

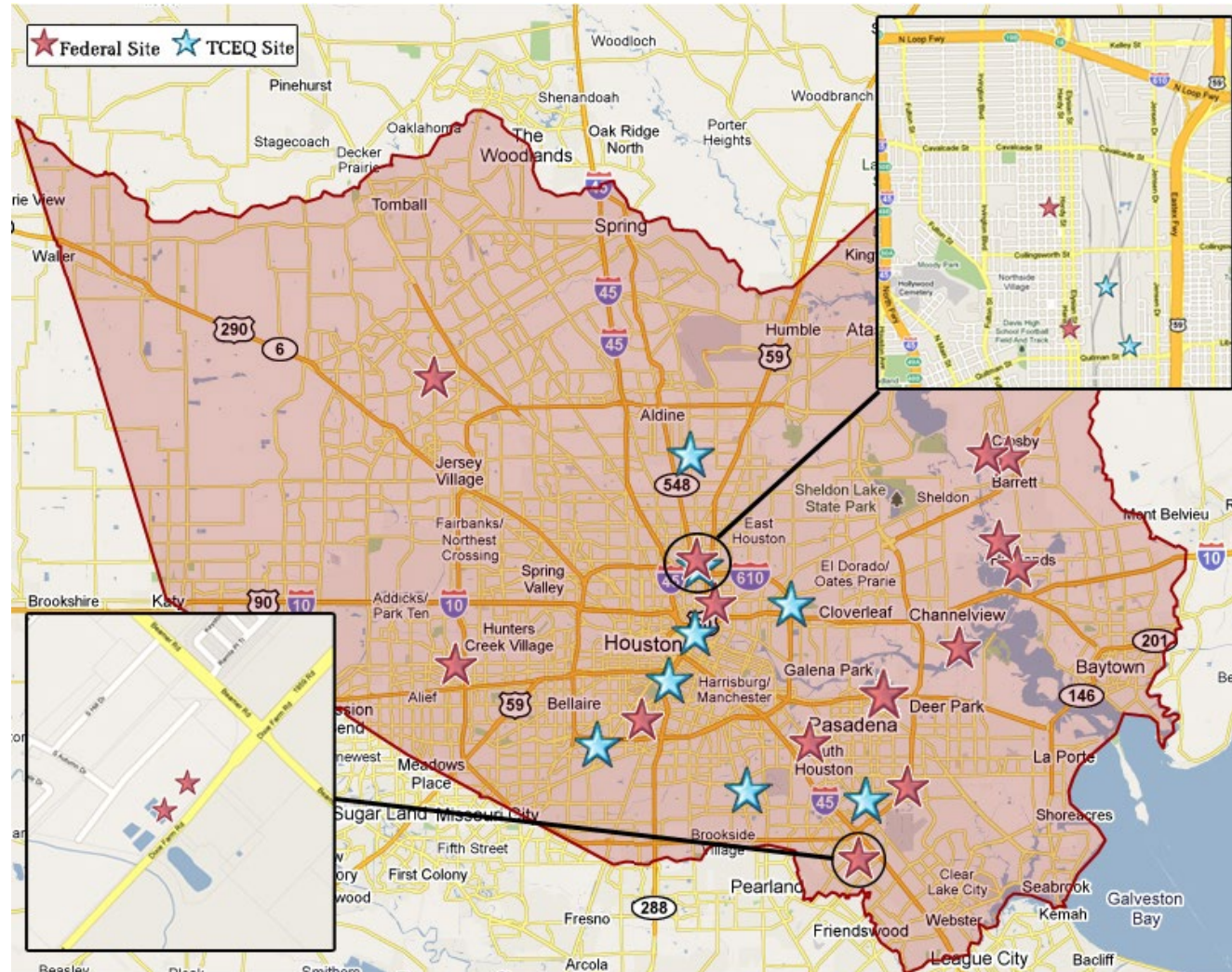
BCM-Rice Superfund Research Program

Polycyclic Aromatic Hydrocarbons (PAHs): Maternal Exposure, Toxicity, and Remediation



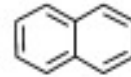
Principal Investigator/Program Director
Bhagavatula Moorthy, Ph.D.
Baylor College of Medicine, Houston, TX

Harris County has 24 remediated or active Superfund Sites

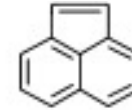


Polycyclic aromatic hydrocarbons (PAHs)

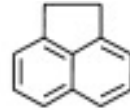
- PAHs are a large group of chemicals made up of multiple fused aromatic (benzene-like) rings.
- There are more than 100 different PAHs, with 16 considered as priority chemicals due to their known toxicity.
- They are formed during incomplete combustion of organic materials including coal, oil, gas, wood, tobacco, and food cooked at very high temperatures.
- Exposure occurs through many modalities including ambient air, vehicular exhaust, water, grilled meat, tobacco smoke & wood smoke
- PAHs are contaminants of concern, not only at Houston-based Superfund sites, but at multiple sites nationwide



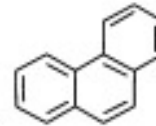
Naphthalene



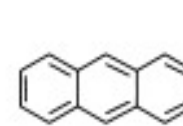
Acenaphthylene



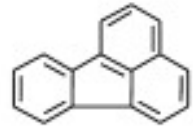
Acenaphthene



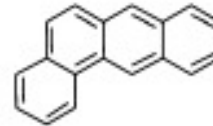
Phenanthrene



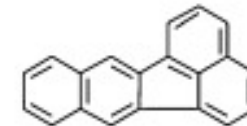
Anthracene



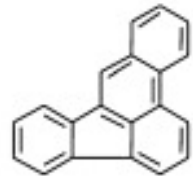
Fluoranthene



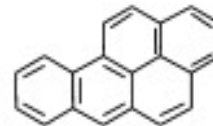
Benz[a]anthracene



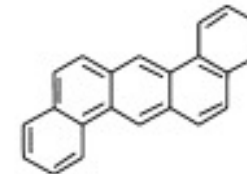
Benzo[k]fluoranthene



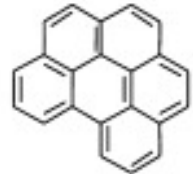
Benzo[b]fluoranthene



Benzo[a]pyrene

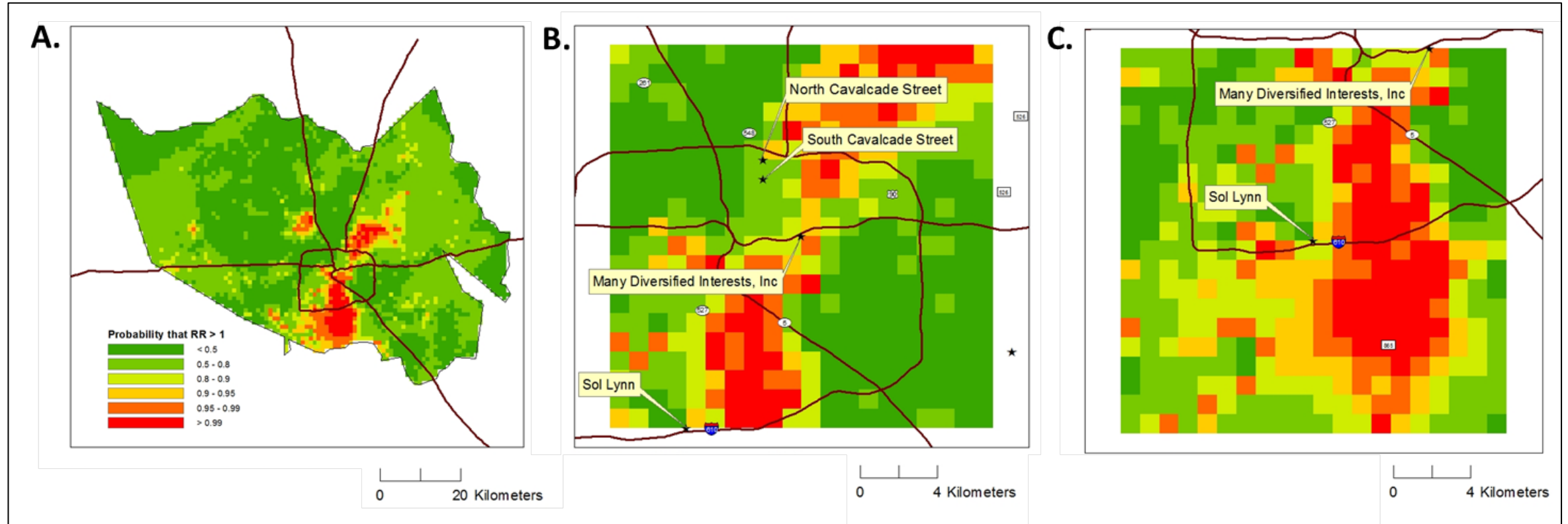


Dibenz[a,h]anthracene



Benzo[g,h,i]perylene

Geostatistical analysis reveals higher risk of preterm birth around 4 Superfund sites



PAHs are contaminants of concern at 3 of 4 sites

Table 1. PAHs are contaminants of concern at Superfund sites with clusters of high incidence of preterm birth and very low birth weight babies

North Cavalcade	Biphenyl, trimethylbenzene, dihydroacenaphthylene, dimethylphenol, methylnaphthalene, methylphenol, carbazole, fluorine, acenaphthylene , anthracene , arsenic, benzene, benzo(b)fluoranthene , benzo(k)fluoranthene , benzo(a)anthracene , benzo(a)pyrene , carcinogenic polycyclic aromatic hydrocarbons , chrysene , copper, ethylbenzene, fluoranthene , indenopyrene , naphthalene , phenanthrene , phenol, pyrene , toluene, xylene, zinc
South Cavalcade	Arsenic, benzene, carcinogenic polycyclic aromatic hydrocarbons , chromium, copper, ethylbenzene, lead, toluene, xylene, zinc
Many Diversified Interests	Benzo[a]pyrene , lead, manganese, molybdenum, total petroleum hydrocarbons
Sol Lynn Industrial Transformers	Chloroethene, dichloroethene, polychlorinated biphenols, trichloroethene

Preterm Birth is a Major Challenge in Maternal and Neonatal Health

- Preterm birth is defined as delivery of the baby before 37 weeks of gestation has been completed.
- Depending on how early the baby is born, there are many morbidities that are associated with a preterm delivery
 - Babies born too soon may not be able to feed on their own, and need supplemental nutrition for weeks before learning to feed
 - Preterm infants are at higher risk of infections and may have lifelong neurodevelopmental impairment
 - Preterm infants are also unable to breathe well on their own. They may suffer from chronic lung disease including bronchopulmonary dysplasia (BPD)

BCM-Rice Superfund Research Program

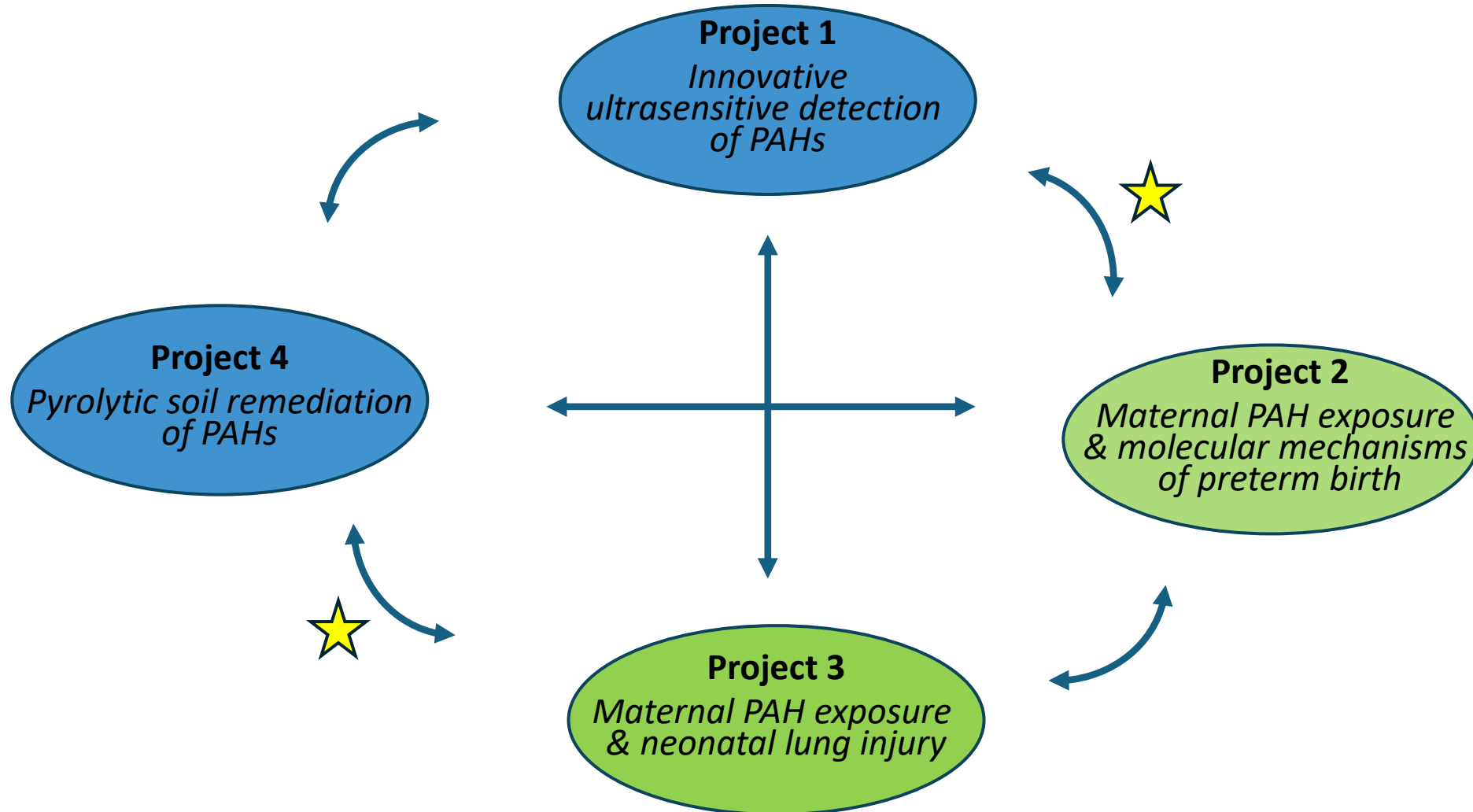
Hypothesis

Maternal exposure to PAHs as well as other environmental chemicals which are present in Superfund sites, increases the risks for preterm birth and augments the major morbidities associated with preterm birth such as chronic lung disease.

BCM-Rice SRP Scientific Goals

- Develop ultra-sensitive detection methods for PAHs and other Superfund-related chemicals ([Project 1](#))
- Uncover mechanisms behind the increased risk of preterm birth with *in utero* exposure to PAHs ([Project 2](#))
- Determine mechanisms by which maternal PAH exposures cause an increased risk of chronic neonatal lung disease ([Project 3](#)).
- Determine optimal conditions to treat PAH-contaminated soils to eliminate toxicity and recover soil fertility ([Project 4](#)).

Integrated Science Across the BCM-Rice SRP

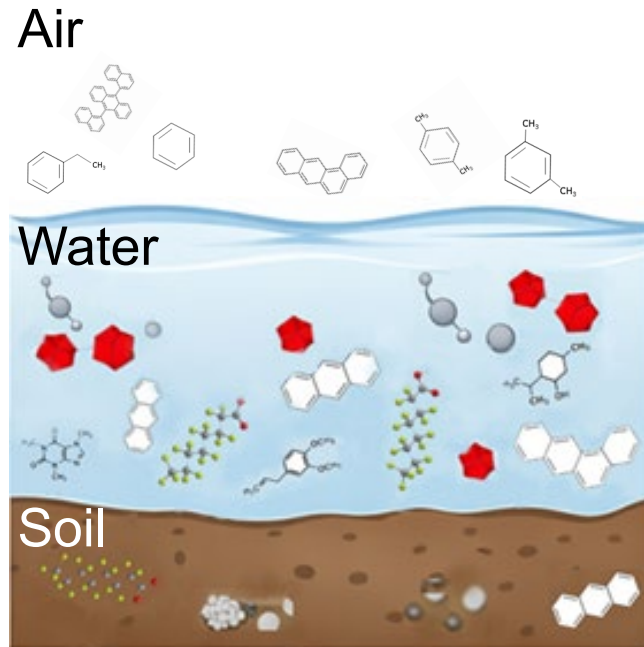


Supporting Cores:

Administrative * Data Management * Community Engagement * Training * Research Support

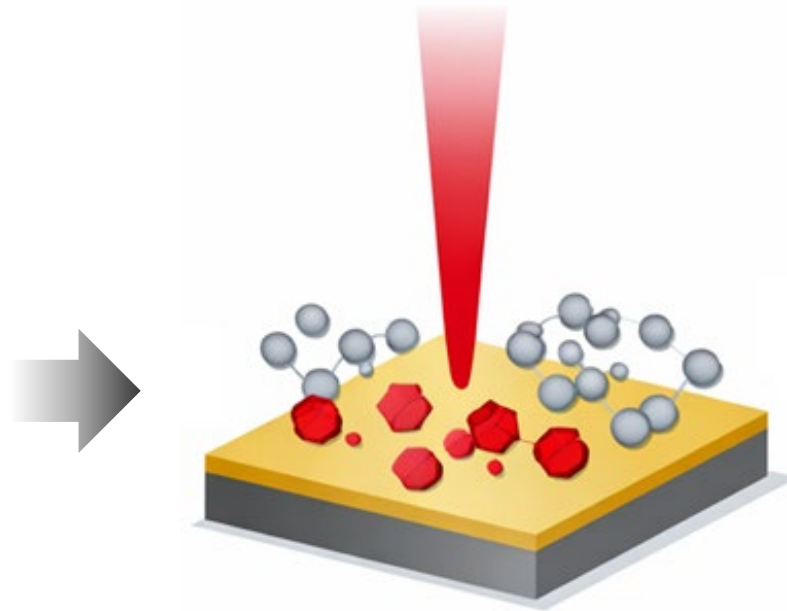
Project 1. Tackling Current Challenges in Trace Molecular Detection

Trace Analytes in Complex Matrices



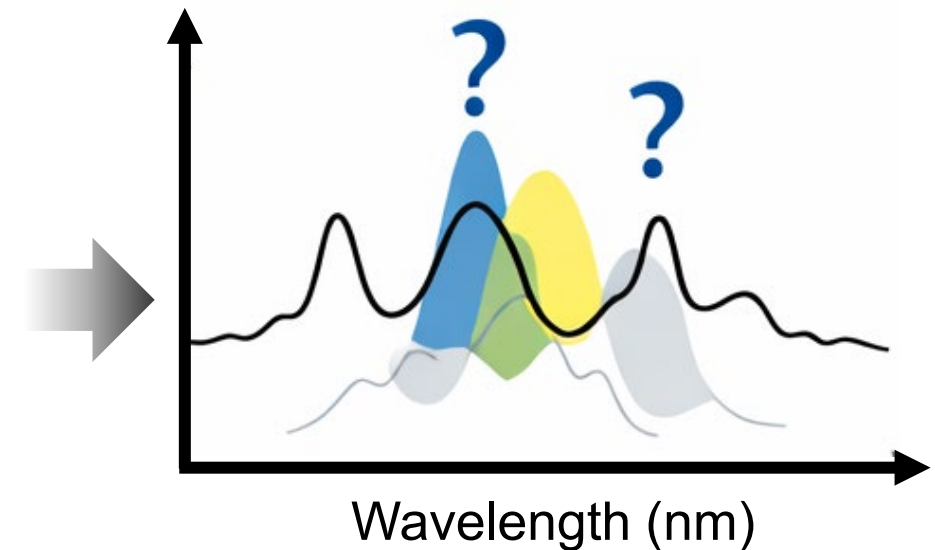
- Trace concentration
- Matrix interference

Matrix Interference and spectral overlap



- Very few target molecules
- Many interfering species
- Weak or overlapping spectral signals

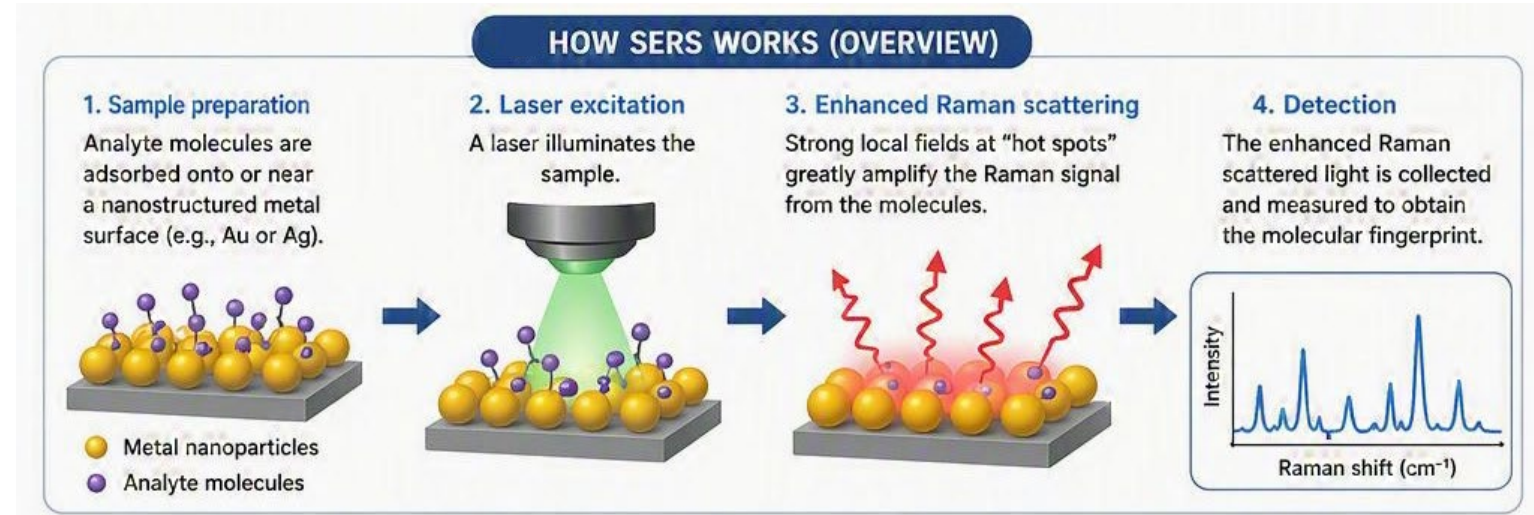
Difficult Spectral Discrimination



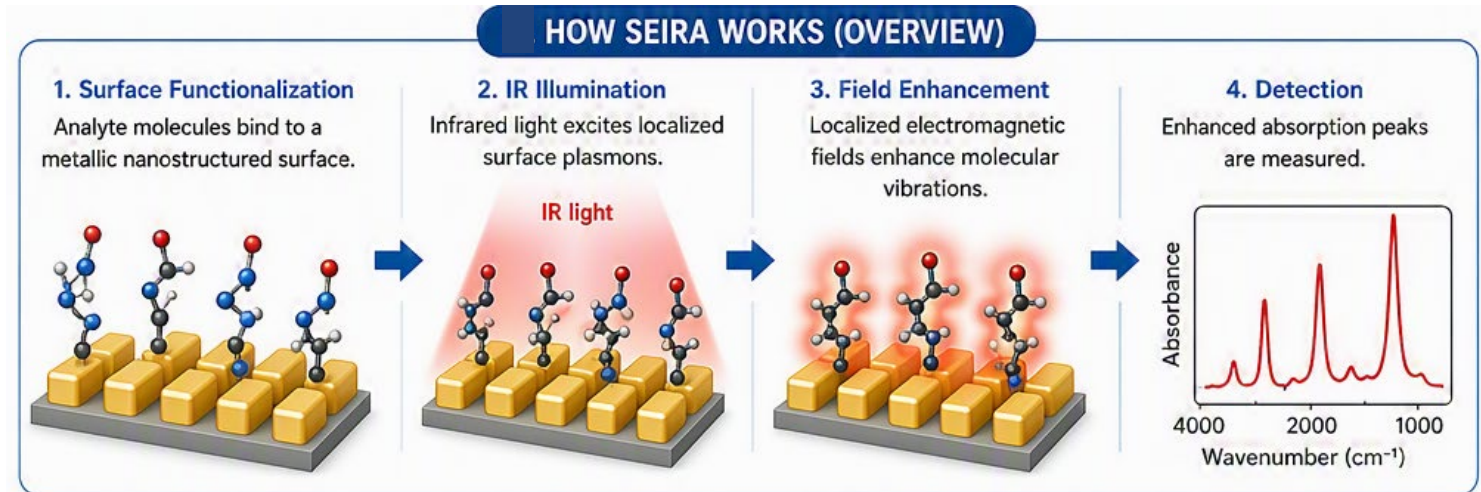
- Weak peaks
- Analyte is unknown
- Noisy baseline

Using SERS and SEIRA for *ultra-sensitive* detection of complex mixtures

Surface Enhanced Raman Spectroscopy (SERS)

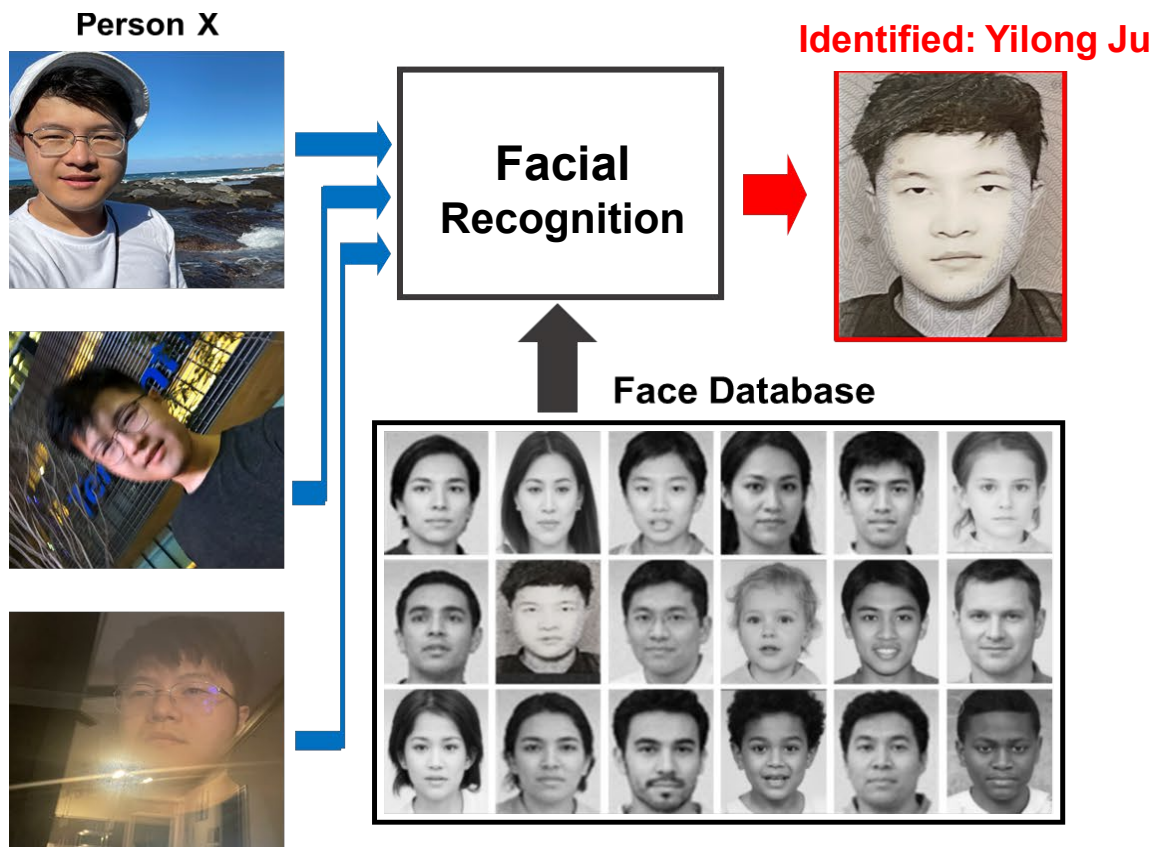


Surface Enhanced Infrared Absorption (SEIRA)

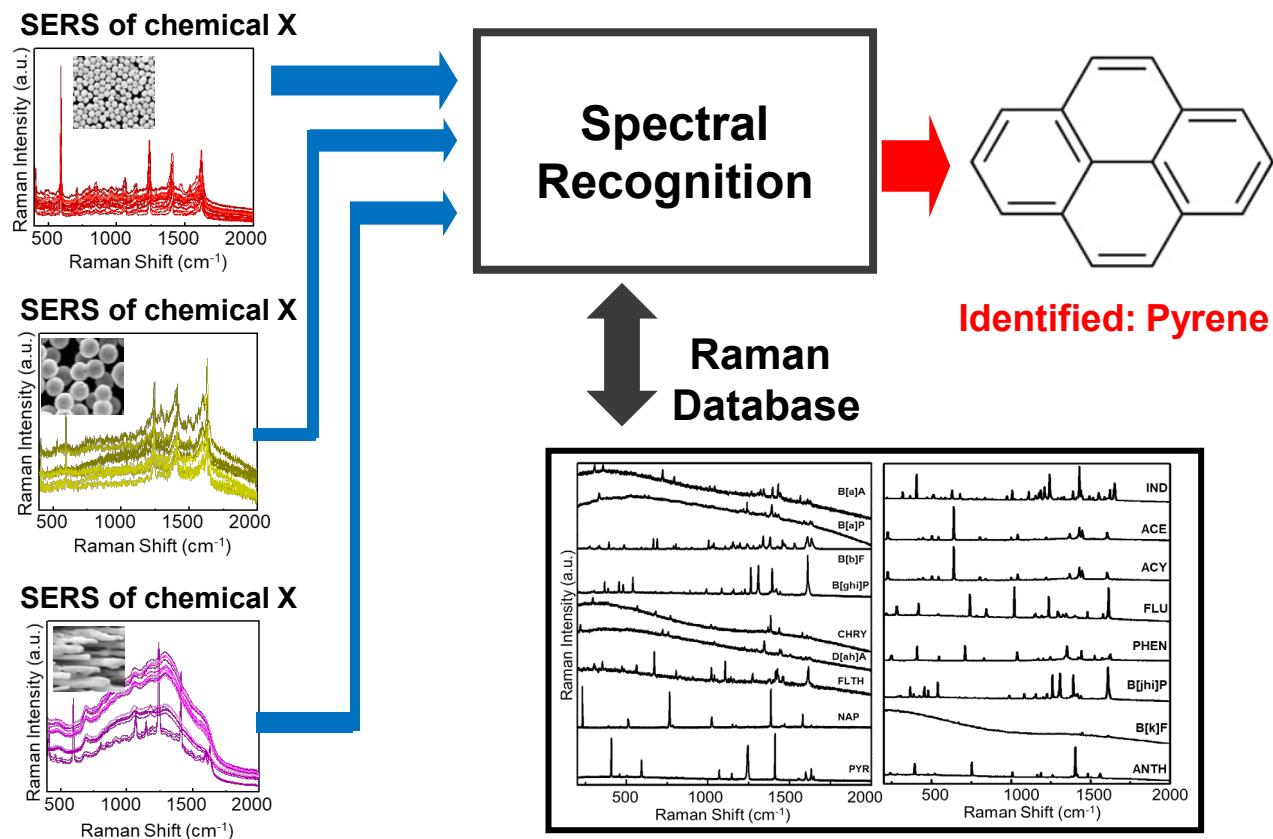


Using Facial Recognition Approaches to identify SERS spectra of molecules using a Raman Database

Characteristic Feature Extraction



Characteristic Peak Extraction

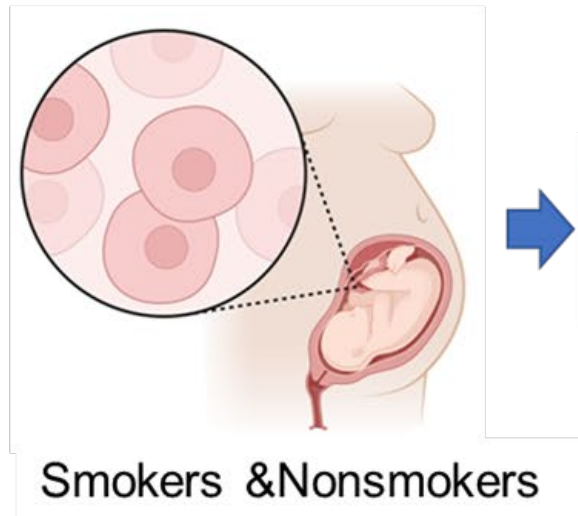


Projects 1 & 2 Collaboration

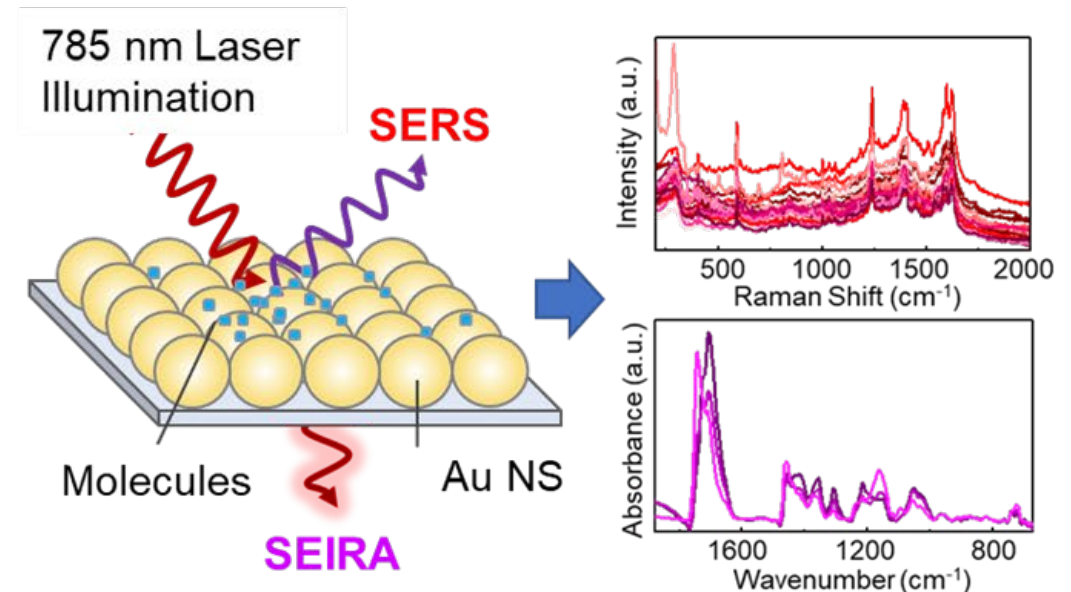
Using SERS, SEIRA & Machine Learning to Detect PAHs in Placenta

Can we use SERS + ML to detect PAH/PACs in the placenta of mothers who are smokers?

Sample Preparation

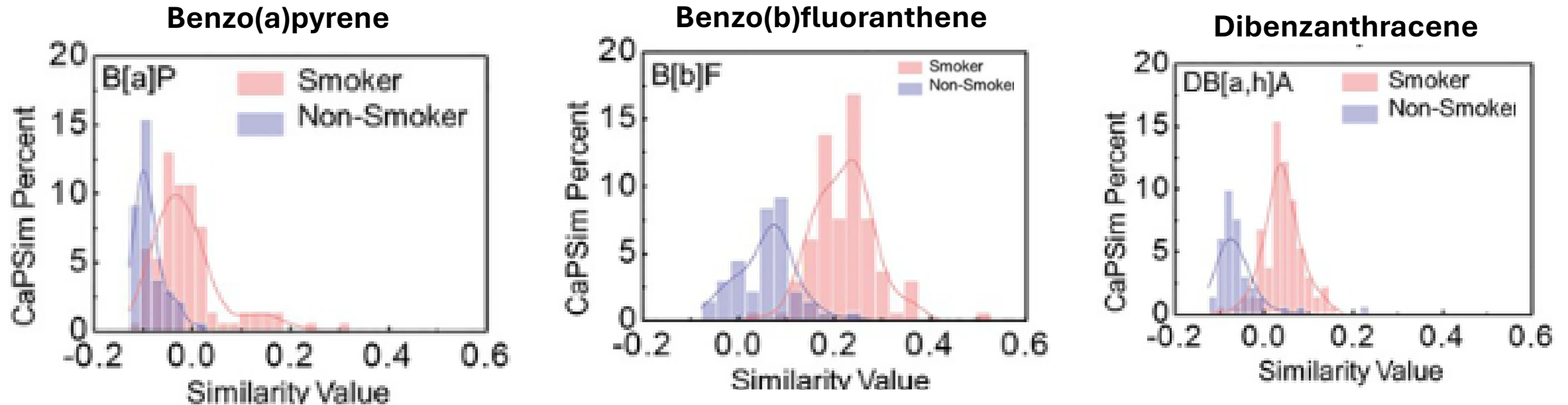


Data Collection and Analysis



Projects 1 & 2 Collaboration

More placental PAHs in smokers compared with non-smokers



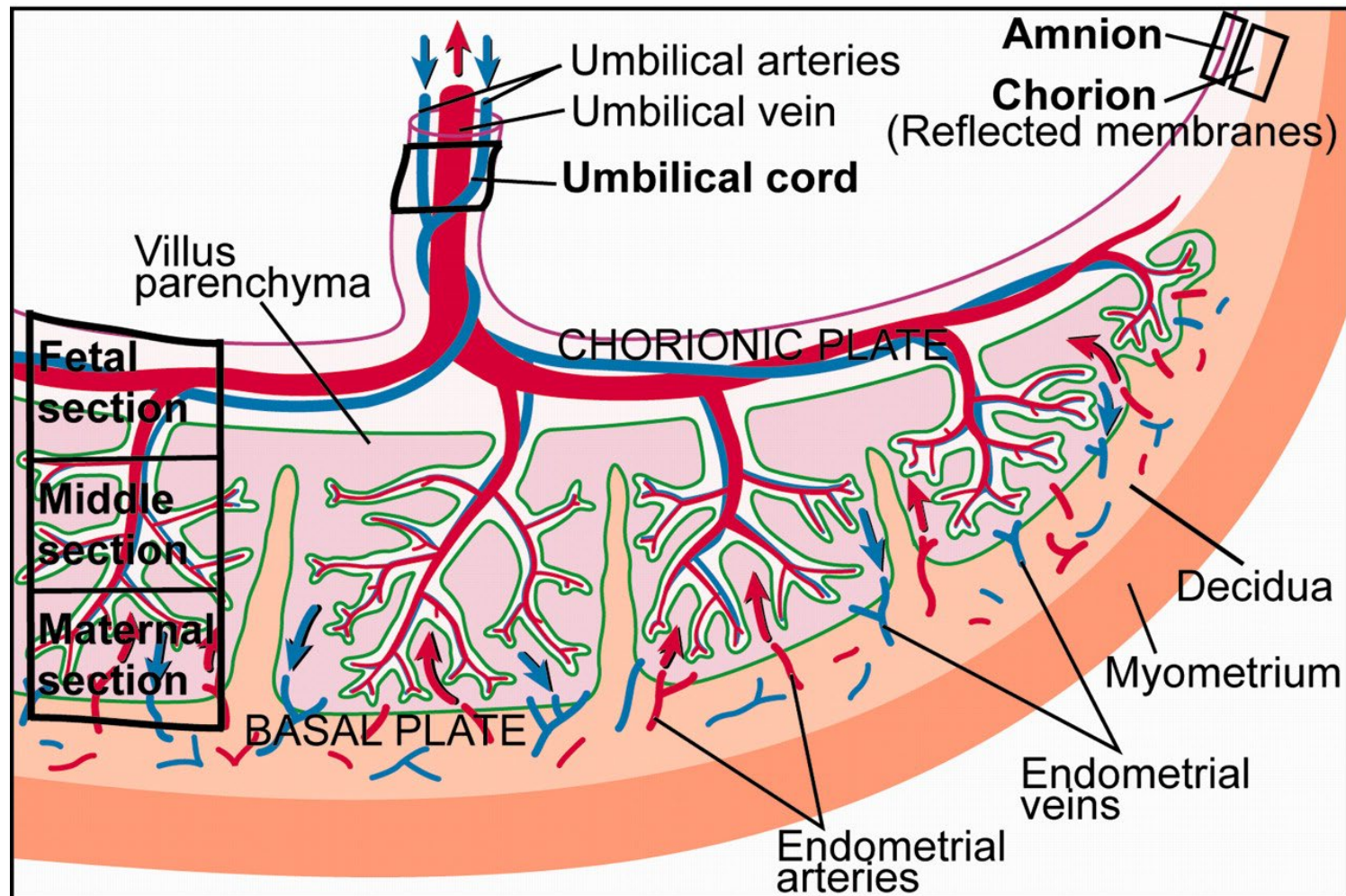
Machine Learning Algorithms:
Characteristic Peak Extraction (CaPE) and Characteristic Peak Similarity (CaPSim)



Andres Sanchez-Alvarado
Graduate Student, Halas Lab
Rice University
Project 1 Trainee

Project 2. Molecular mechanisms behind PAH exposures and preterm birth

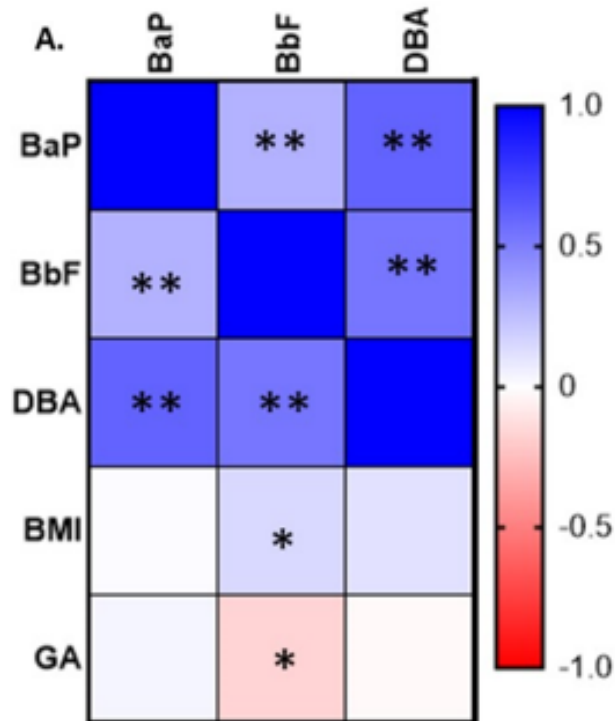
The placenta contains a footprint of the in utero experience



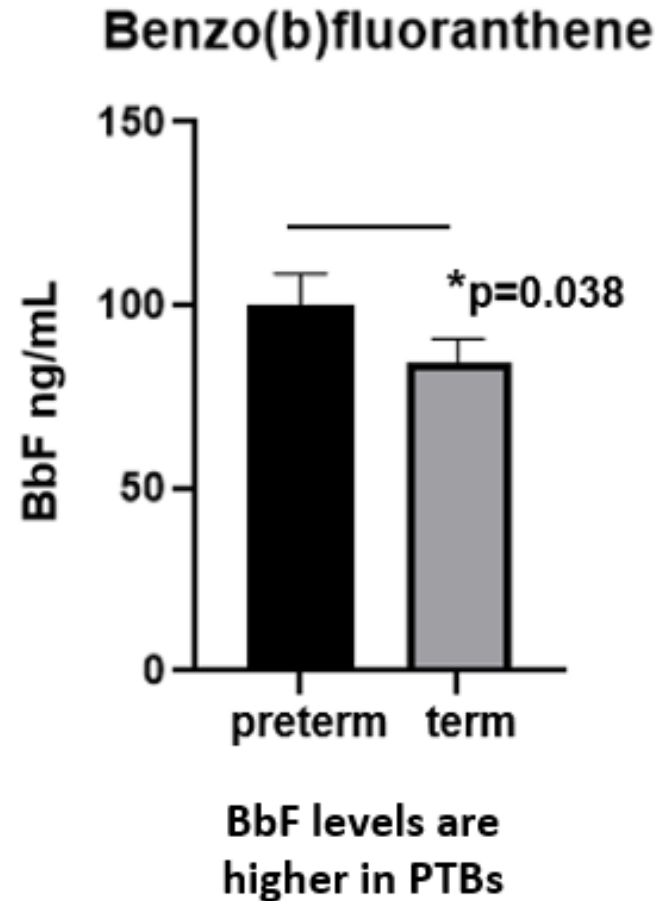
Project 2 & Research Support Core Collaboration

Maternal PAH exposures are associated with *spontaneous* preterm birth

N=323 placenta samples



BbF negatively correlates with gestational age at delivery

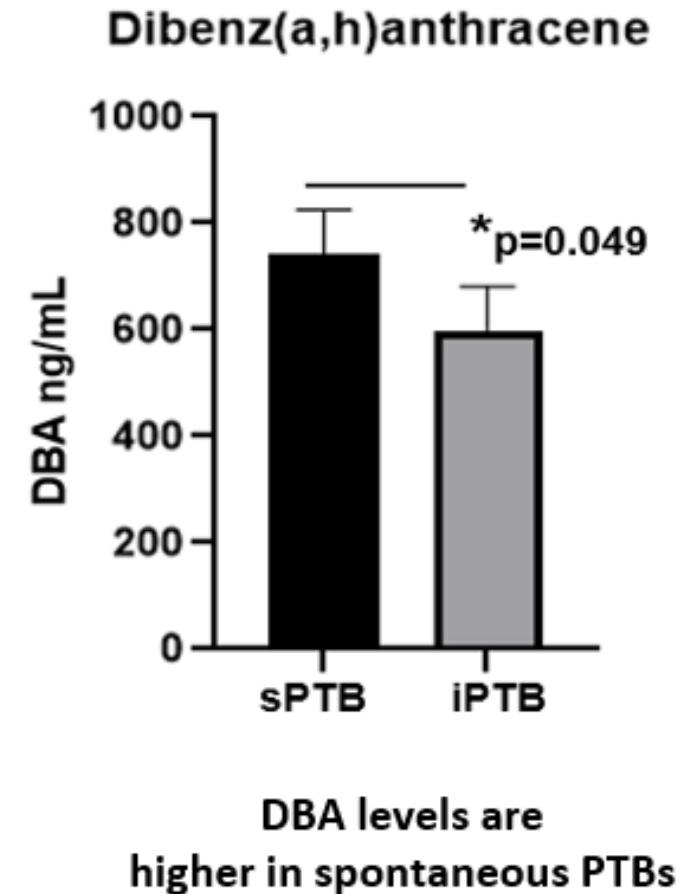


Gwen Hummel
Graduate Student
Baylor College of Medicine
Project 2 Trainee

Project 2 & Research Support Core Collaboration

Maternal PAH exposures are associated with *spontaneous* preterm birth

- Spontaneous vs. indicated preterm birth
- **Spontaneous**- This is when the body goes into labor or the membranes rupture on their own, before 37 weeks of gestation.
- **Indicated**- This is when a healthcare provider decides that continuing the pregnancy is riskier than delivering the baby early.

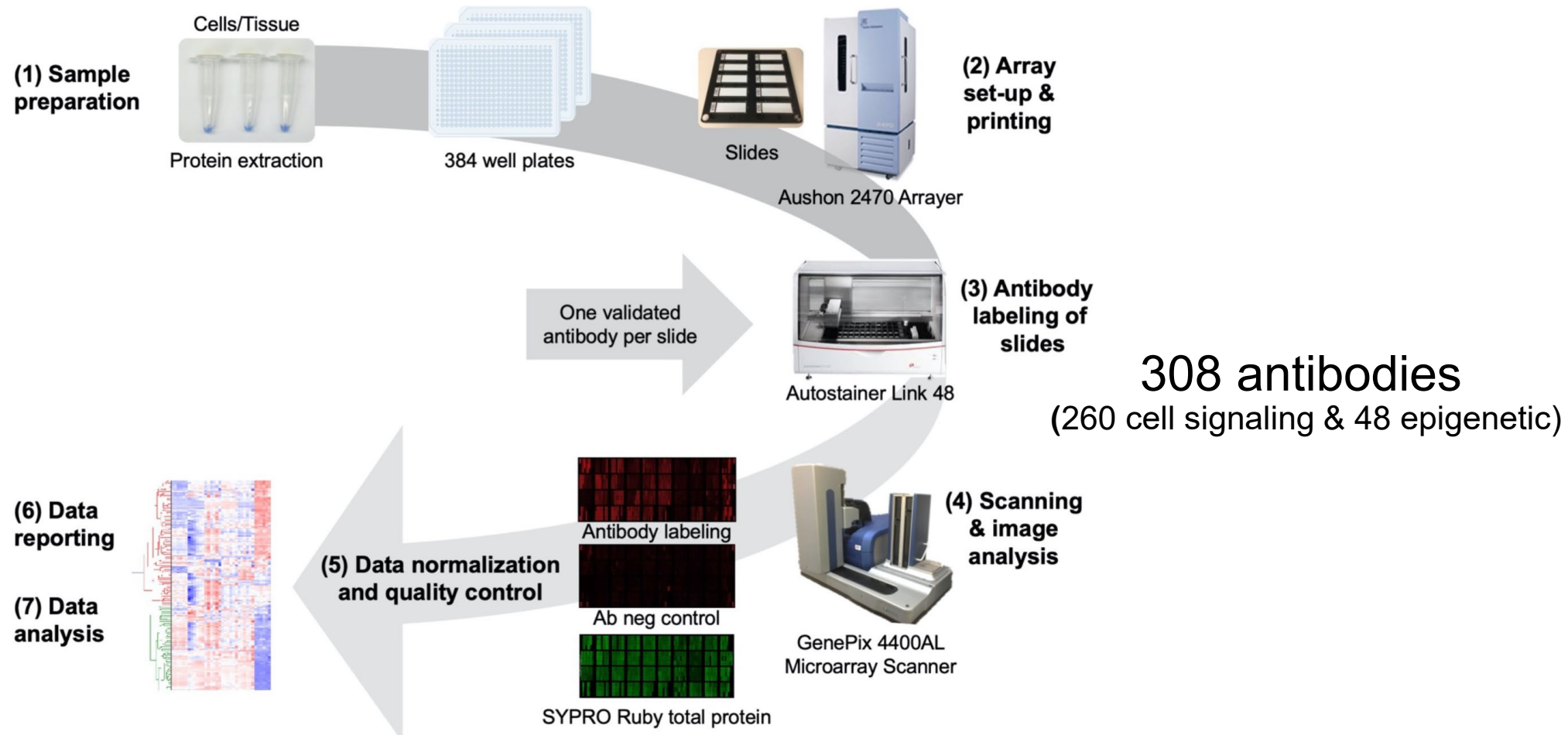


How might PAHs contribute to PTB?

Alterations to the placental proteome

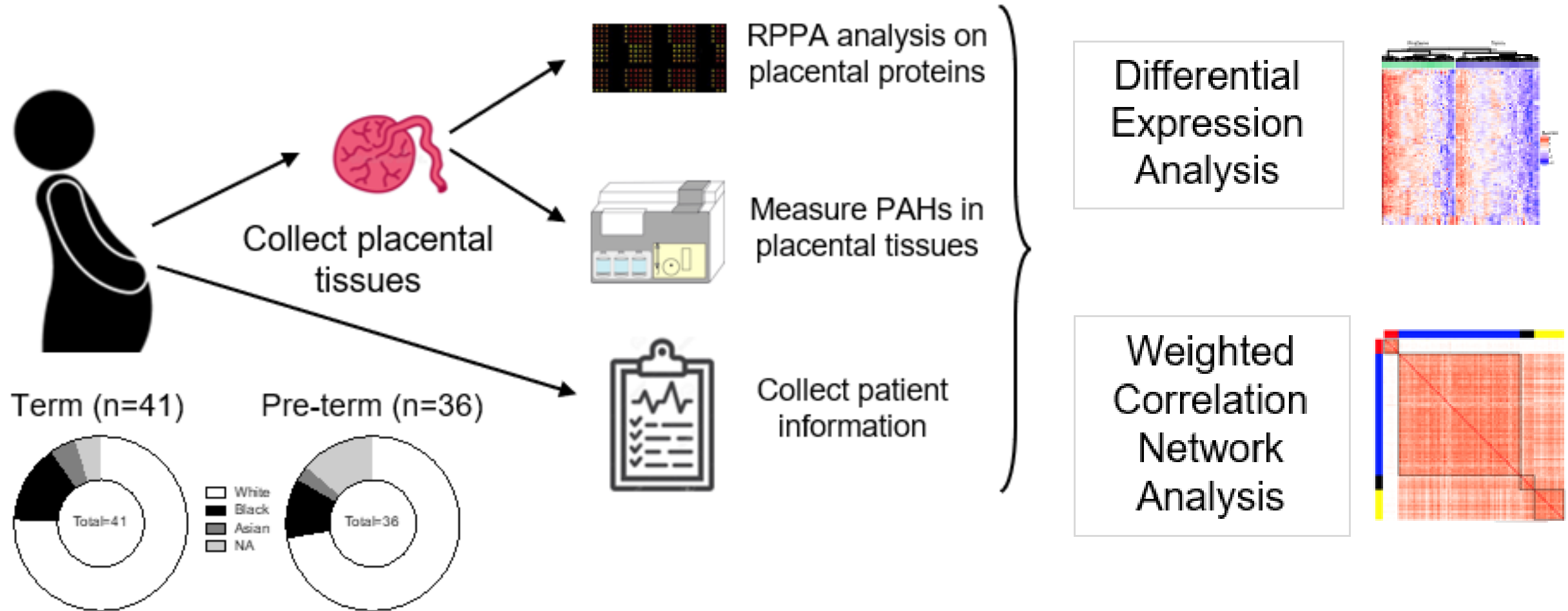
Project 1, RSC & DMAC Collaboration

Reverse phase protein arrays (RPPA): High throughput protein quantification



Project 1 & DMAC Collaboration

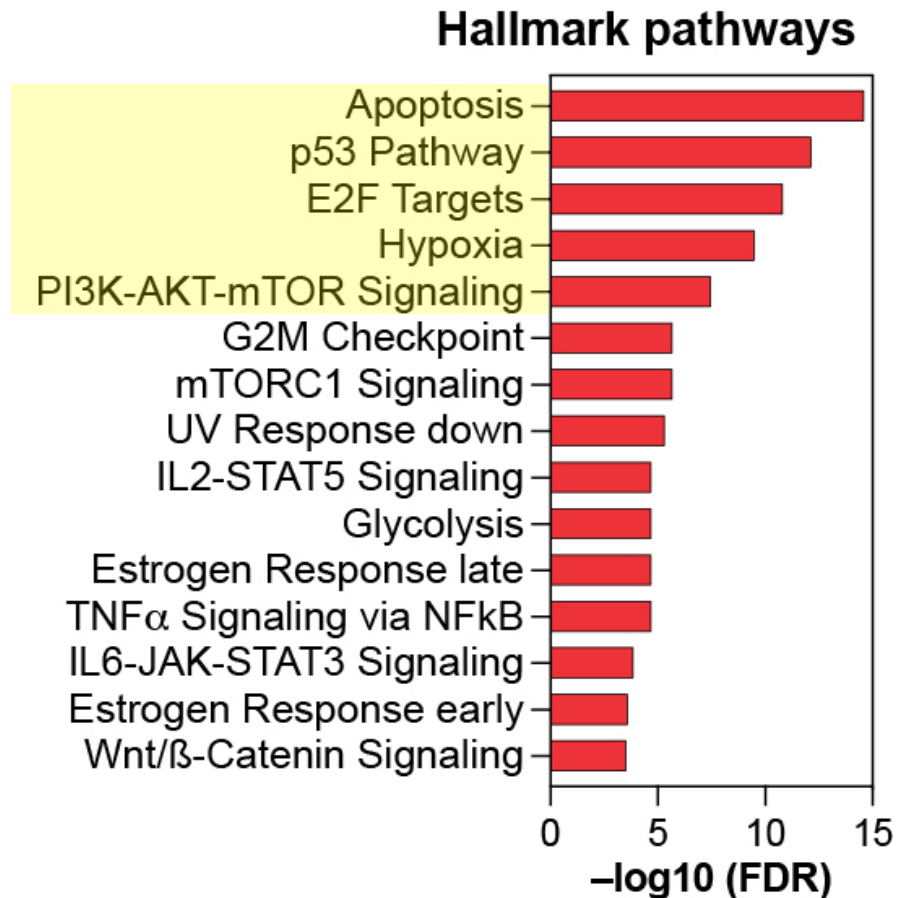
Associations between PAH levels and placenta proteins



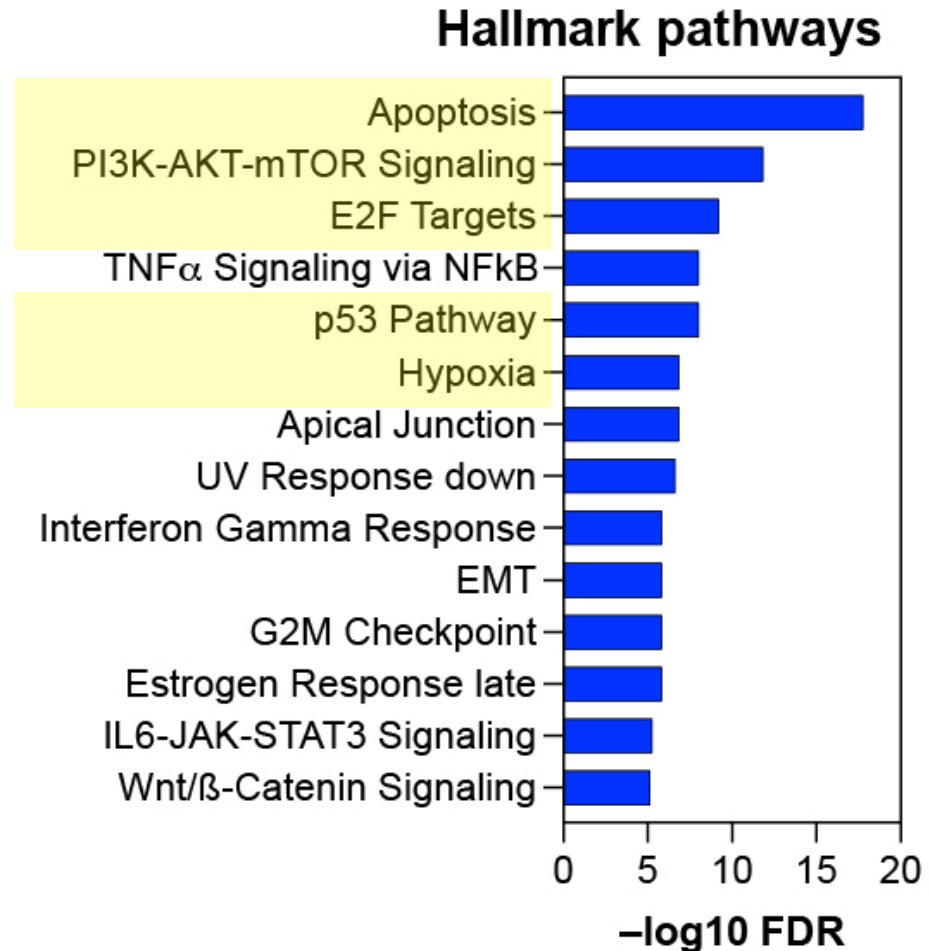
Differential Expression

Similar pathways altered with PTB & PAHs

Preterm vs Term



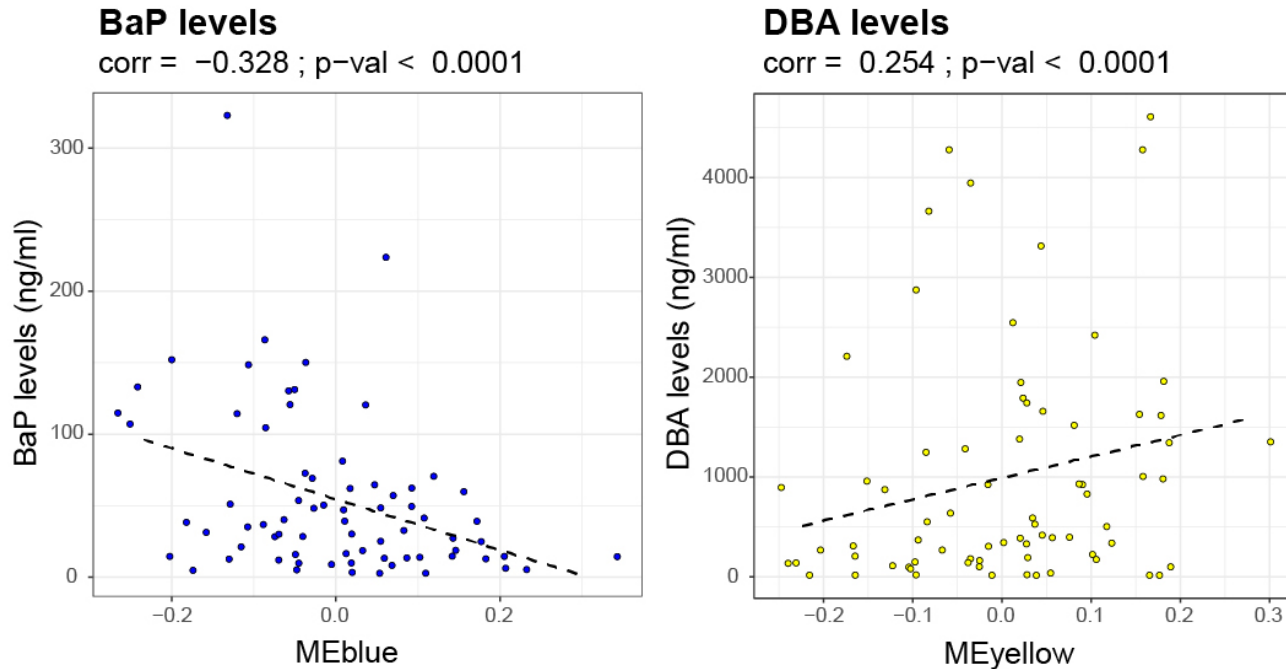
High vs. Low PAHs



Weighted Correlation Network Analysis (WCNA)

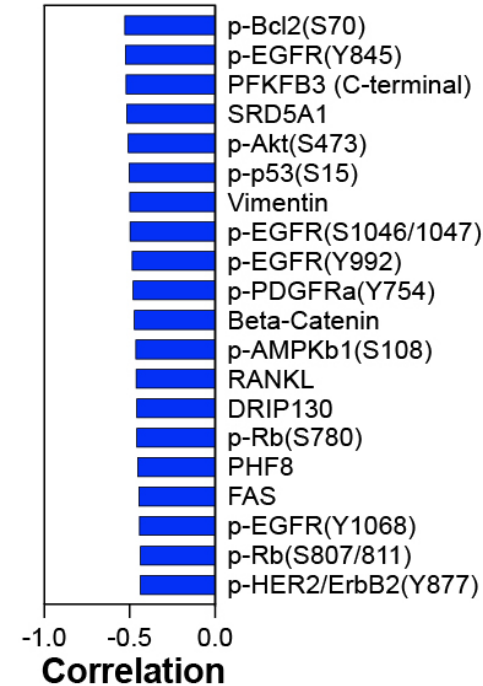
Unique cell signaling changes for each PAH

A WGCNA module-trait correlations

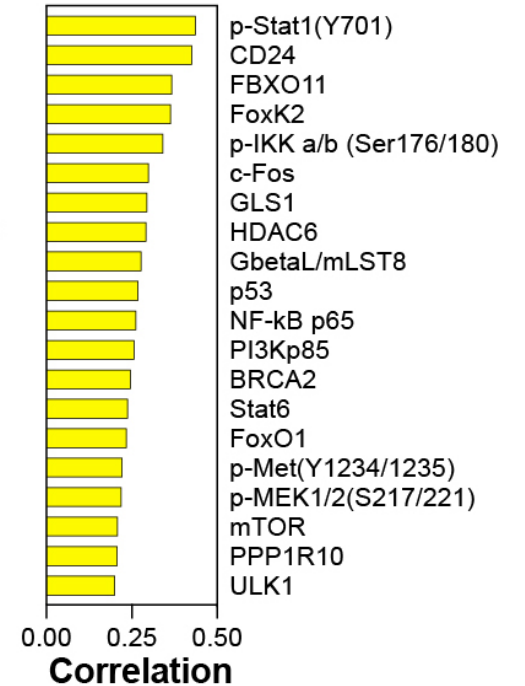


B

BaP top proteins



DBA top proteins



The cellular response is likely unique to individual PAHs

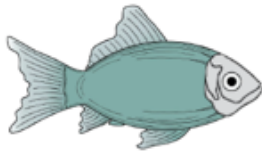
Projects 2 & Community Engagement Core Collaboration

Prenatal Education on Environmental Exposures during Pregnancy Study (PEEPS)

Everything you need to know about Seafood



Seafood at its Finest



Everything You Need to Know About Omega-3 Fatty Acids

Omega-3s are a family of particularly long-chained polyunsaturated fats. These nutrients are essential for human health due to their cardiac, metabolic, visual, and immune benefits. There are three main types of Omega-3:

DHA

DHA is a structural component of the visual and nervous system, and is vital for fetal and infant development.

EPA

EPA produces eicosanoids, which are needed to reduce inflammation, and help reduce the risk of physiological disorders.

ALA

Commonly found in plants, ALA is mostly used for energy storage, and a portion converts into EPA and DHA.

Although humans can manufacture some types of fatty acids in the body, the two fatty acids essential for good health, Omega-3s and Omega-6s, can only be obtained from diets.

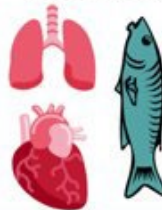
Omega-3

Anti-inflammatory fatty acids, Omega-3s are best found in seafood and plants such as soybean, canola, flaxseed, and purslane

Omega-6

Pro-inflammatory fatty acids, Omega-6s can be found in seafood, but the main source are plants such as sunflower seeds, corn, and soybean.

How does Omega-3 Prevent or Relieve Disease?



Omega-3s control the production of a hormone called eicosanoid, which uncontrolled increases the risk of arthritis, asthma, heart disease, strokes, and other health disorders.

Omega-3 produces anti-inflammatory eicosanoids, while Omega-6 produces pro-inflammatory eicosanoids. This is important to show a balance must be created when consuming seafood - otherwise, there will be an uncontrolled production of eicosanoids. So always remember: **balance your diet!**

Everything You Need to Know About Freezing Fish

Seafood has a limited storage life, which is why the best thing to do for seafood that will not be consumed immediately is to place it in the coldest part of the refrigerator, at temperatures close to 32°F, as soon as possible.

Steps to Freeze Fish

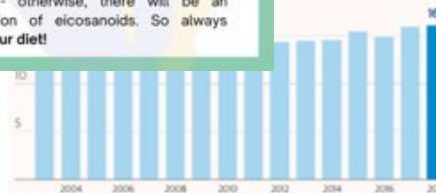
- Clean, rinse, and pat dry fish
- Wrap with plastic wrap, excluding as much air as possible
- Wrap a second time with freezer wrap, a freezer bag, or aluminum foil

Additional Recommendations

- Seal, label, and date all seafood products before putting them in the freezer
- When consuming seafood, use the older labeled seafood first
- Aim to consume within 3 to 6 months from purchase date

Seafood Consumption Cont.

in pounds

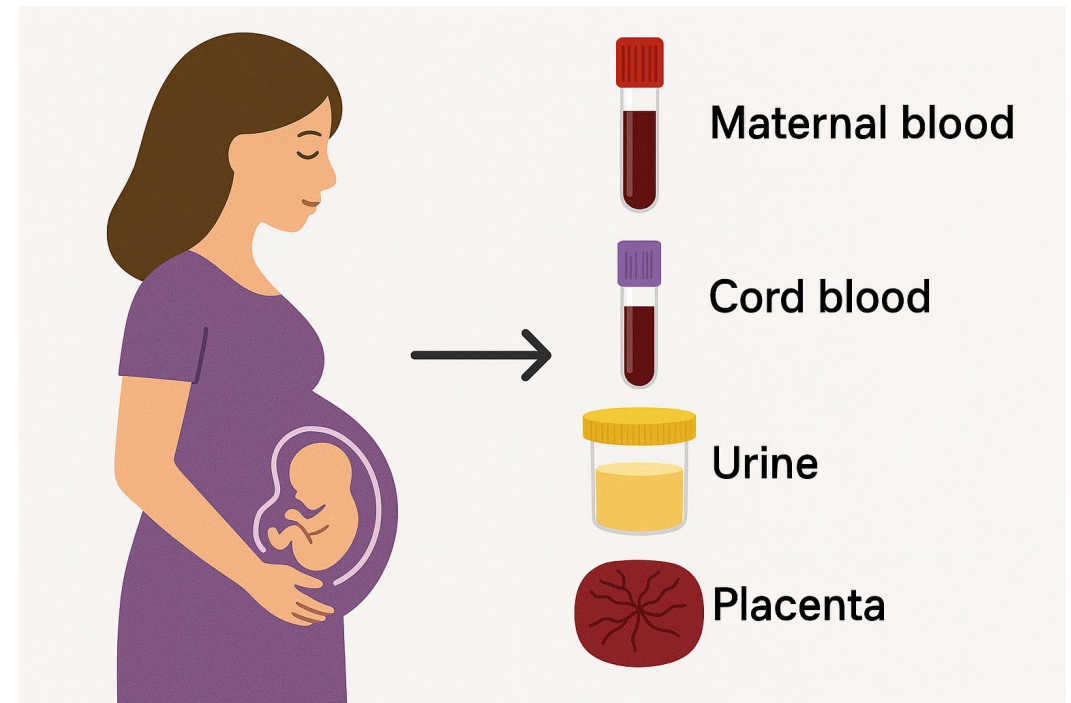


Per Capita consumption in pounds
Chart: NOAA - Source: NOAA

Projects 2 & 3 Collaboration

Prospective birth cohort study design

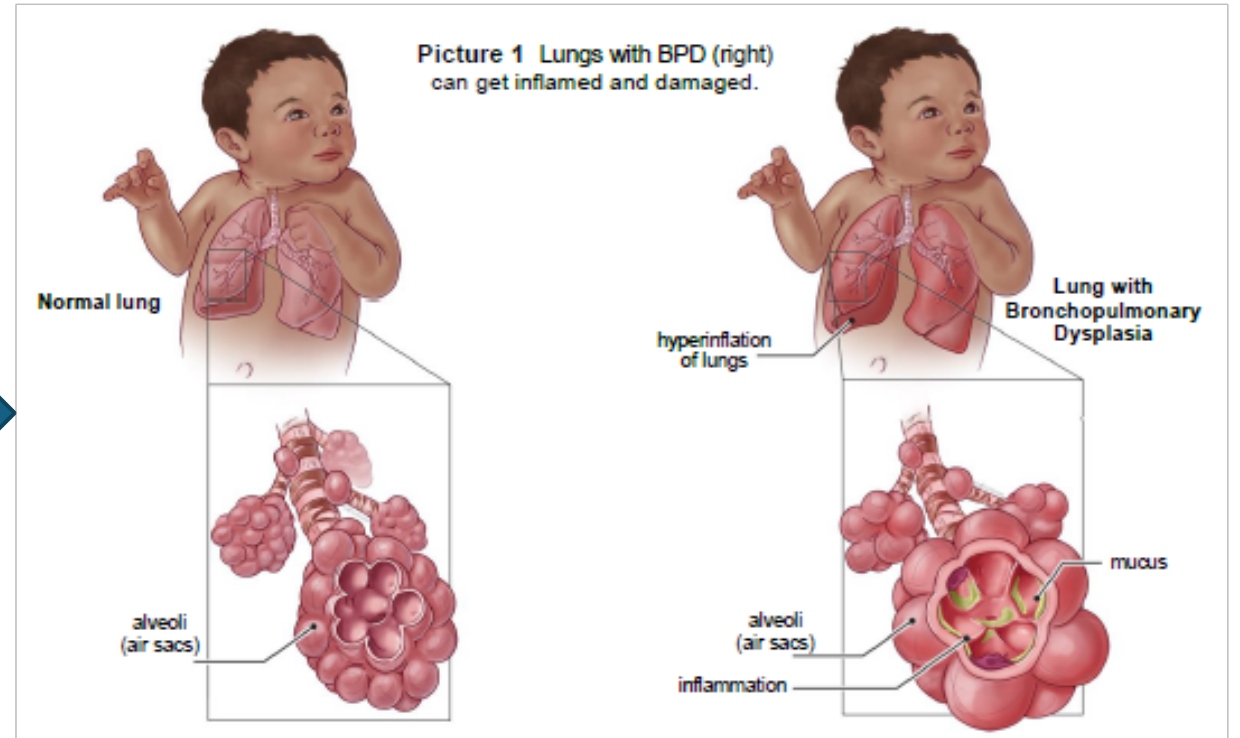
- Enroll moms in L&D or before a Cesarean delivery and collect maternal and cord serum, urine and placenta
- If the baby goes to the [NICU](#), consent for collection of tracheal aspirates, (scavenged) neonatal blood and breastmilk
- Prospective study design so that address-level/ nearest intersection data can be collected



Project 3. Uncovering molecular changes in neonatal lungs after in utero exposure to PAHs

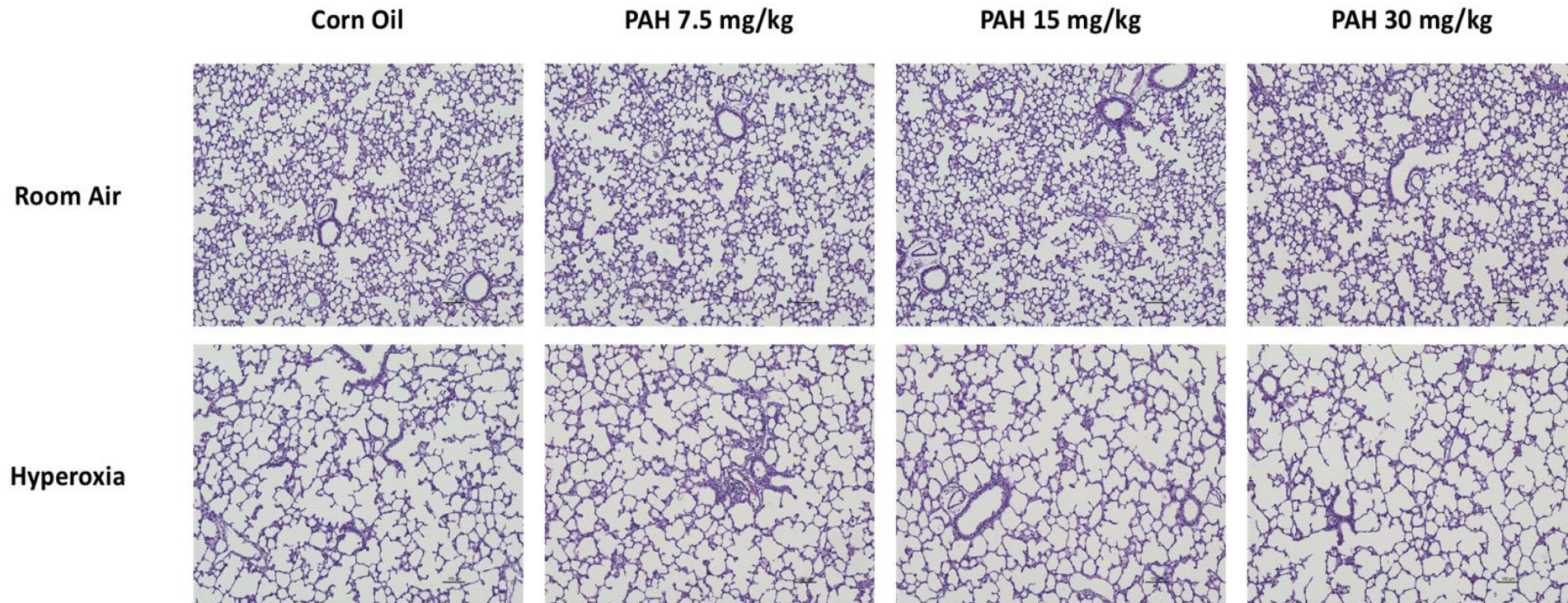


In 2021, **1 in 10** babies was born too early in the United States.

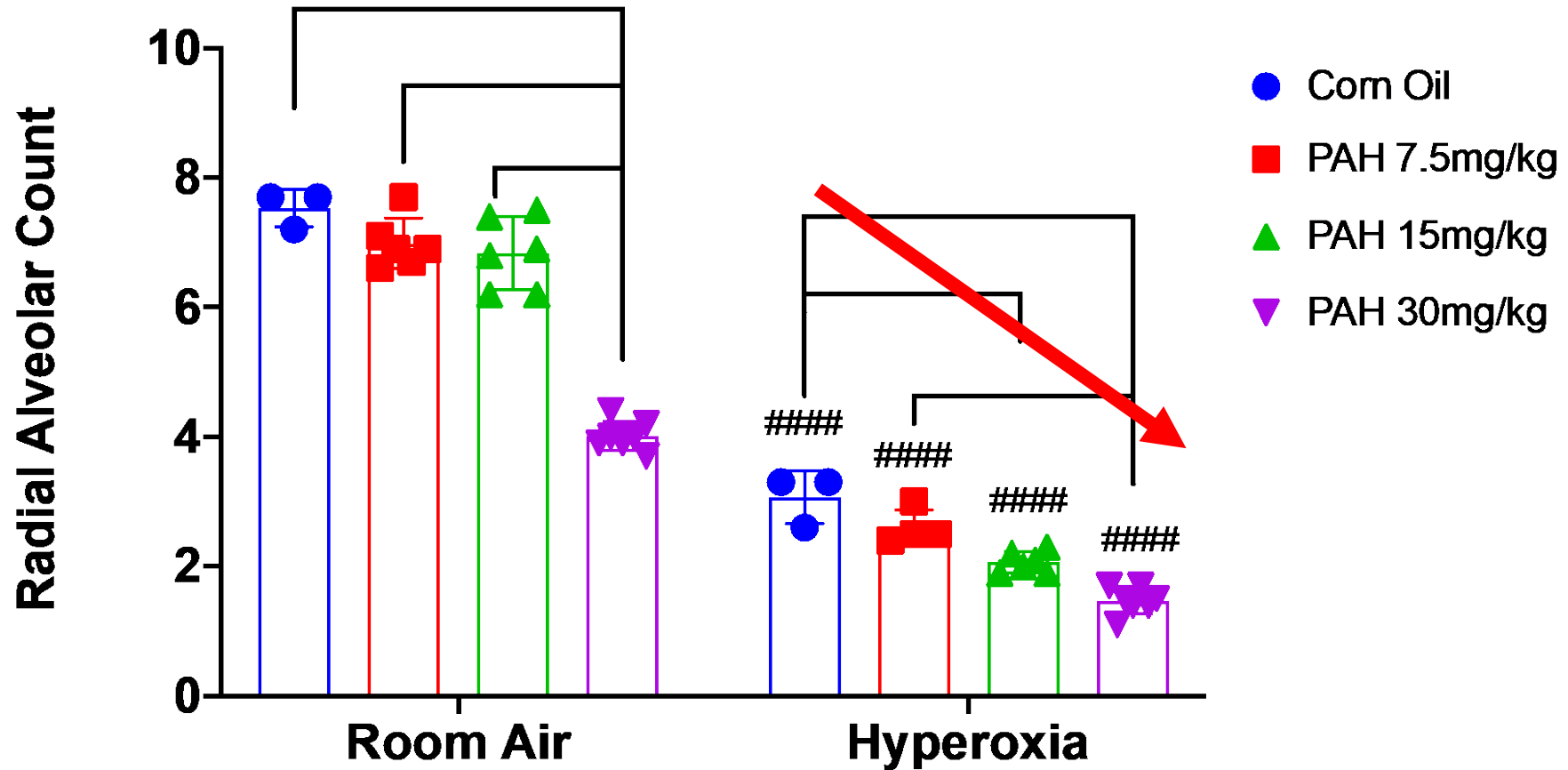


Supplemental oxygen can induce lung injury and bronchopulmonary dysplasia (BPD)

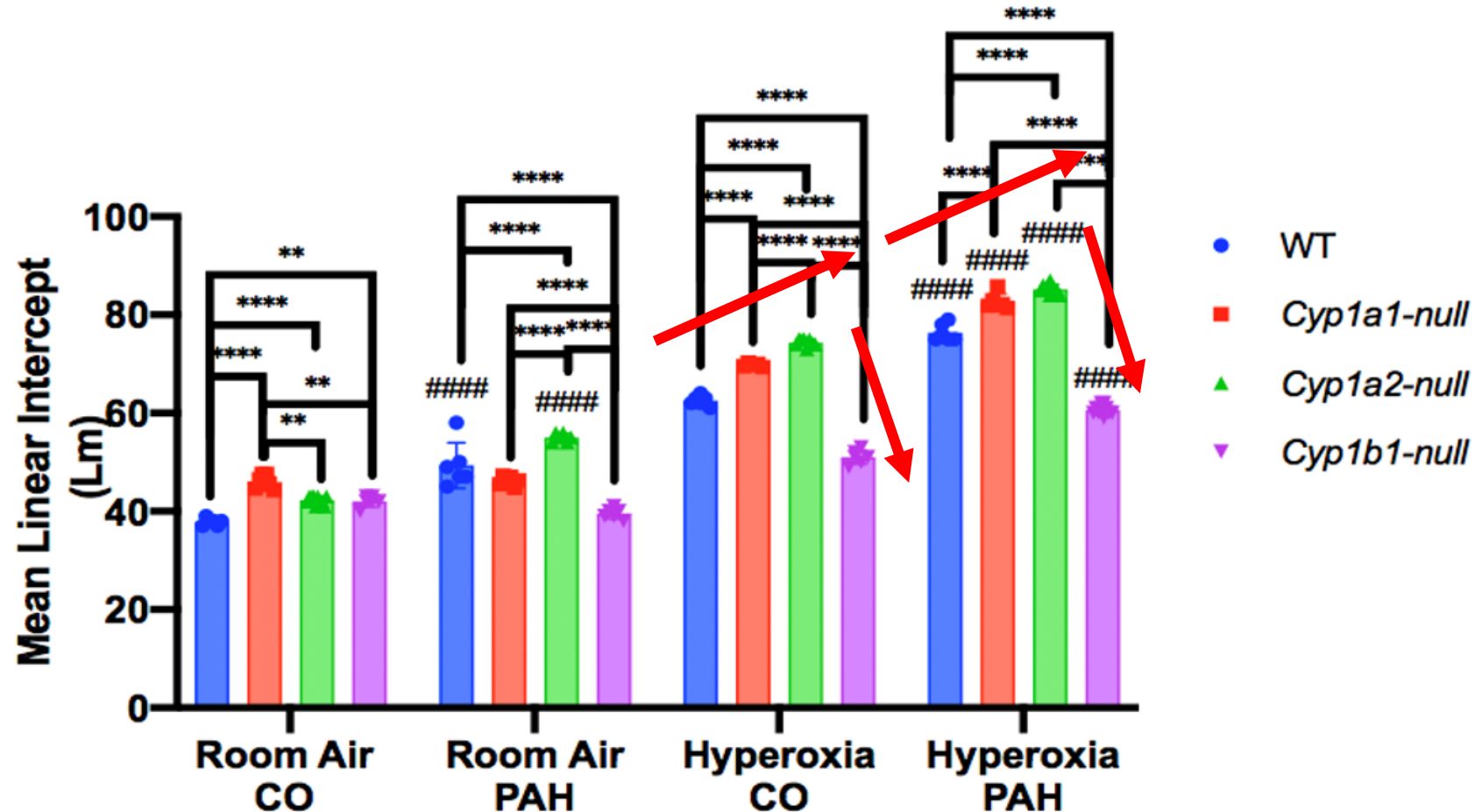
Prenatal PAH exposure exacerbates hyperoxic lung injury in neonatal mice



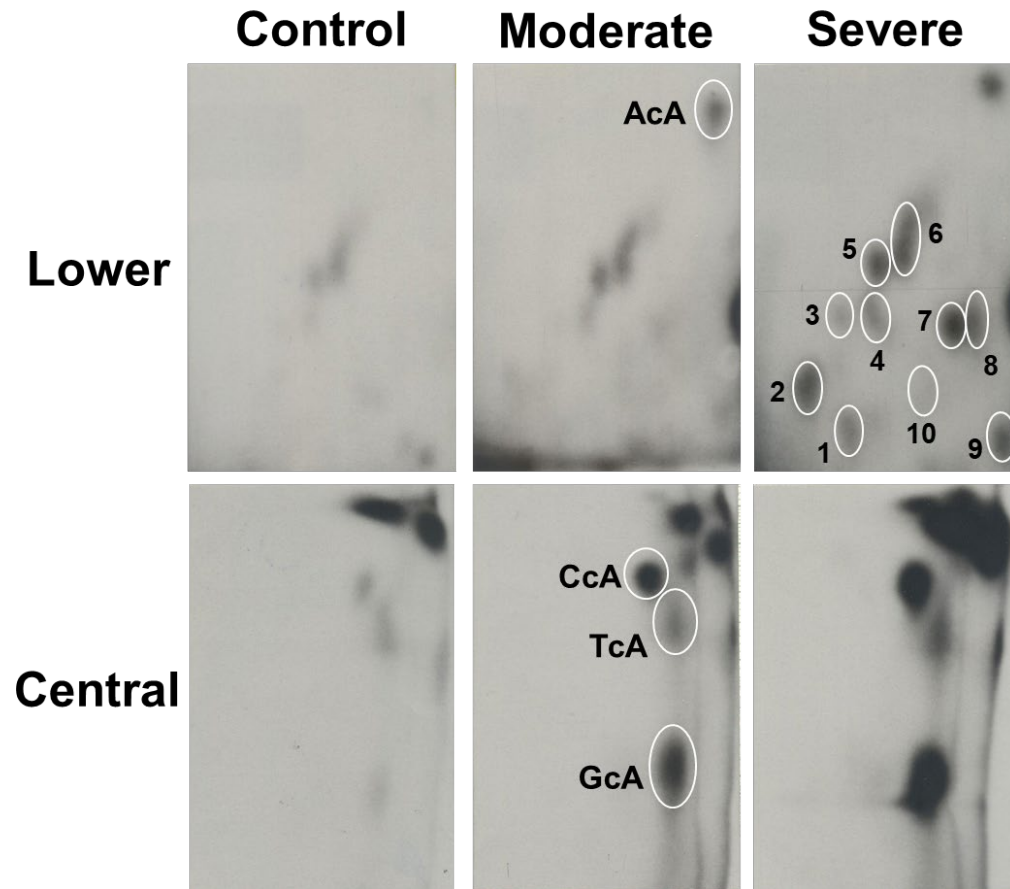
Histological analysis of prenatal PAH exposure on hyperoxic lung injury in WT mice



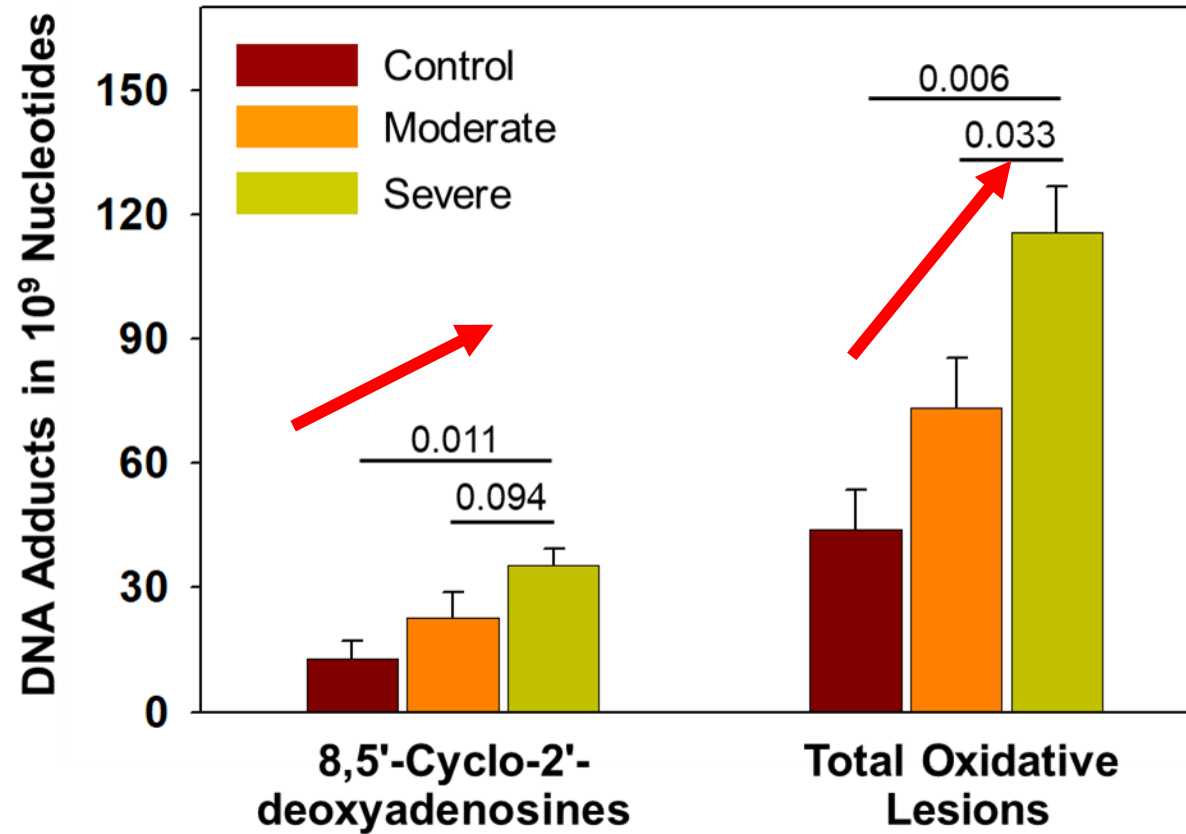
Histological analysis of prenatal PAH exposure on hyperoxic lung injury in WT, *Cyp1a1*-null, *Cyp1a2*-null, *Cyp1b1*-null mice



Representative DNA adduct profiles in tracheal aspirate from BPD patients

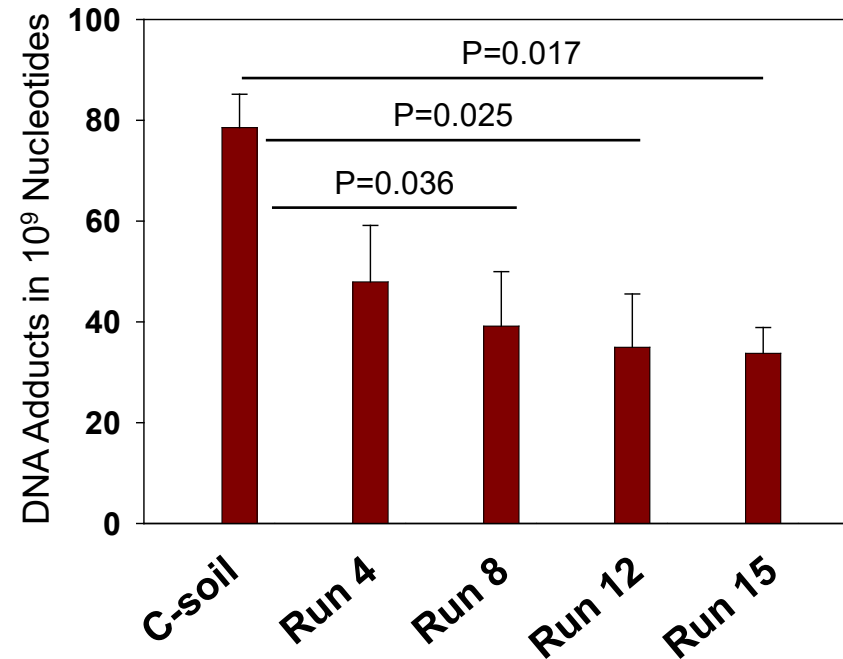
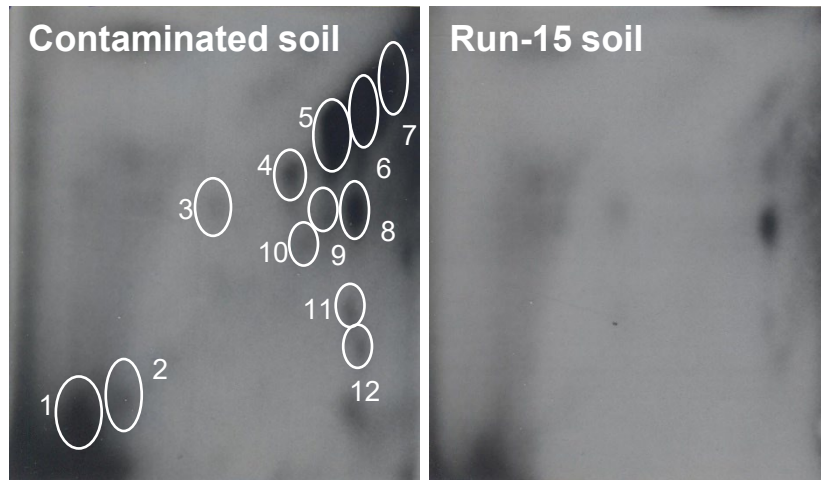


Levels of DNA adducts in tracheal aspirate from BPD patients



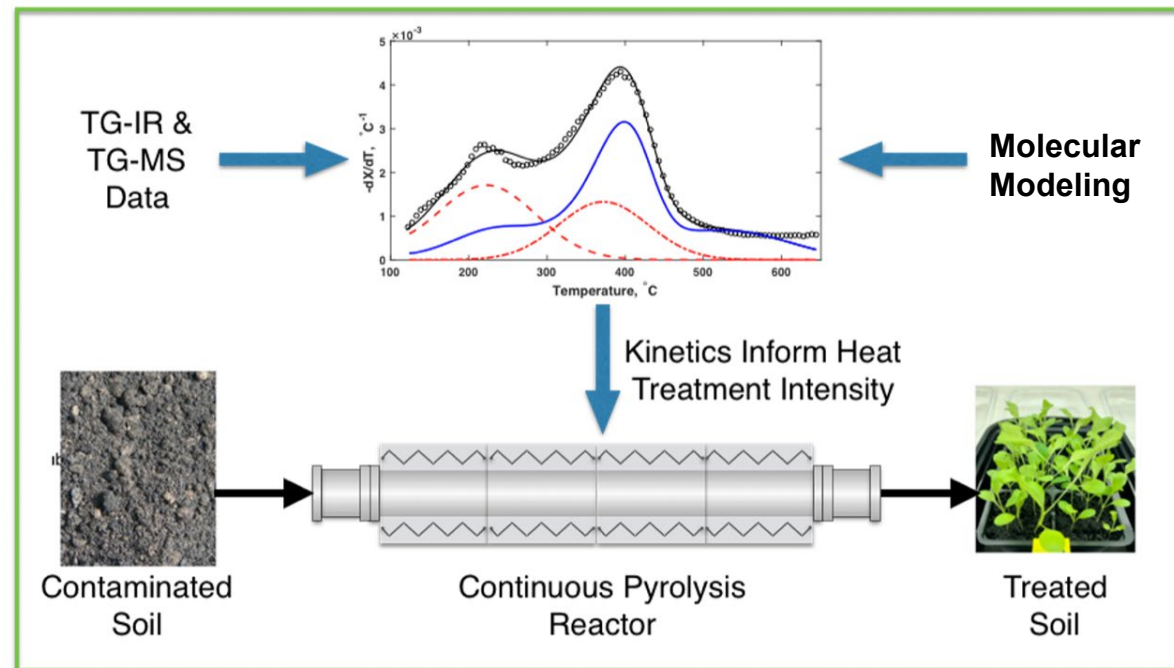
Projects 3 & 4 Collaboration

DNA adducts of mice treated with soil extracts from Superfund sites before and after remediation



Project 4. Pyrolytic Treatment of PAH-Contaminated Soils to Eliminate Toxicity and Enhance Soil Fertility

Pyrolysis of contaminated soils converts PAHs into char, meeting cleanup standards, eliminating toxicity and enhancing soil fertility. Common transition metals (e.g., Fe(III)) can catalyze pyrolytic degradation and decrease required temperature and contact time to significantly decrease energy requirements.



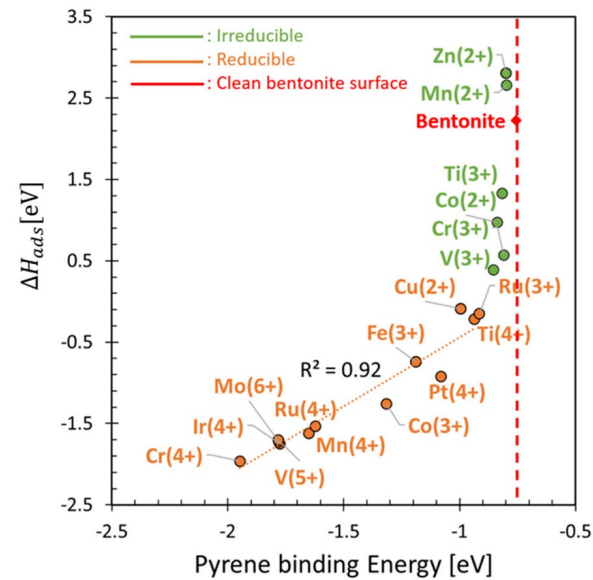
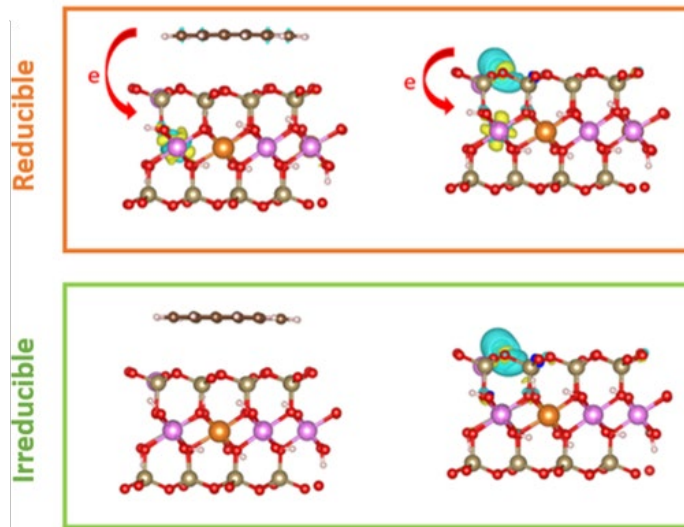
Benefits: Unprecedentedly mild treatment temperatures decrease required energy; shorter contact times increase throughput capacity.

Treated soil remain fertile for regreening efforts

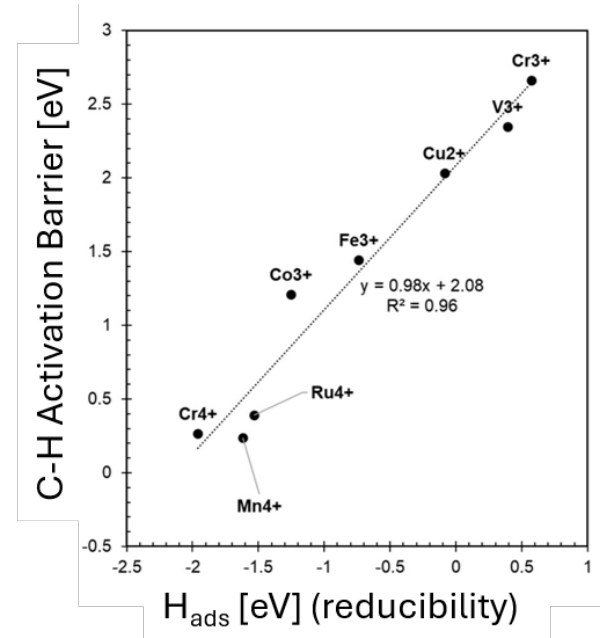
DFT calculations reveal how the metal cation center reduced the PAH degradation temperature

The metal cation center accepts an electron from the PAH

PAH binding energy correlates directly to the C-H activation energy



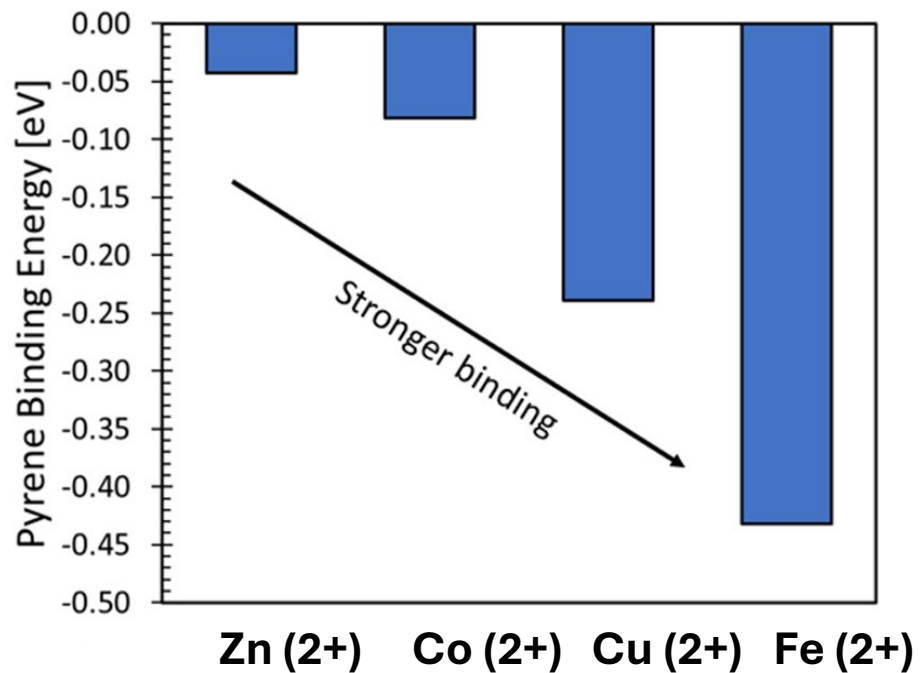
→ Effectiveness of the cation site for binding PAH can be predicted based on site reducibility



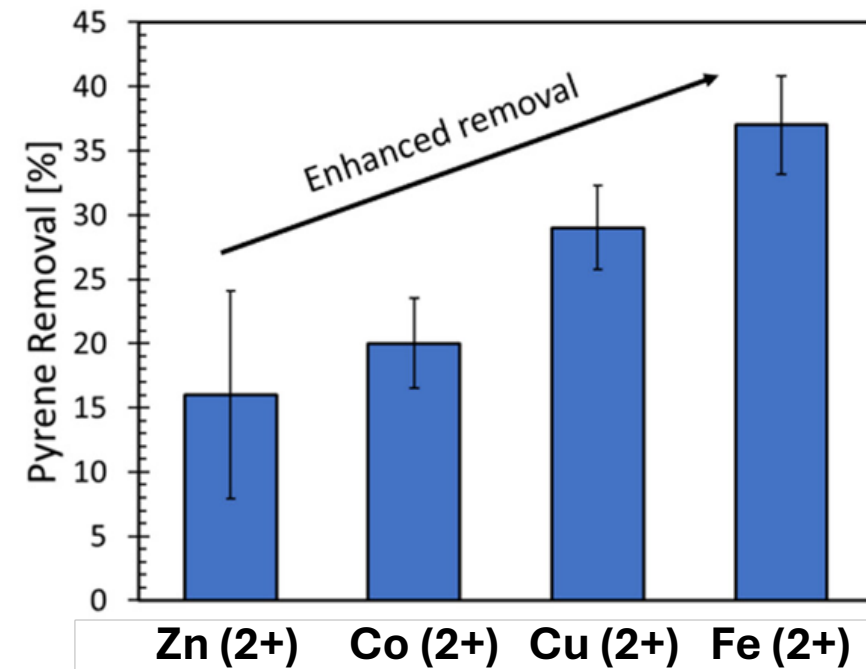
→ Effectiveness of the cation site for PAH activation can be predicted based on site reducibility

Excellent agreement between model and experiment

Predicted PAH degradation trend



Experimental PAH degradation trend



→ PAH degradation trends predicted by the DFT model agree with experimentally observed trends

Projects 1 & 4 Collaboration.

Enhanced detection of PAHs before and after soil remediation



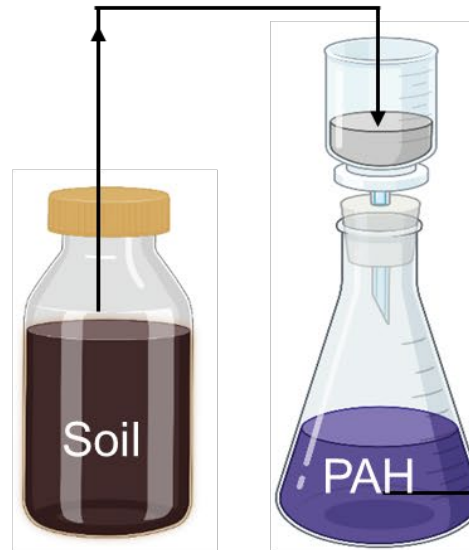
Thomas Senftle

Yilong Ju, Oara Neumann, Sara Denison, Peixuan Jin, Andres B. Sanchez-Alvarado, Peter Nordlander, Thomas P. Senftle, Pedro J. J. Alvarez, Ankit Patel, and NJH PNAS (2025).

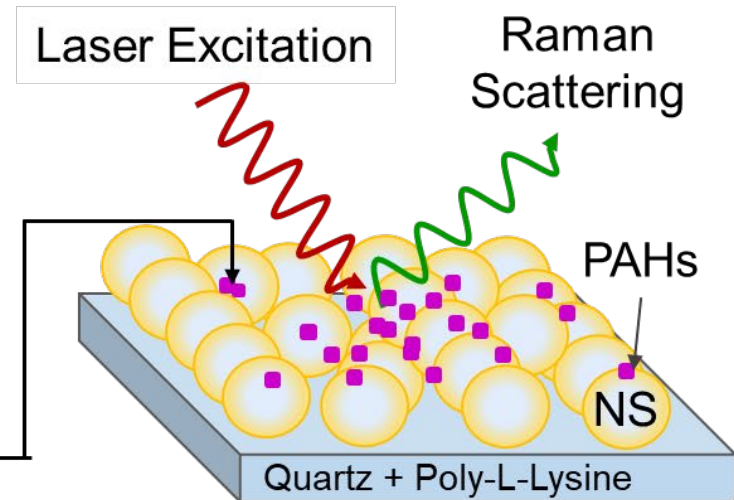


Peixuan Jim

Sample Collection and PAHs Extraction



SERS Substrate Preparation



pyrene, anthracene contamination

Community Engagement Core

Hydroponics/Urban Gardening Project

GARDENS FOR REDUCING EXPOSURES AND ENHANCING NUTRITION - HYDROPONICS AND AQUACULTURE FOR URBAN SUSTAINABILITY (GREEN HAUS)

- Establish an aquaponics prototype as a proof-of-concept for efficient, affordable fish and produce production in communities facing food insecurity or soil/water contamination.
- Engage underserved communities through soil and water sampling to identify environmental hazards affecting food production.
- Provide educational workshops on aquaponics and offer resources to help partners develop their own self-sustaining systems.



Community Responsive Studio

Perspectives of Community Members Near Superfund Sites



Conclusions

- Ultra-sensitive detection methods, coupled to machine learning technologies, can enhance detection of environmental chemicals in human tissues
- Exposure to PAHs in pregnancy is associated with adverse pregnancy outcomes, including spontaneous preterm birth
- Exposure to PAHs in pregnancy can make the lung injuries experienced by premature infants worse
- Pyrolysis is a low cost, effective method for large scale remediation of soils
- Collaborative science, combining engineering, physics, chemistry, computer science and the biomedical sciences improves discovery

Baylor College of Medicine- Rice Superfund Research Program



BCM-RICE
SUPERFUND
RESEARCH
PROGRAM



RICE



National Institute of
Environmental Health Sciences
Superfund Research Program

5P42ES027725-07