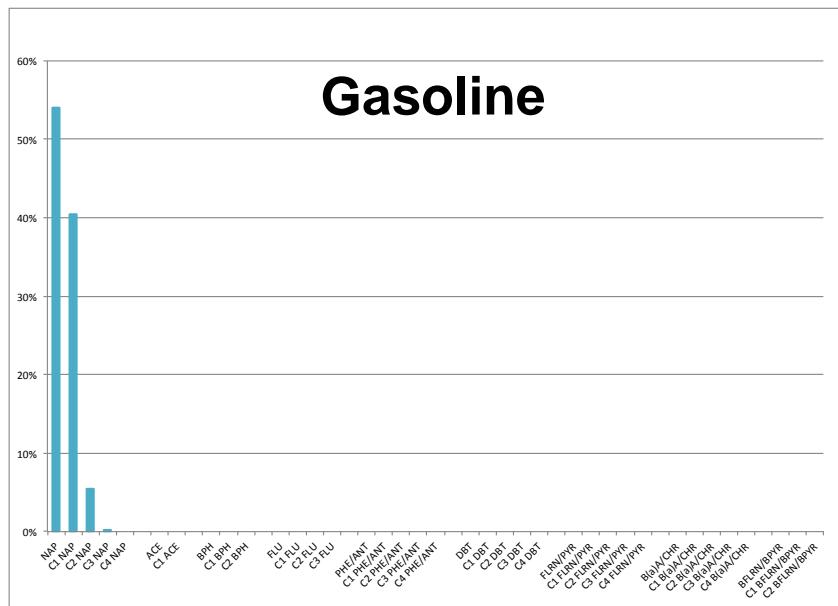
Light PAHs dominant
Nice bell-shaped patterns



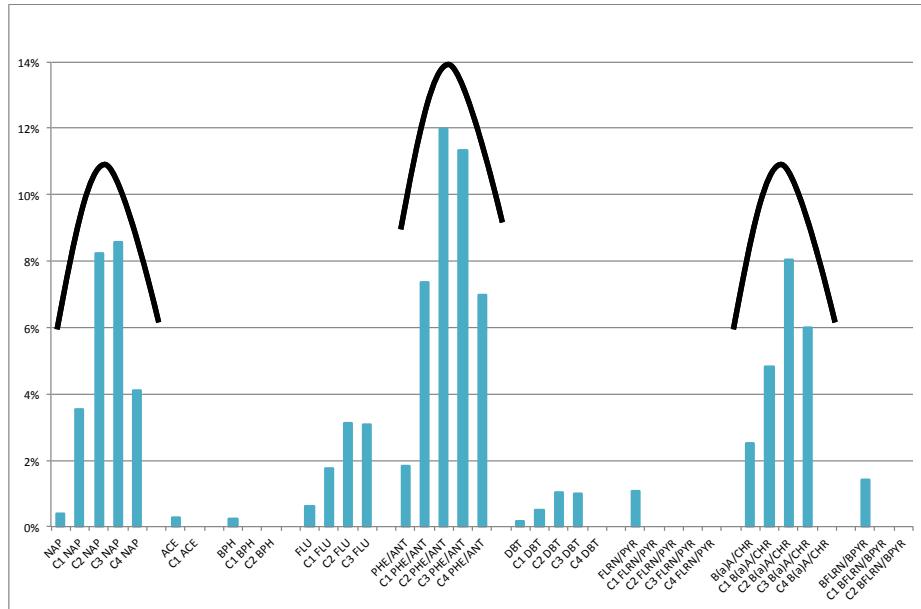
Bitumen

Heavy PAHs dominant
Mixed patterns

Product Types

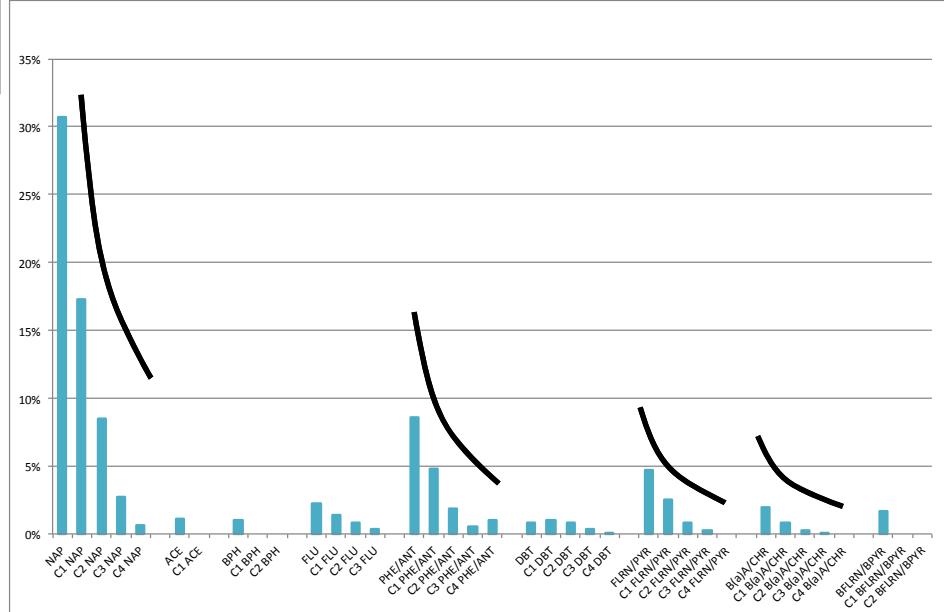


Petrogenic / Pyrogenic



Petrogenic
Bell-shaped family groups
Oil products

Pyrogenic
scree-shaped family groups
Combustion products



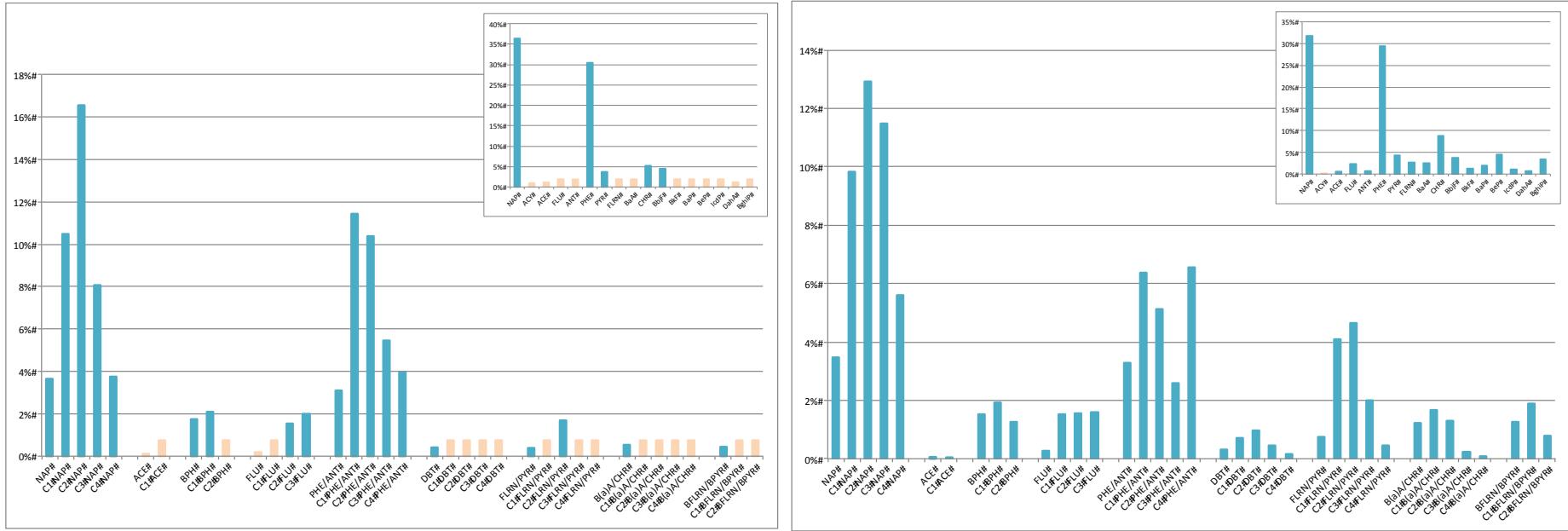
Natural background

Background is not zero.

- Dependent on type of system...



Natural background



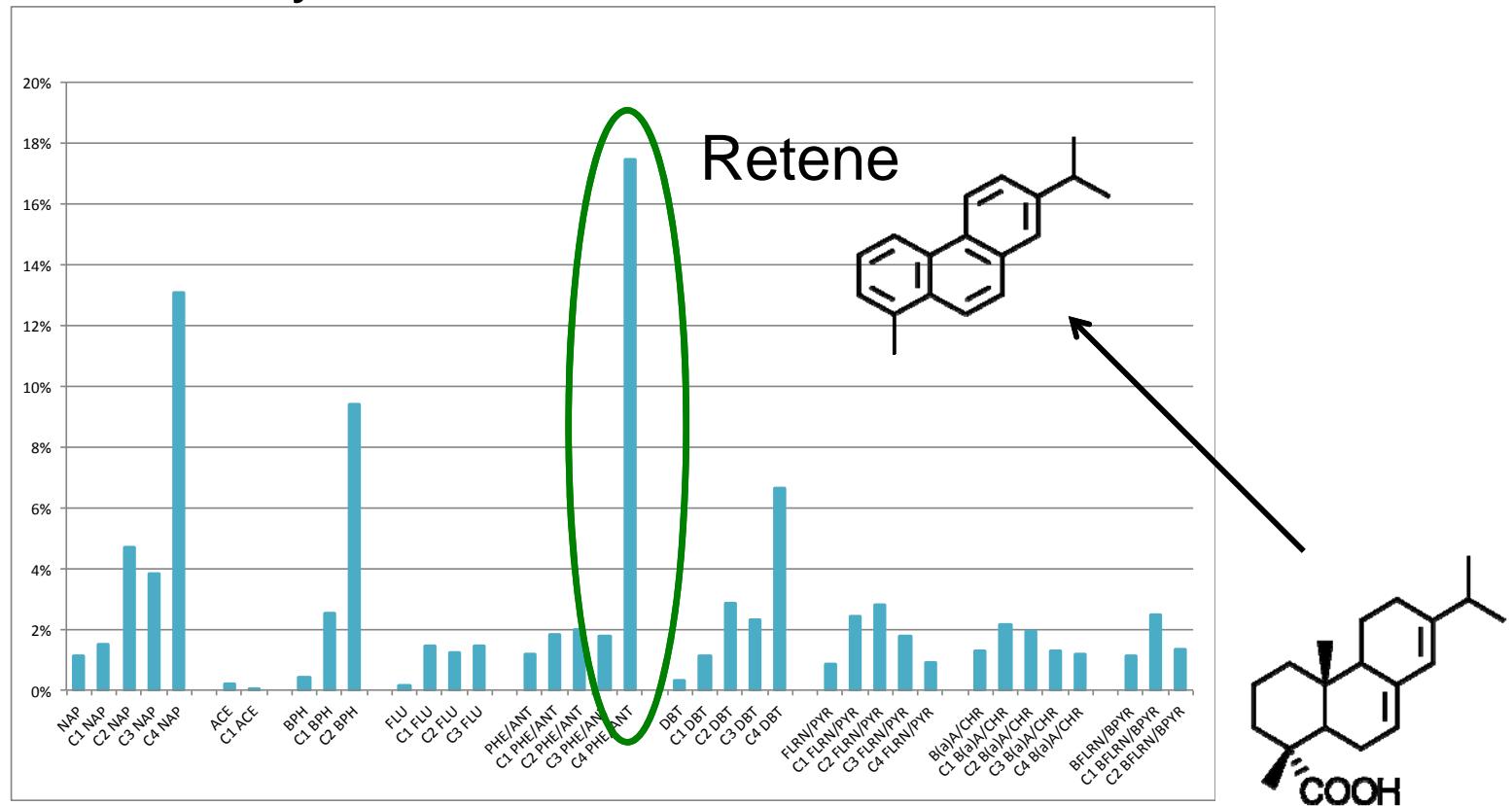
Floodplains are natural sinks.
Expect lots of guideline exceedances.

Naphthalenes and phenanthrenes are very common worldwide

Natural background

Muskeg – can detect lots of PAHs!

C4-PAHs are a key natural indicator...

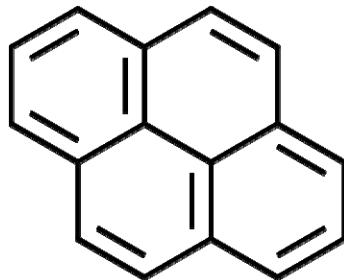


Retene is a breakdown product of terpenes from coniferous trees

Diagnostic Ratios

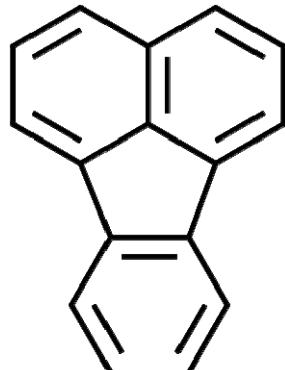
Certain PAHs are really key to understanding the origin of the family.

Kinetic and thermodynamic stability



Pyrene

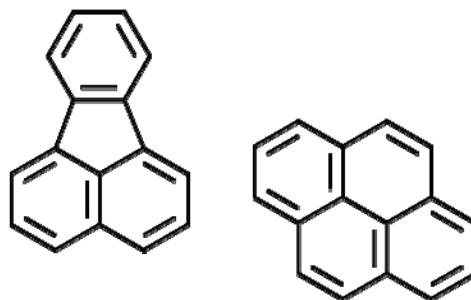
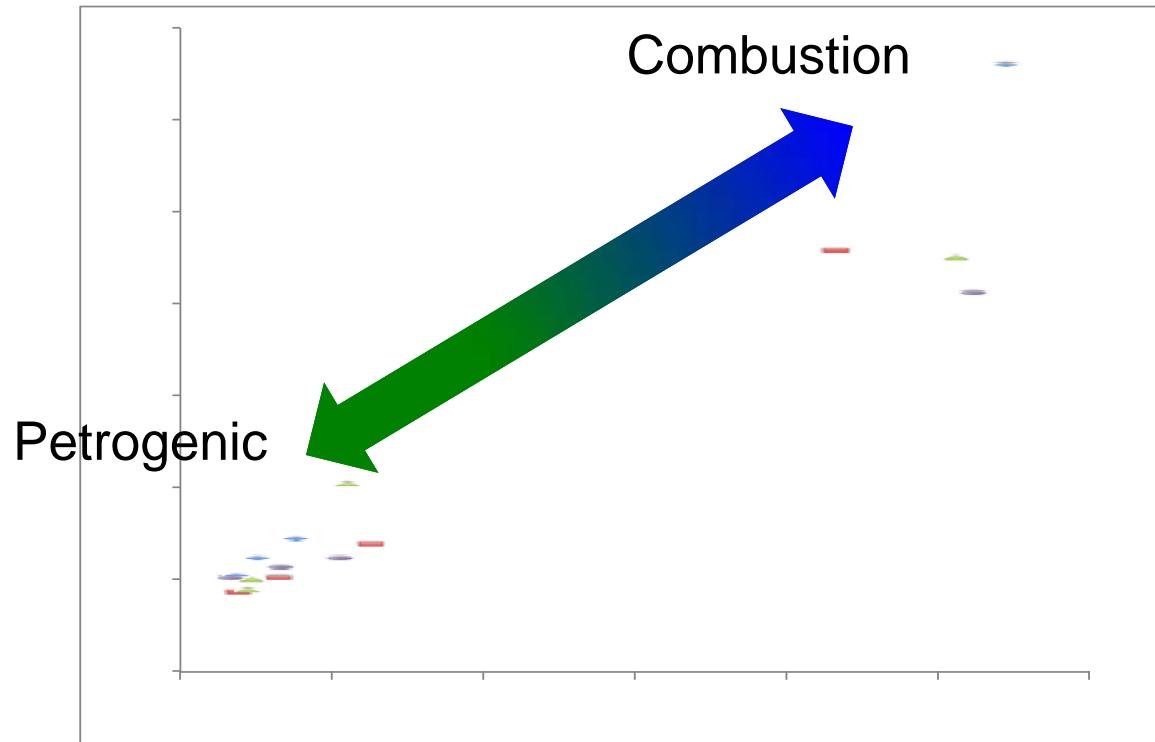
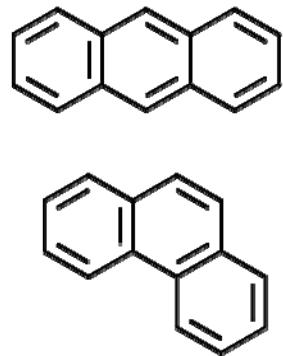
Thermodynamically favored



Fluoranthene

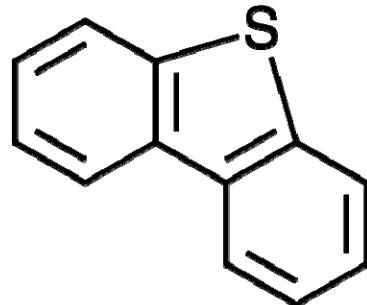
Kinetically favored

Diagnostic Ratios

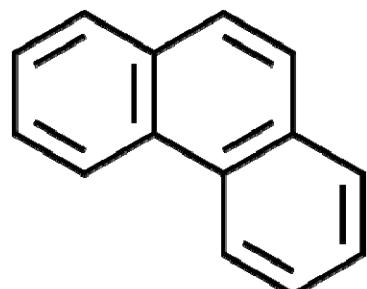


Diagnostic Ratios

Sulfur-containing PAHs.



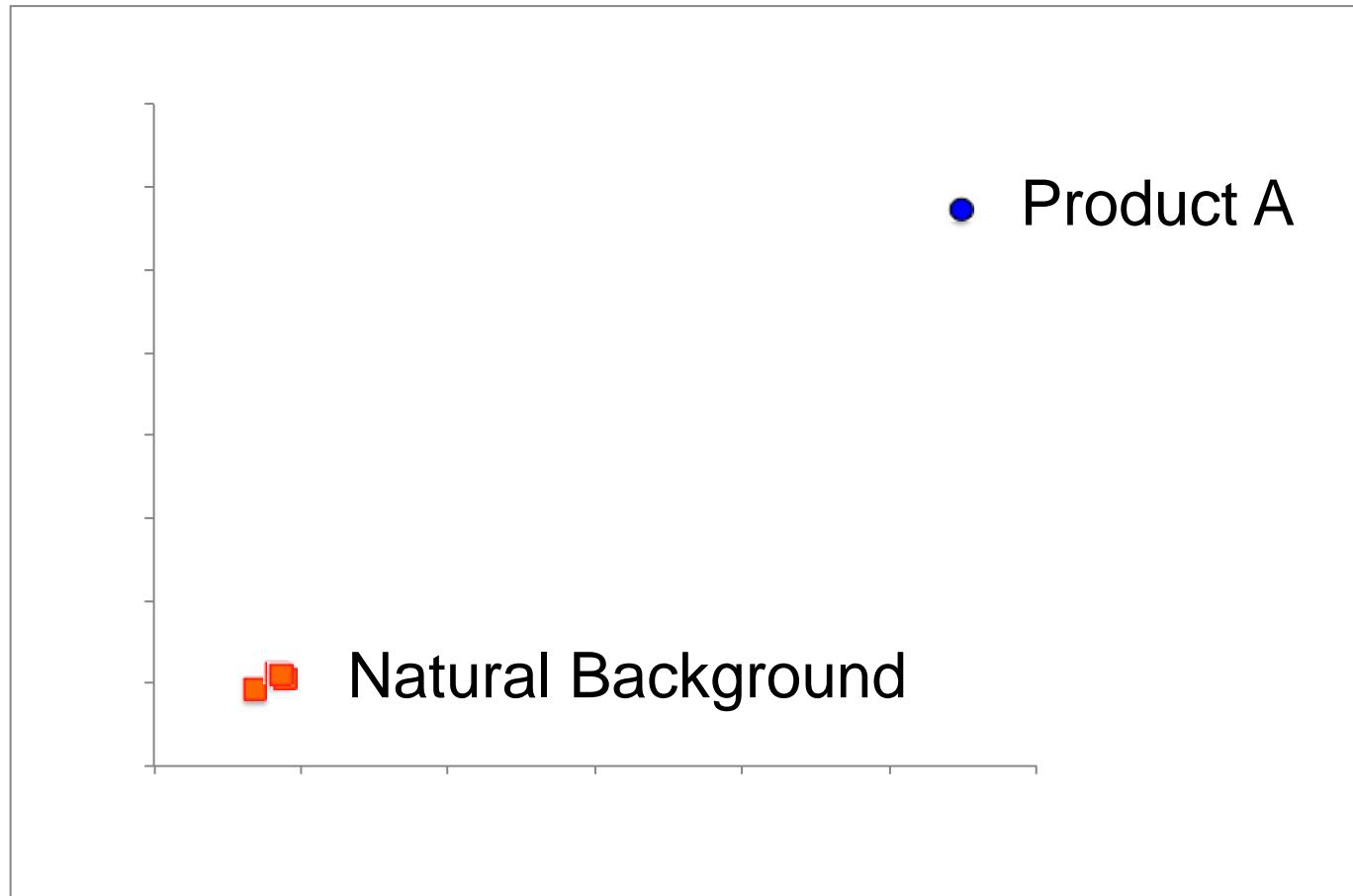
Dibenzothiophene



Phenanthrene

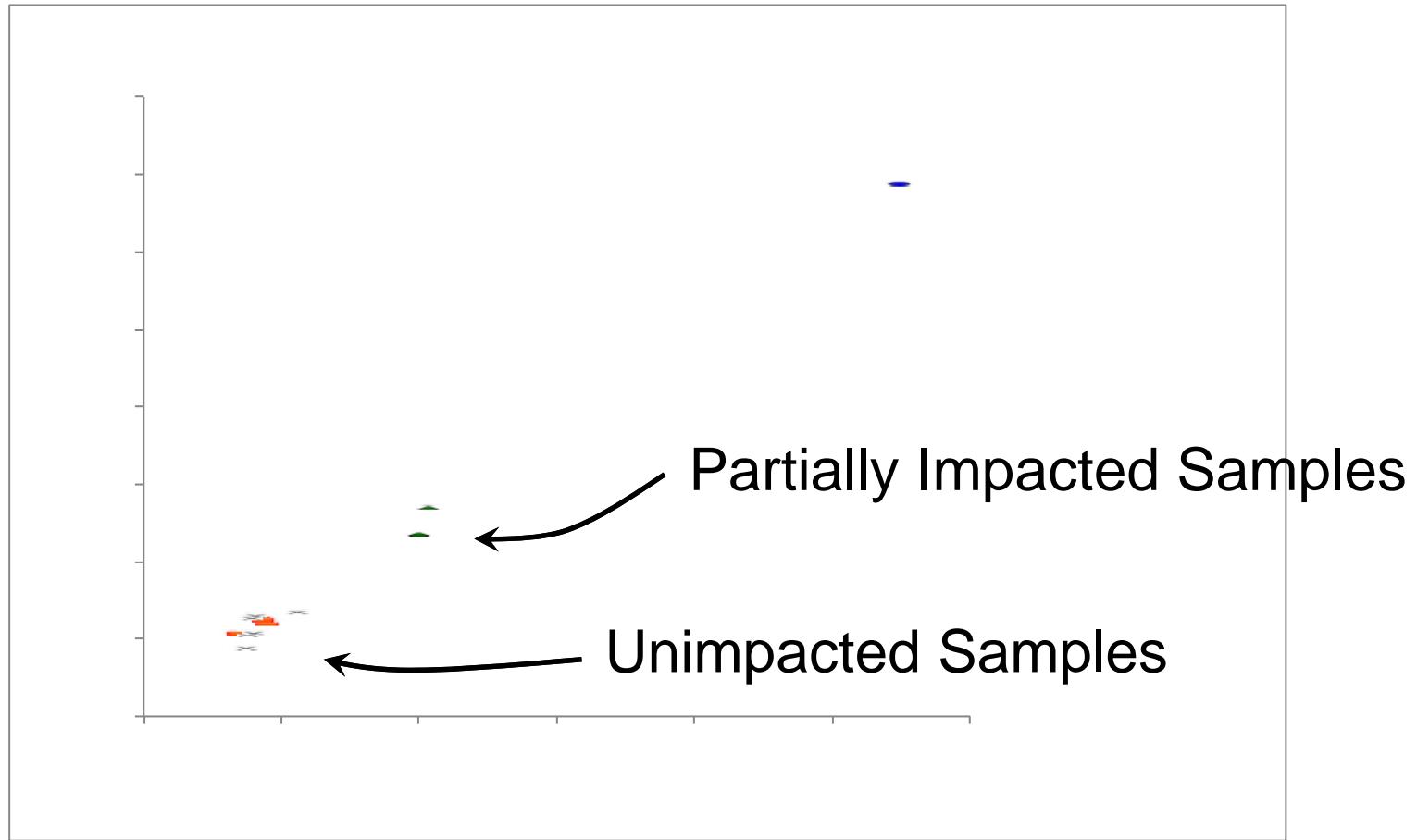
Diagnostic Ratios

Sulfur content



Diagnostic Ratios

Sulfur content



Statistical Analysis

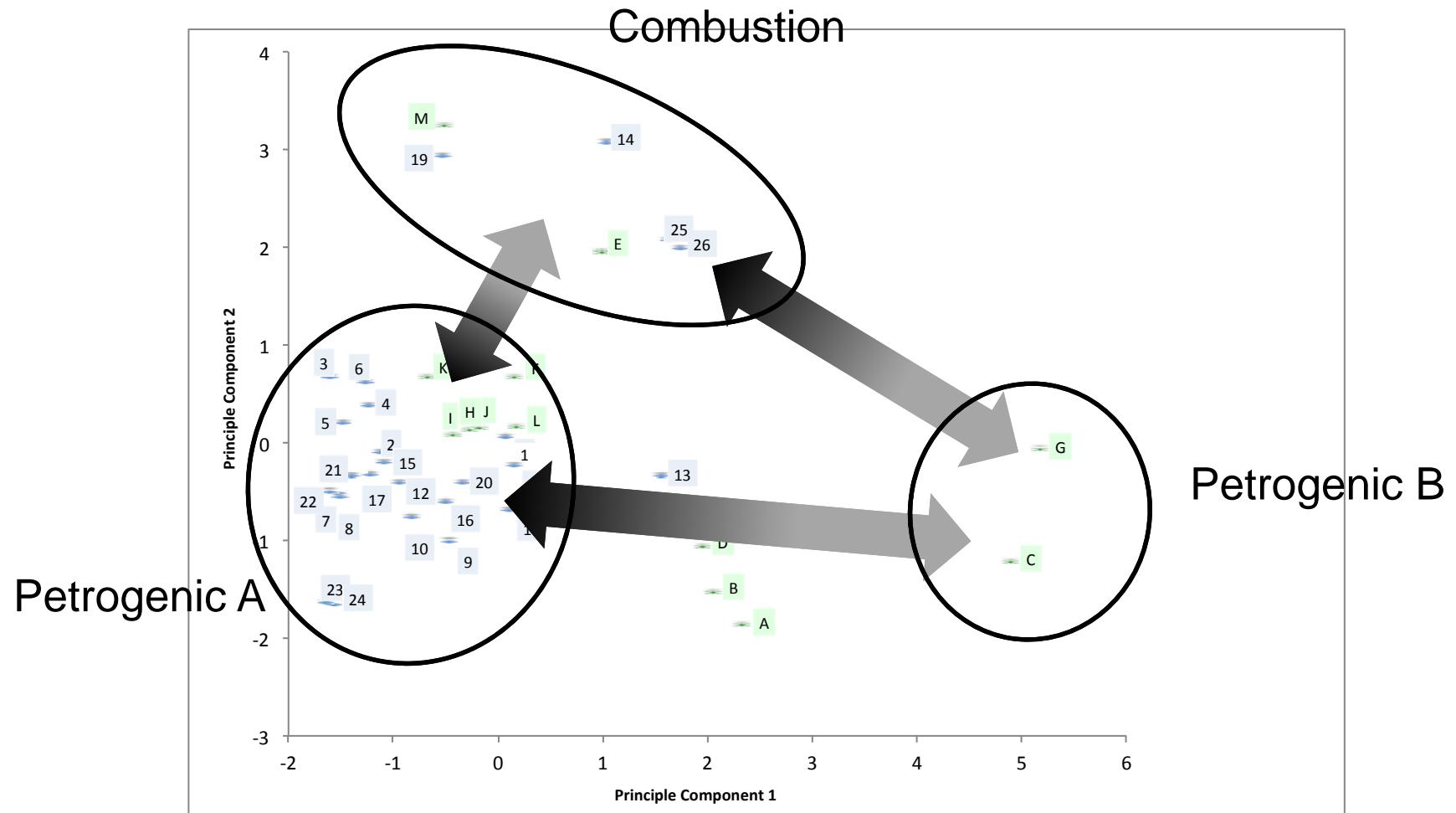
Diagnostic ratios are indicators for 2 chemicals.

Other statistical analyses can use all PAH data.

Principle Components Analysis (PCA)



Statistical Analysis



Summary

- PAHs are everywhere, take care with the data.
- Natural exceedances are likely in many types of area.

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Thank You



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