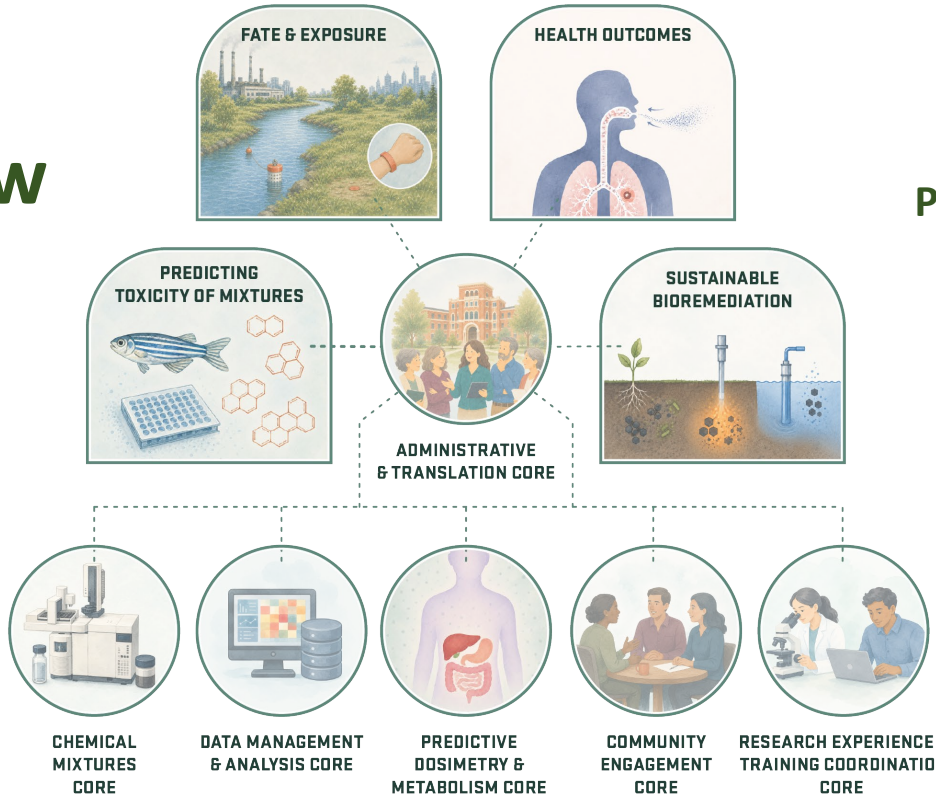
The Center for Science, Technology and Emerging Health Risks of PAHs

Robyn Tanguay, Director

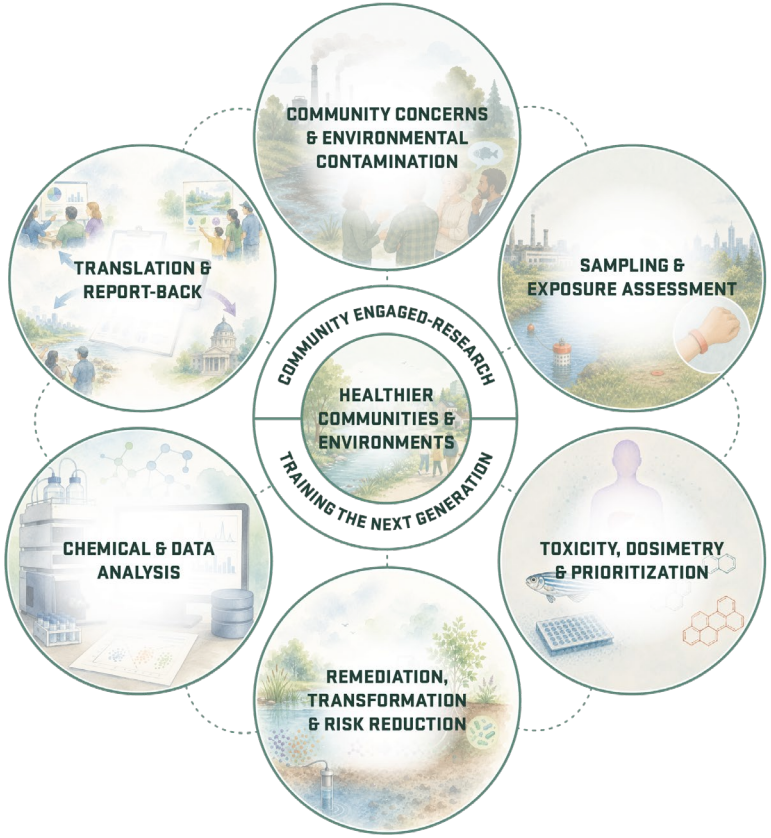
Center Overview



Projects

Support Cores

Integrated Research Process



Evaluation of Pure Bacteria Cultures that Initiate the Oxidation of Alkylated and Non-alkylated PAHs with Either Monooxygenase or Dioxygenase Enzymes

Lewis Semprini

School of Chemical, Biological, and Environmental Engineering

Oregon State University

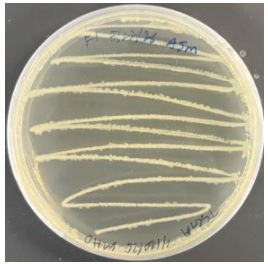
SRP Progress in Research Summer 2026 Webinar Series

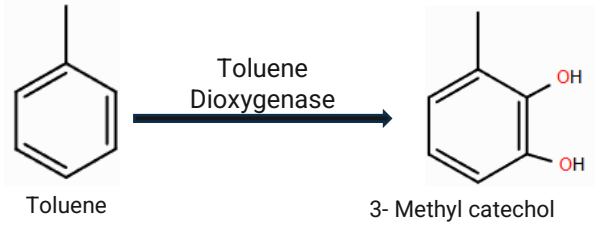
June 1, 2026

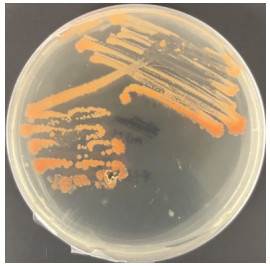
Pure Bacteria Cultures Used to Investigate the Transformation of PAHs and the Production of Transformation Products

Dioxygenase

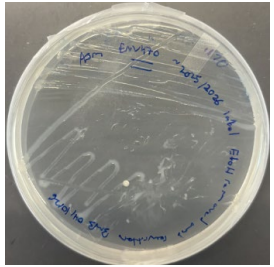
Pseudomonas putida F1

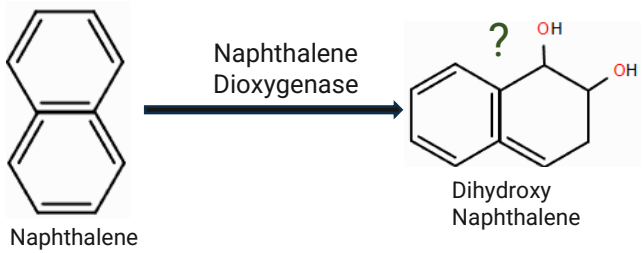


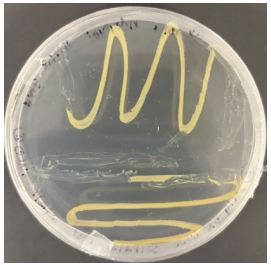




ENV 470

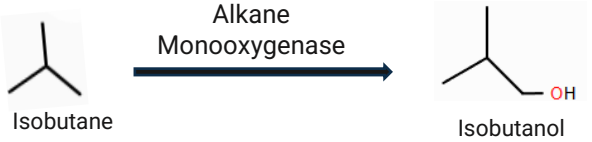




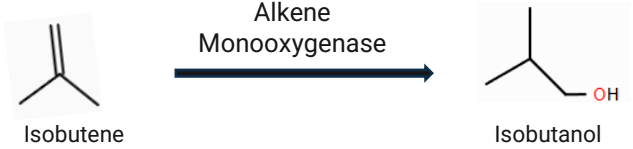


Monooxygenase

Rhodococcus Rhodochrous ATCC 21198



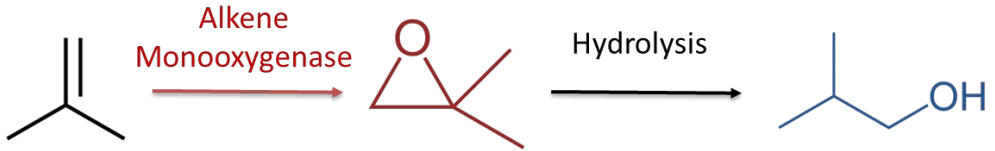
Mycobacterium sp. ELW1



Formation of Developmentally Toxic Phenanthrene Metabolite Mixtures by Mycobacterium sp. ELW1

Schrlau et al. ES&T 2017, 51:8569-8578

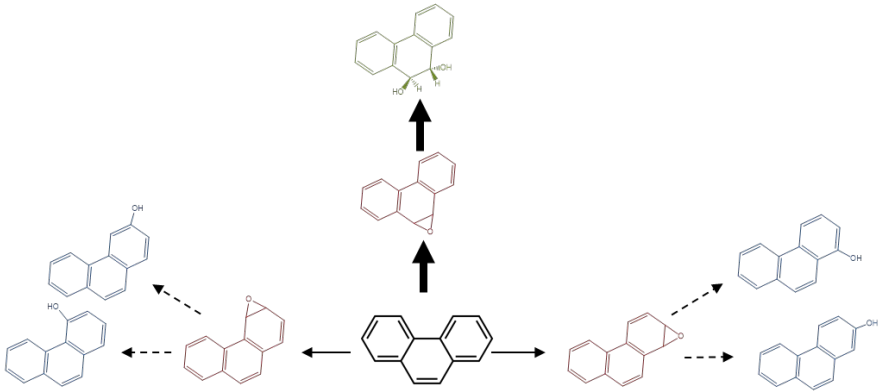
Mycobacterium Strain ELW1

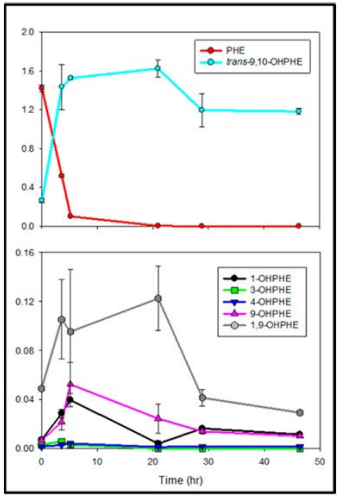


Isobutene
(Primary growth substrate)

Isobutene epoxide

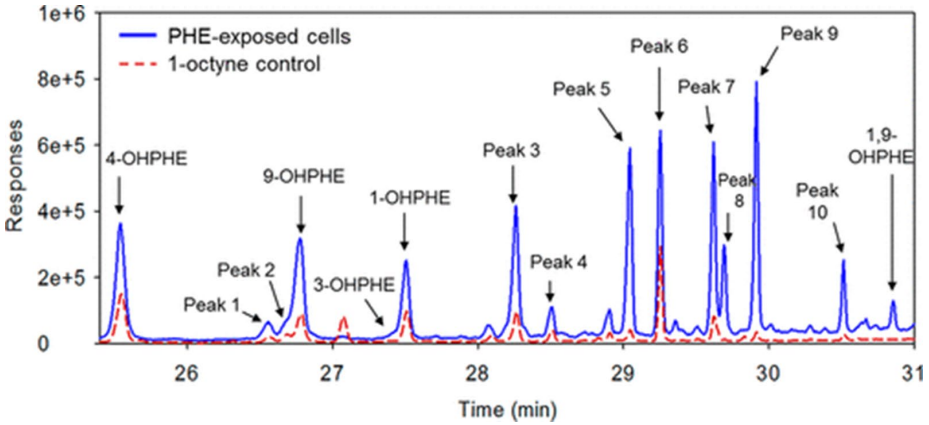
Isobutanol



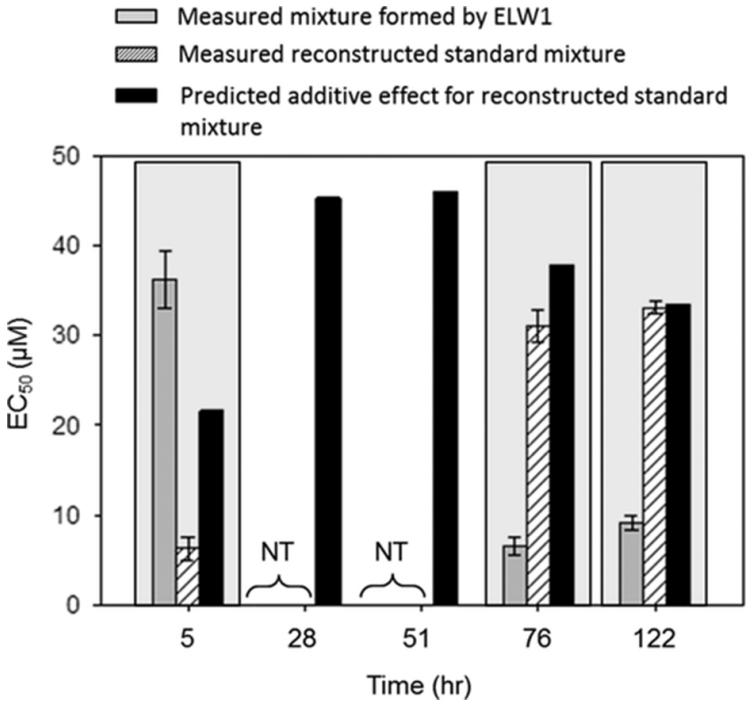


- Methods used for chemical analysis include solid phase extraction, N_2 concentration, derivatization, GC/MS

Embryonic Zebrafish Assays of Cometabolic Mixtures formed by ELW1 Transformation of Phenanthrene and Reconstructed Standard Mixtures



Full scan chromatogram between ~26–31 min for derivatized PHE-exposed cells and 1-octyne controls collected at 122 h



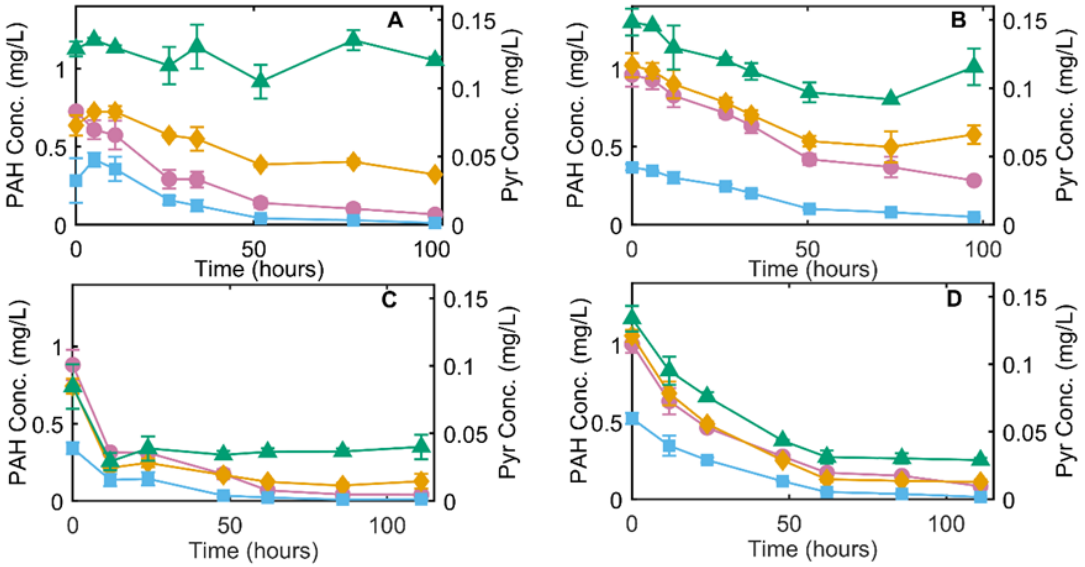
Schrlau et al. ES&T 2017, 51:8569-8578

PAH bioremediation with *Rhodococcus rhodochrous* ATCC 21198: Impact of cell immobilization and surfactant use on PAH treatment and post-remediation toxicity

Huizenga et al. JHM 2024, 470:134109

Set 1:
Suspended Cells

Set 2:
Suspended Cells + TW80



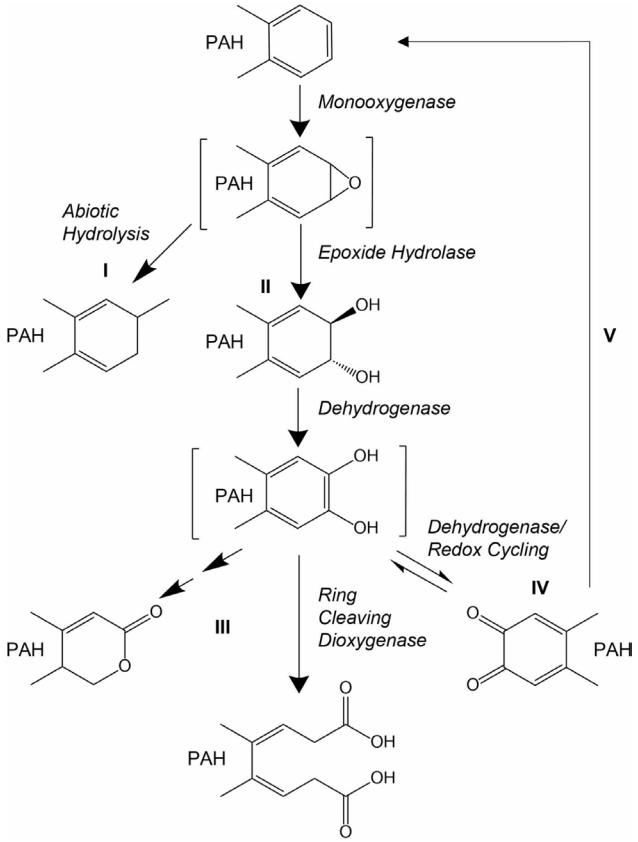
Set 3:
Immobilized Cells

Set 4:
Immobilized Cells + TW80

- Significant degradation of LMW PAHs
  - Ant>Flu>Phe>>Pyr
- Immobilized cells outperformed suspended cells
- Tween 80 improved Pyr degradation

Proposed generic pathway for PAH transformation by *Rhodococcus rhodochrous* ATCC 21198

Huizenga et al. JHM 2024, 470:134109 and Huizenga et al. ES&T 2025, 23:46-58



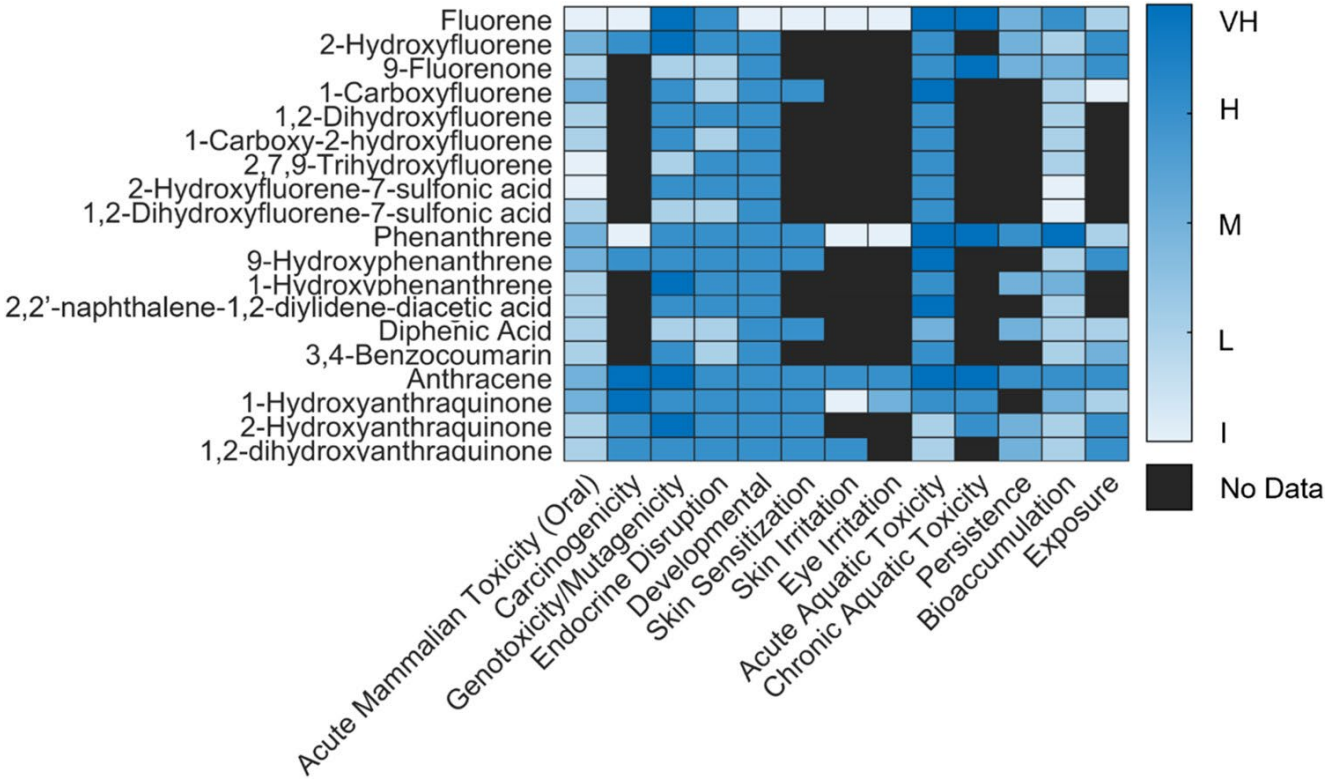
Ultra-high performance liquid chromatography (UPLC – Sciex ExionLC AD) coupled to high-resolution mass spectrometry (HRMS – Sciex ZenoTOF 7600) were used for the identification of PAH transformation products

Compounds in brackets represent undetected intermediates, while others represent compound classes identified in treated samples with high confidence:
I – hydroxylated, II – dihydroxylated, III – ring fission, IV – quinone, and V – hydroxy-/dihydroxy-quinone

Nontarget screening approaches allowed the tentative identification 16 PAH transformation products

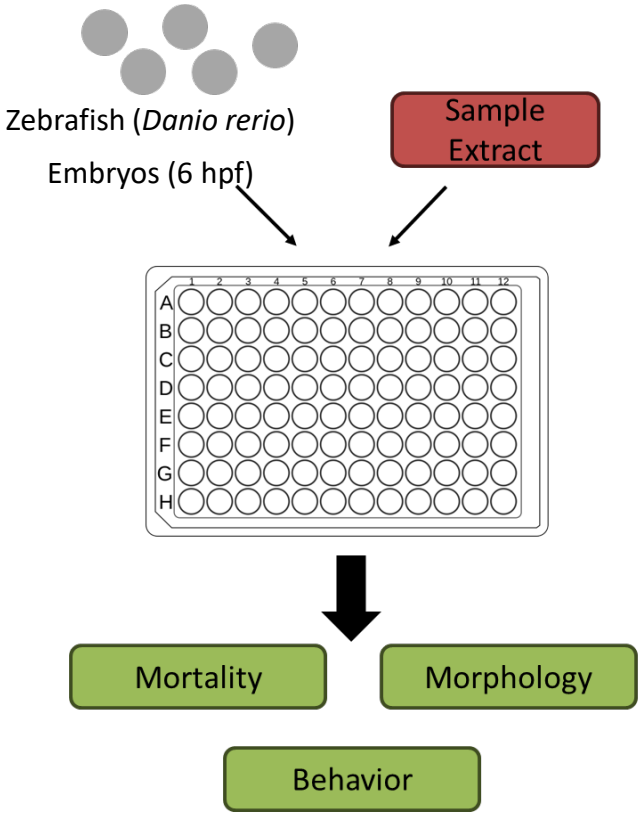
Heatmap of the predicted toxicity of the PAH-TPs and their parent compounds by the US EPA Hazard Cheminformatics Module (HCM)

Huizenga et al. ES&T 2025, 23:46-58



Results of Post-Remediation Toxicity Testing

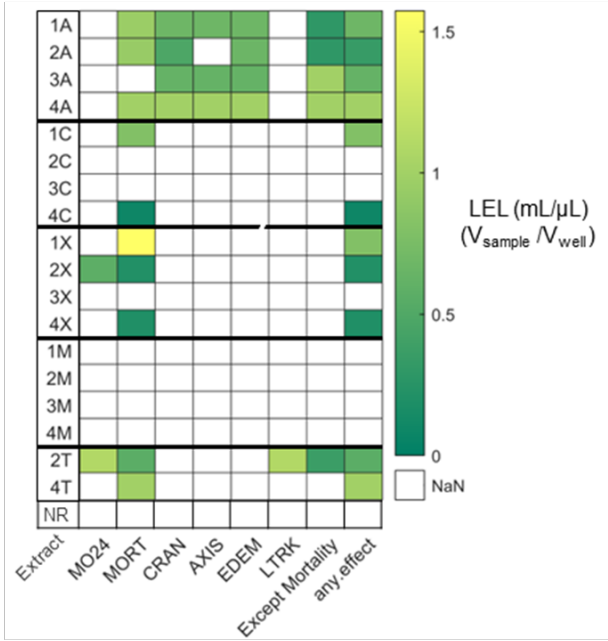
Huizenga et al. JHM 2024, 470:134109



Lowest Effect Level (LEL) = lowest dose where adverse effect was observed

Lower the LEL -> higher the toxicity

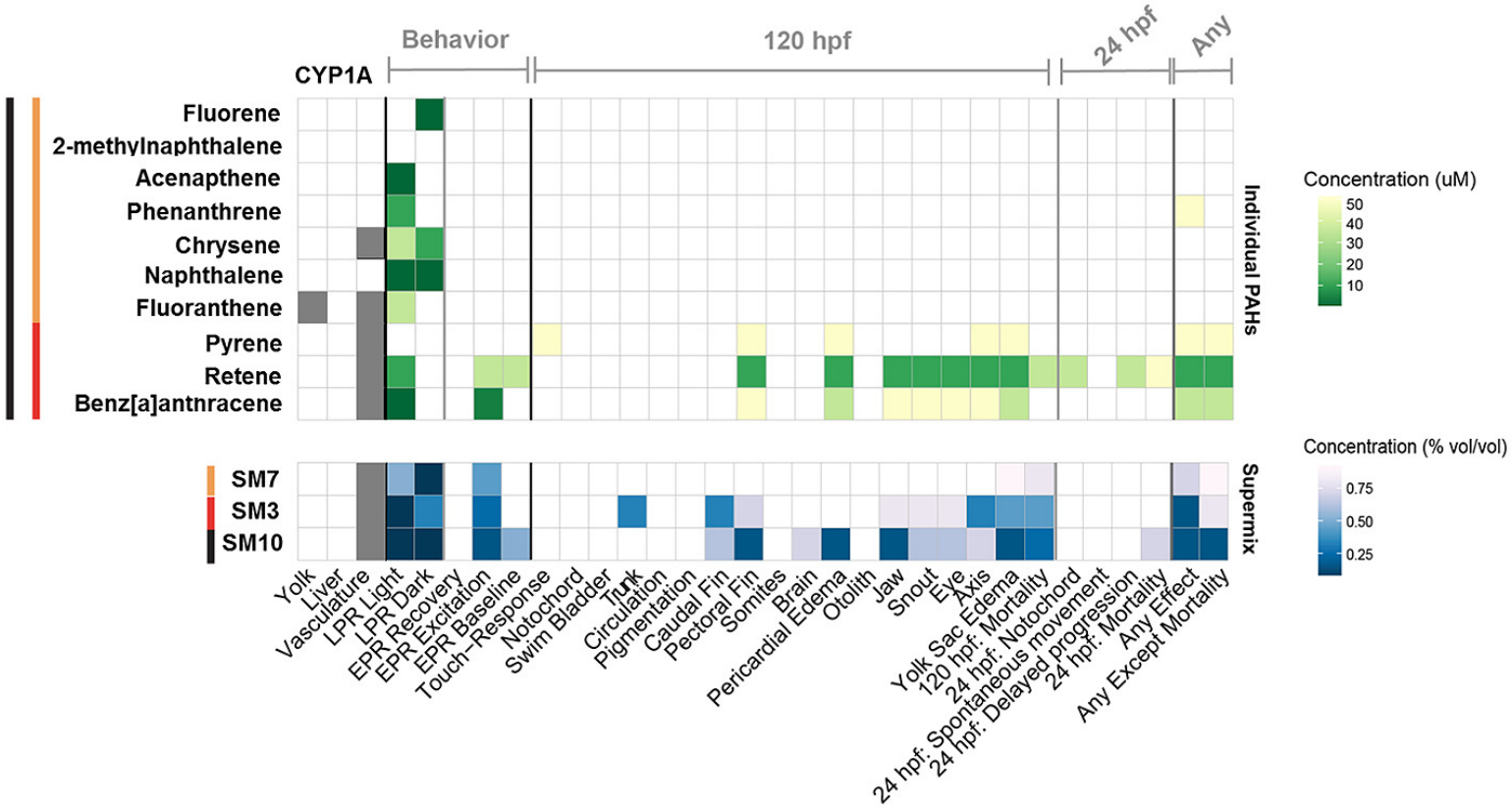
$$\frac{\text{Sample Volume}}{\text{Well Volume}}$$



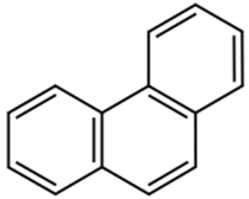
Active (A), autoclaved control (C), abiotic control (X), media extraction blanks (M), T80 control (T), and not remediated (NR)

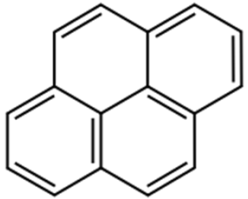
Systematic developmental neurotoxicity assessment of a representative PAH Superfund mixture using zebrafish

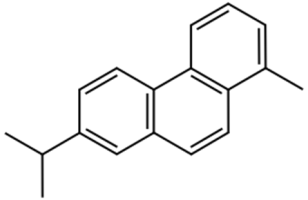
Geier et al. Toxicology and Applied Pharmacology 2018, 345:115-125

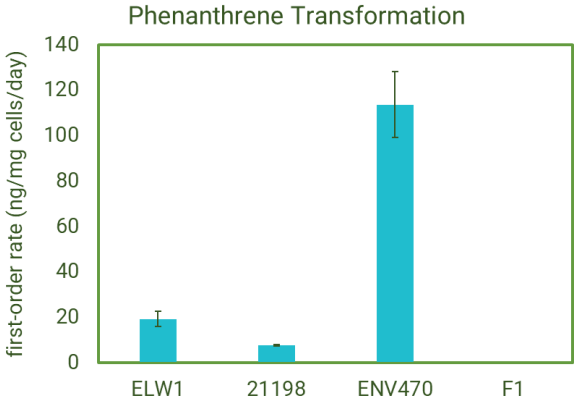


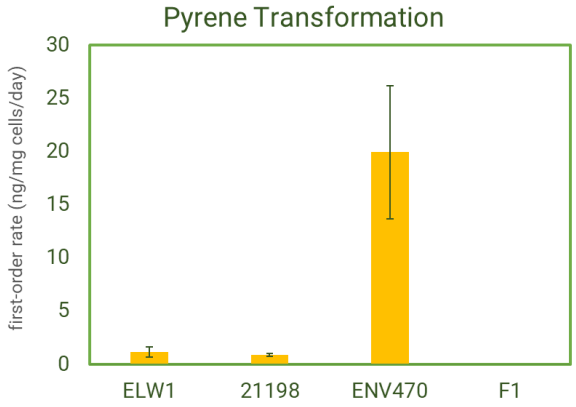
Estimated transformation rates for selected microorganisms when grown on specific substrates:
ELW1 (Isobutene); 21198 (Isobutane); ENV 470 (Naphthalene); F1 (Toluene)

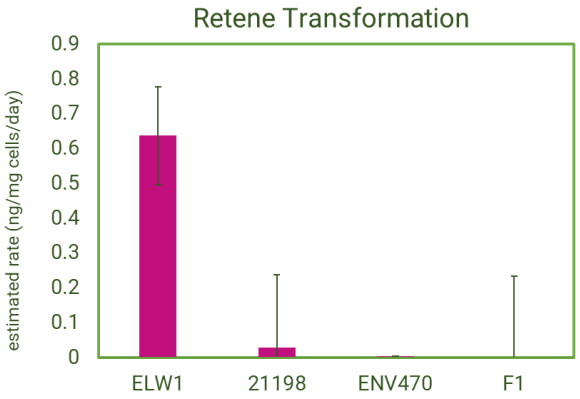






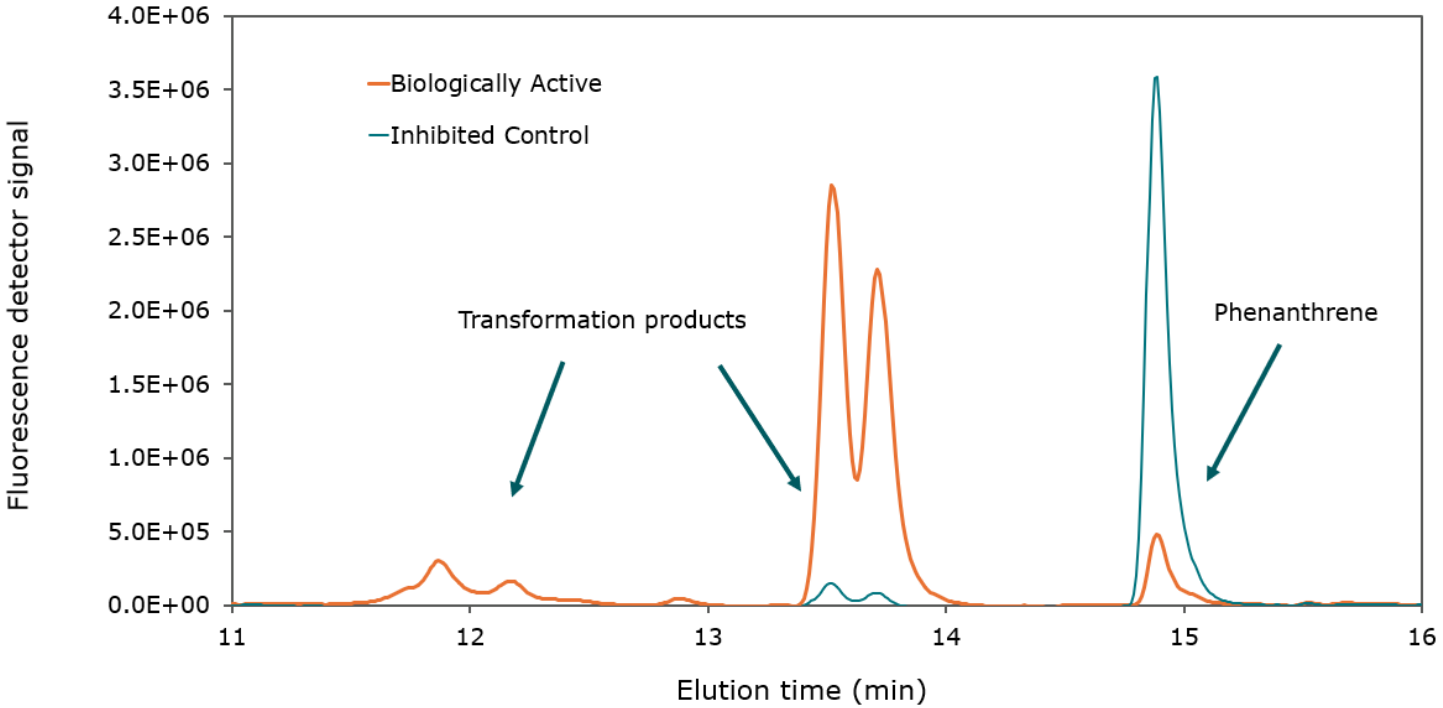




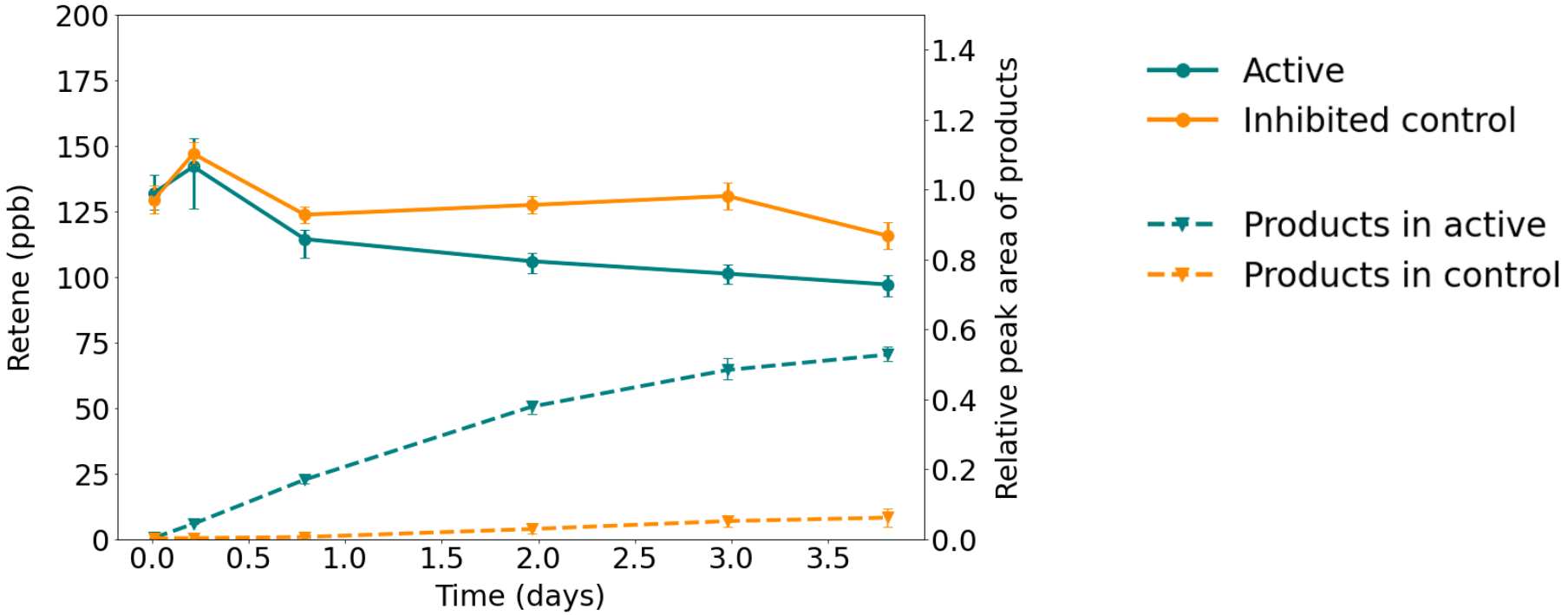


Phenanthrene Transformation by *Rhodococcus rhodochrous* ATCC 21198 Grown on Isobutane

HPLC analysis with measurement using a Fluorescence Detection

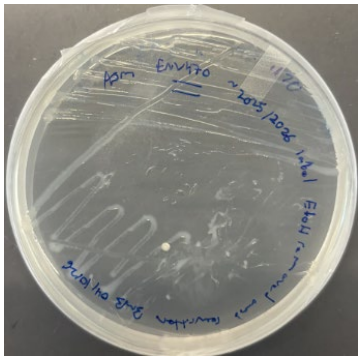


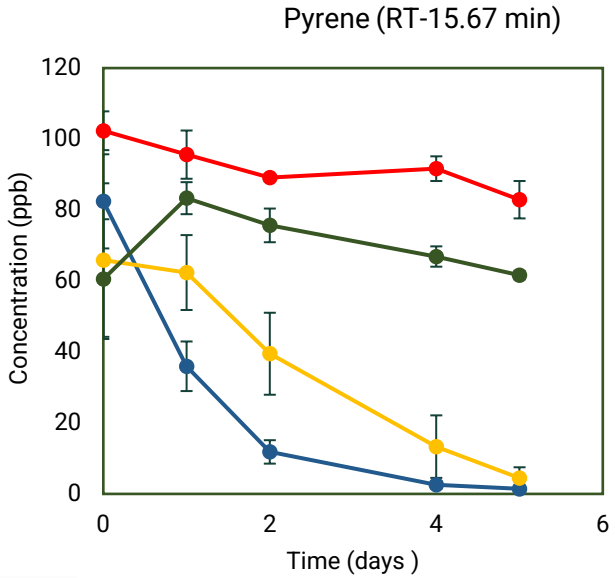
Transformation of Retene by *M.* sp. ELW1 Grown on Isobutene

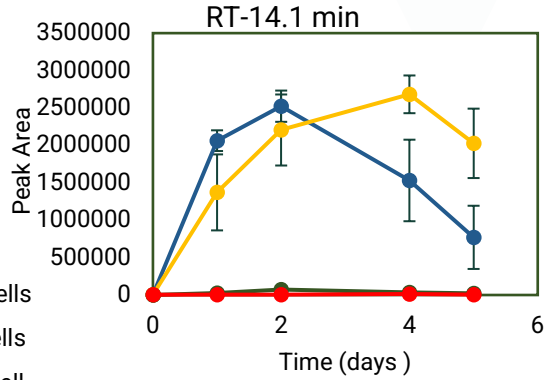


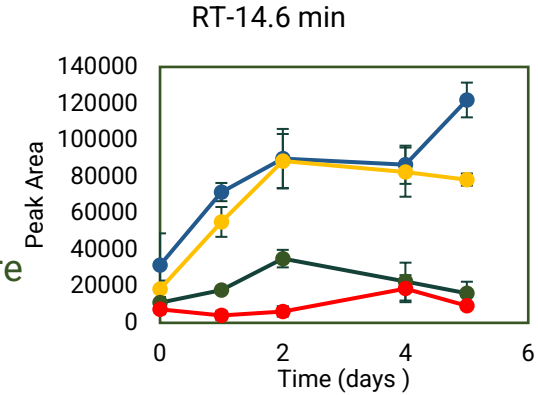
Pyrene Transformation and Product Formation by ENV 470 Grown on Naphthalene

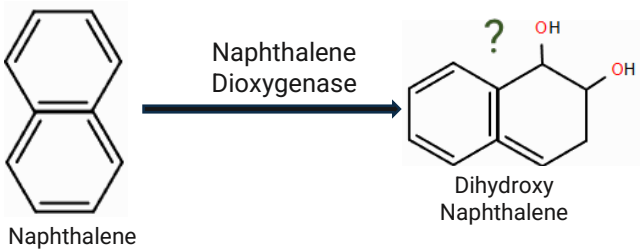
ENV 470











- Rapid transformation of pyrene
- Formation to products that are more hydrophilic

Predicting and Measuring Dosimetry and Metabolism of Polycyclic Aromatic Hydrocarbons (PAHs) for Improved Risk Assessment

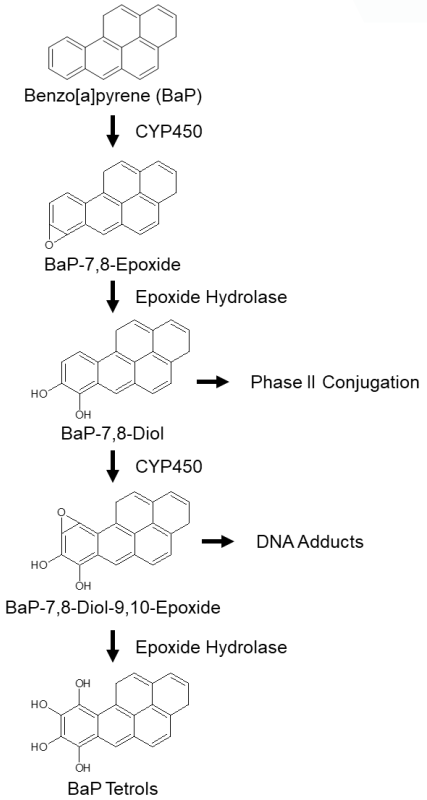
Jordan Ned Smith

Predictive Metabolism and Dosimetry Core (PDMC)

June 1, 2026

Challenges with Risk Assessment of PAHs

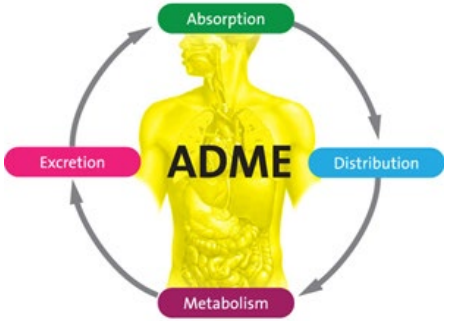
- Few available reference standards
  - Especially true
    - Substituted PAHs
    - Metabolites
- Ultimate toxicant can be unknown for many PAHs
  - May not be the parent compound
  - Rates of bioactivation and detoxication determine the concentration of the ultimate toxicant and toxicity
- Translation across test systems
- Complex Mixtures



Predictive Metabolism and Dosimetry Core (PDMC)

- Identify PAH metabolites using a reference free approach
- Predict chemical properties
- Measure rates of PAH metabolism
- Develop models to translate PAH dosimetry across zebrafish, lung cells, and humans

External Dose

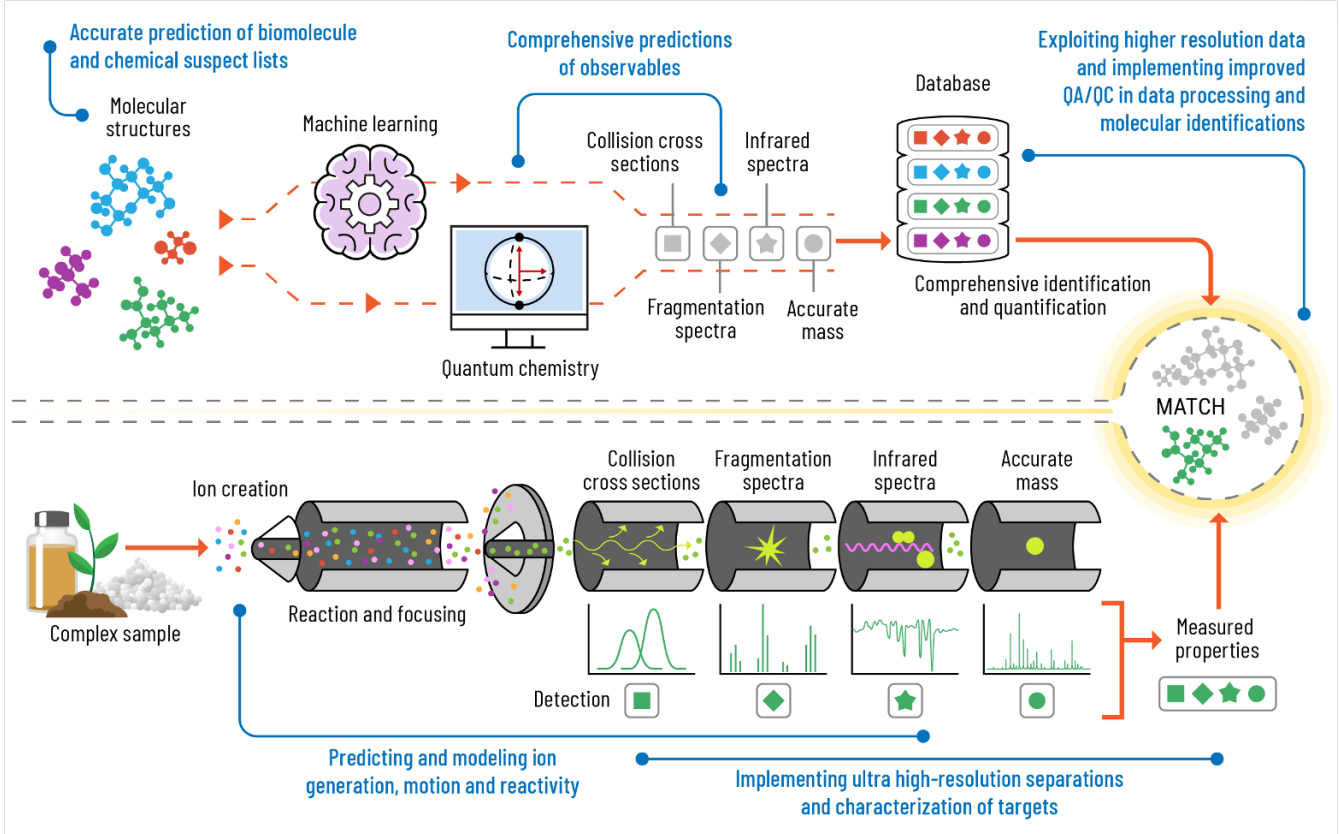


Internal Dose

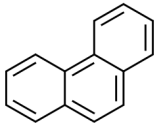
Reference Free Approach to Identify Metabolites

Computational

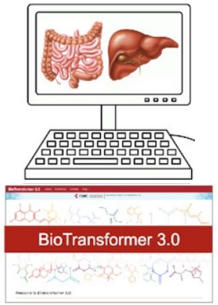
Experimental



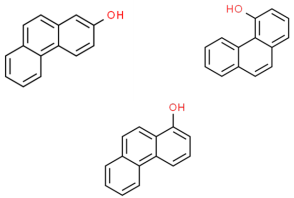
Chemical Property Prediction



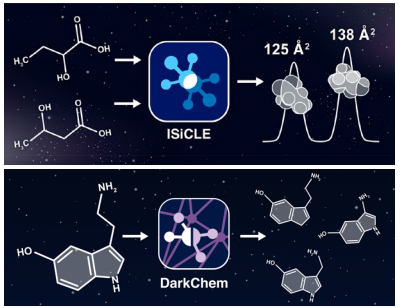
PAHs



Predict Metabolites



N=319 in 3 generations

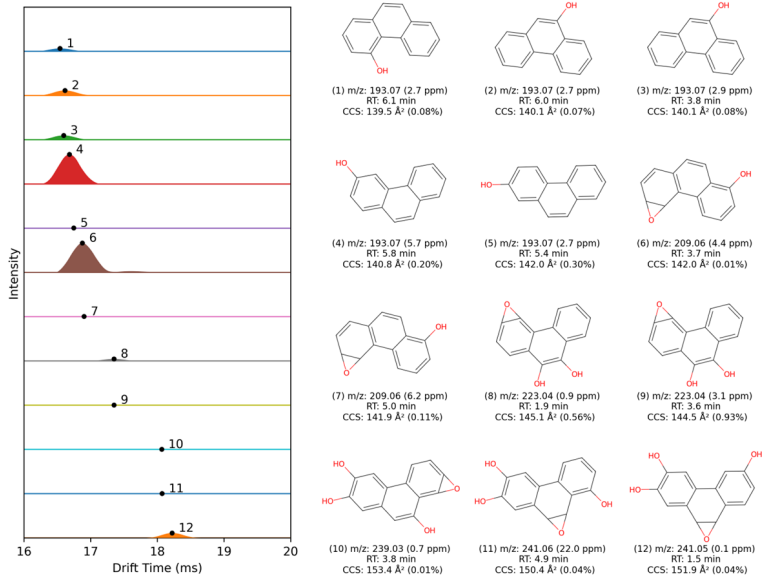


Predict Chemical Signatures

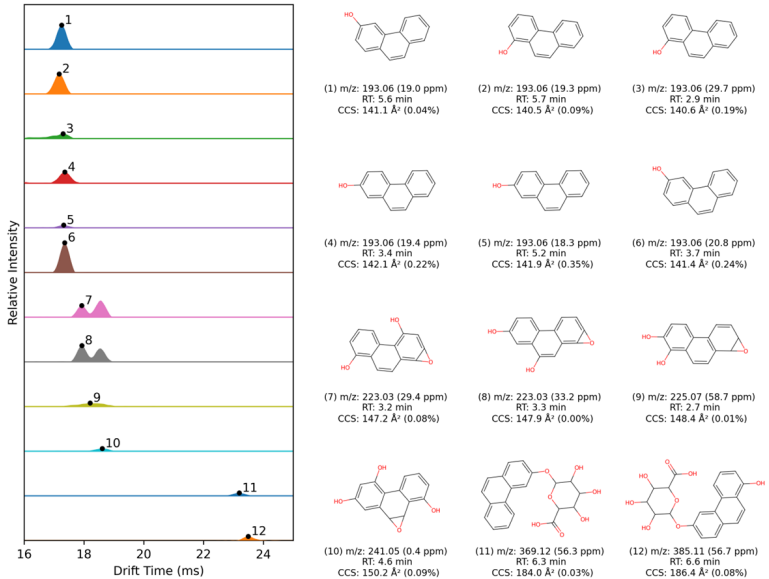
Wishart et al. (2022) *Nucleic Acids Res*. 50(W1):W115-23.
Colby et al. (2019) *Analytical Chemistry* 91(7):4346-4356.
Colby et al. (2020) *Analytical Chemistry* 92(2): 1720-1729.

Putative Metabolite Identification

ELW1

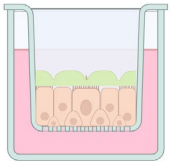


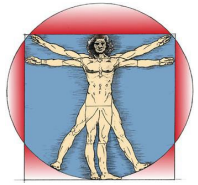
Human Liver Microsomes

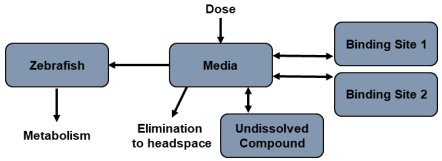


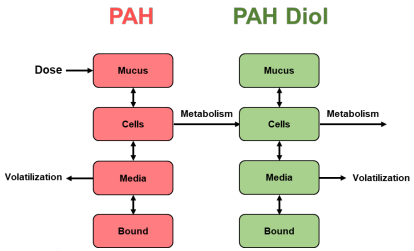
Schrlau et al (2017) *Environ. Sci. Technol. 51*(15) 8569– 8578.

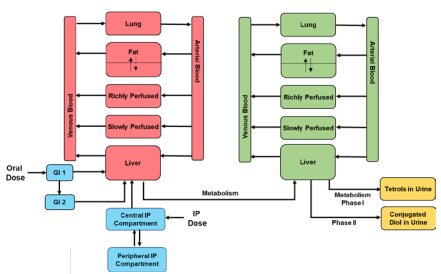
Dosimetry Modeling

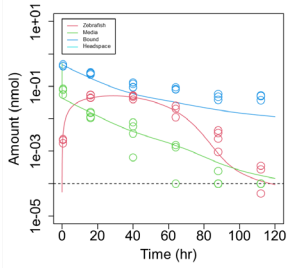


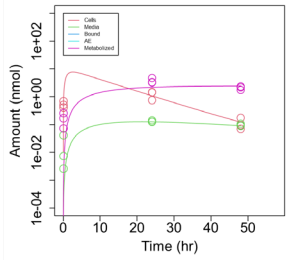


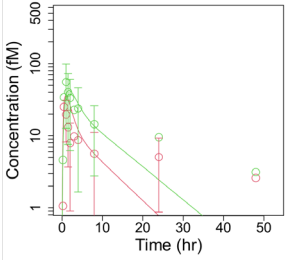












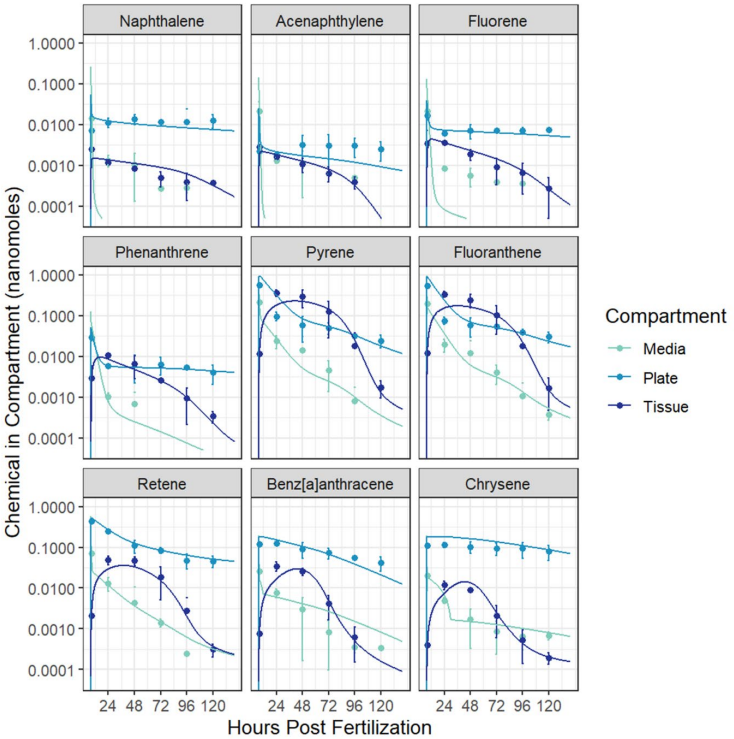
Rude et al. (2025) *Toxicol. Sci.* 205*(2): 326-343.*

Colvin et al. (2025) *Toxicol. Rep. 15:102133.*

Pande et al. (2022) *Toxicol. and Appl. Pharmacol.* 438: 115830.
Smith et al. (2022) *Int. J. Environ. Res. Public Health* 19(14).

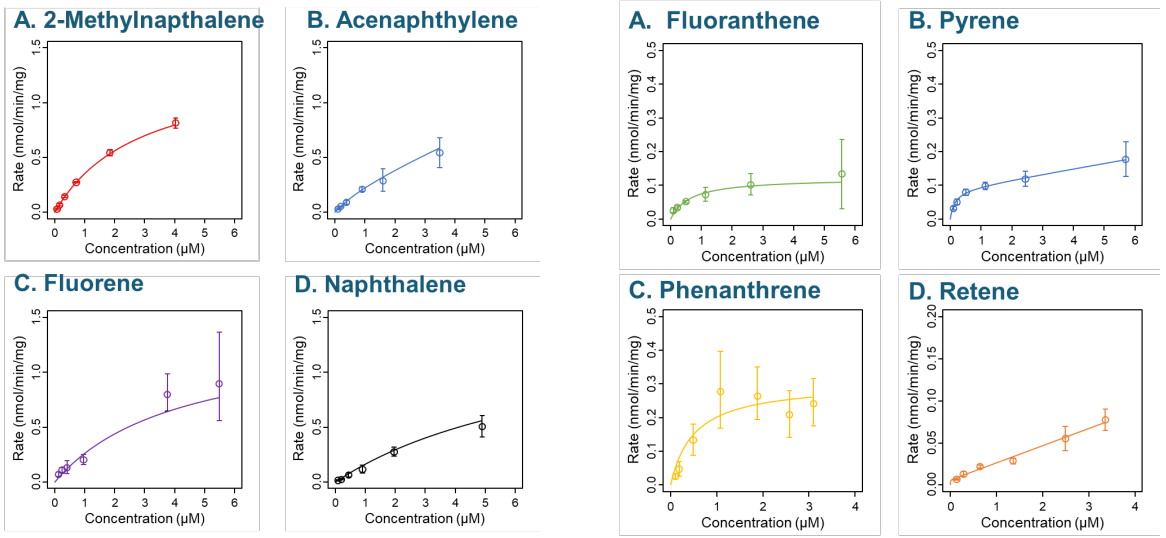
Supermix-10 in Zebrafish

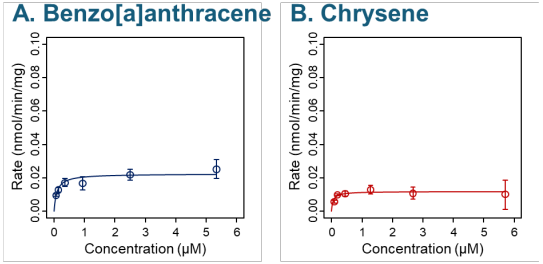
Compound	CAS	Molecular Weight (g/mol)	Structure	Molar Ratio[A]	Molar Fraction	Carcinogenic[B]
naphthalene	91-20-3	128.17		3.48	0.07	EPA, IARC, ACGIH
2-methylnaphthalene	91-57-6	142.2		1.00	0.02	
acenaphthylene	208-96-8	152.19		2.00	0.04	
fluorene	86-73-7	166.22		1.84	0.04	
phenanthrene	85-01-8	178.23		1.72	0.03	
fluoranthene	206-44-0	202.25		14.24	0.28	
pyrene	129-00-0	202.25		14.5	0.28	
benzo[a]anthracene	56-55-3	228.28		2.47	0.05	EPA, IARC, ACGIH
chrysene	218-01-9	228.28		2.59	0.05	EPA, ACGIH
retene	483-65-8	234.3		7.43	0.15	

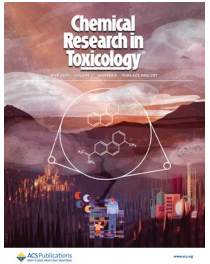


Allan et al. (2011). *Chemosphere*. (85) 920-927.
Rude et al. (2025) *Toxicol. Sci.* 205*(2): 326-343.*

Human Metabolism of Supermix-10

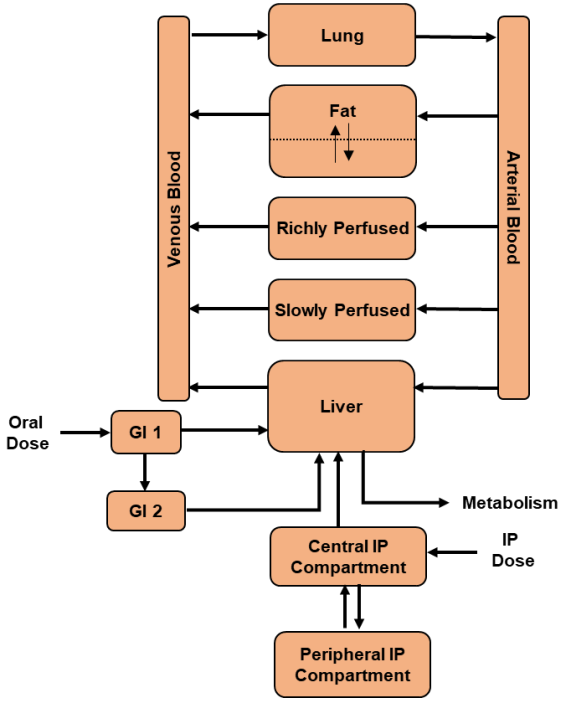


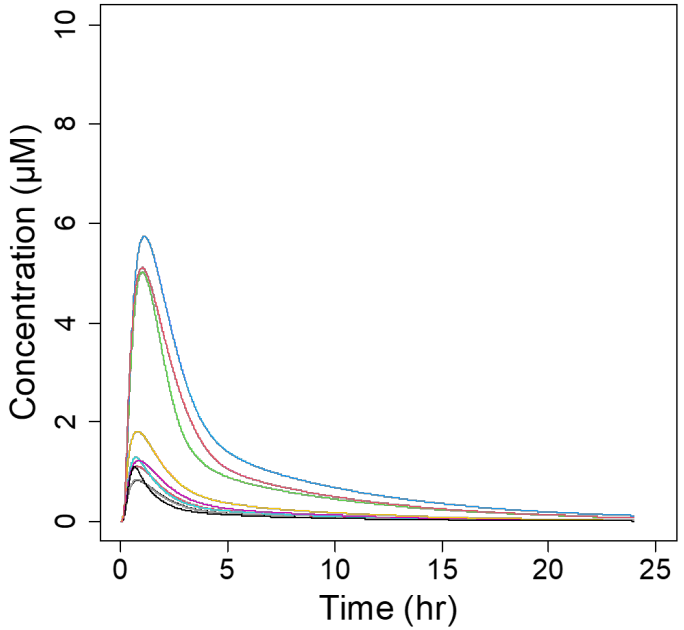




Gaither et al. (2024) *Chem. Res. Toxicol.* 37(5) 711-722.
Gaither et al. (2025) *Toxicol. Lett.* 412:172-181.

Human Supermix-10 Predictions





Pande et al. (2022) *Toxicol. and Appl. Pharmacol.* 438: 115830.
Smith et al. (2022) *Int. J. Environ. Res. Public Health* 19(14).

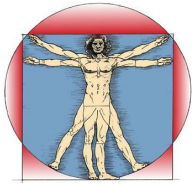
Comparison and extrapolation

Compound	EC_{20} (μM)
retene	5.8
pyrene	20.6
benzo[a]anthracene	38.1
fluoranthene	39.6

External Dose

Compound	Cmax (μM)	Concentraion in Zebrafish AUC (μM×hr)	Concentration Metabolized (μM)	Concentration Metabolized AUC (μM×hr)
retene	201	8940	86	4663
pyrene	1997	113505	1252	66158
benzo[a]anthracene	157	7875	863	40271
fluoranthene	2909	171908	1891	95664

Internal Dose Metric



External Dose

Compound	Dose (mg/kg)		
	Cmax	AUC	Concentration Metabolized
retene	36	211	19
pyrene	381	2713	244
benzo[a]anthracene	21	39	NA
fluoranthene	416	575	NA

Internal Dose Metric

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