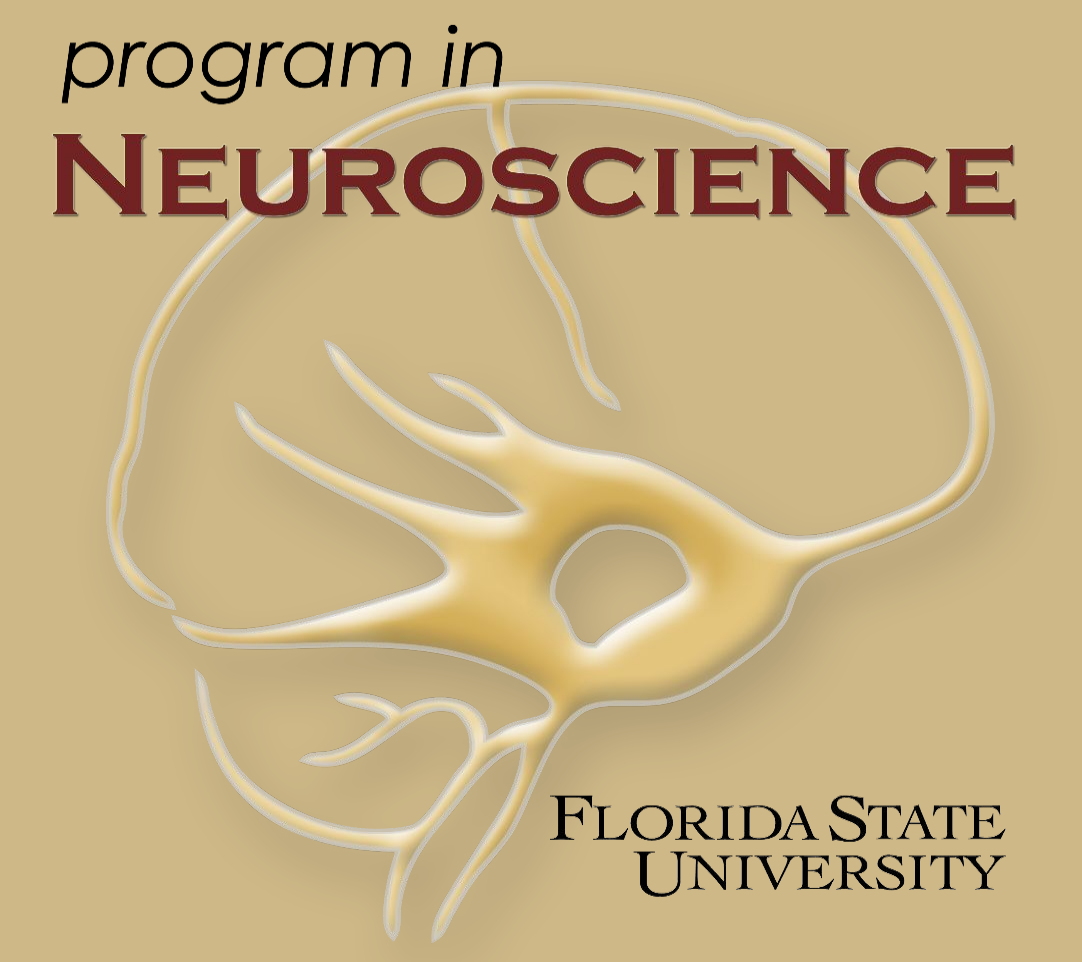# The Relationship between Liquid and Vapor Phase Concentrations for Alkylbenzene Odorants Diluted in Mineral Oil Using a Photoionization Detector-Based Approach
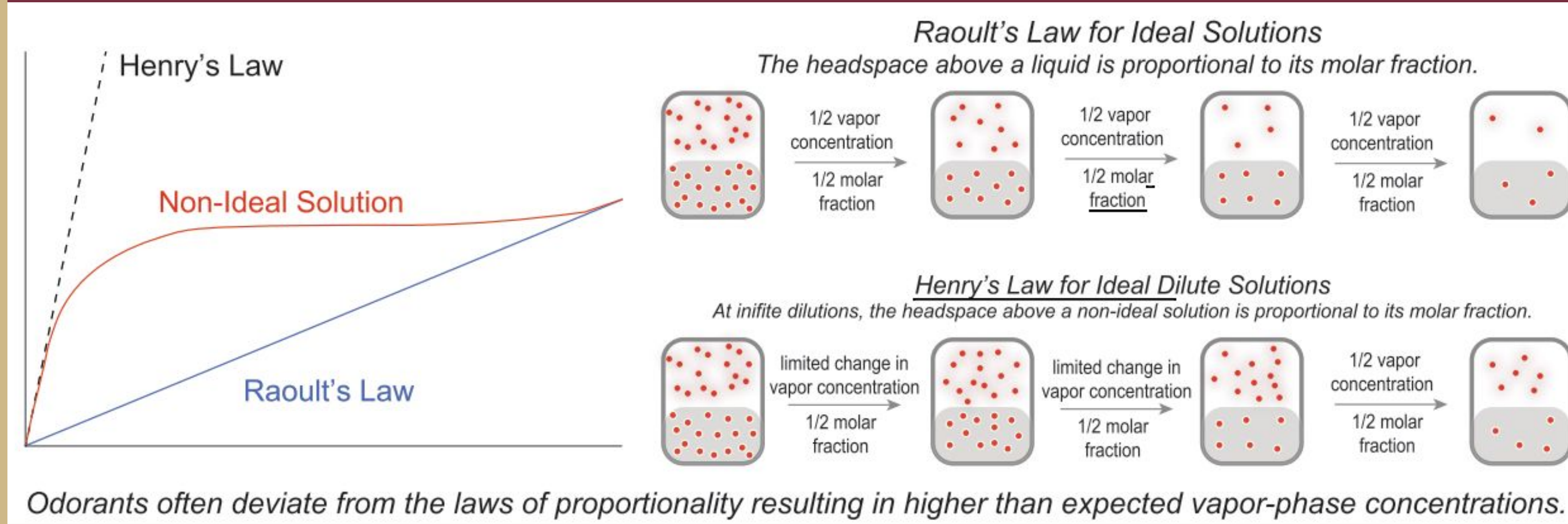
<u>Lena Firlotte</u>, Austin Pauley, and Adam Dewan

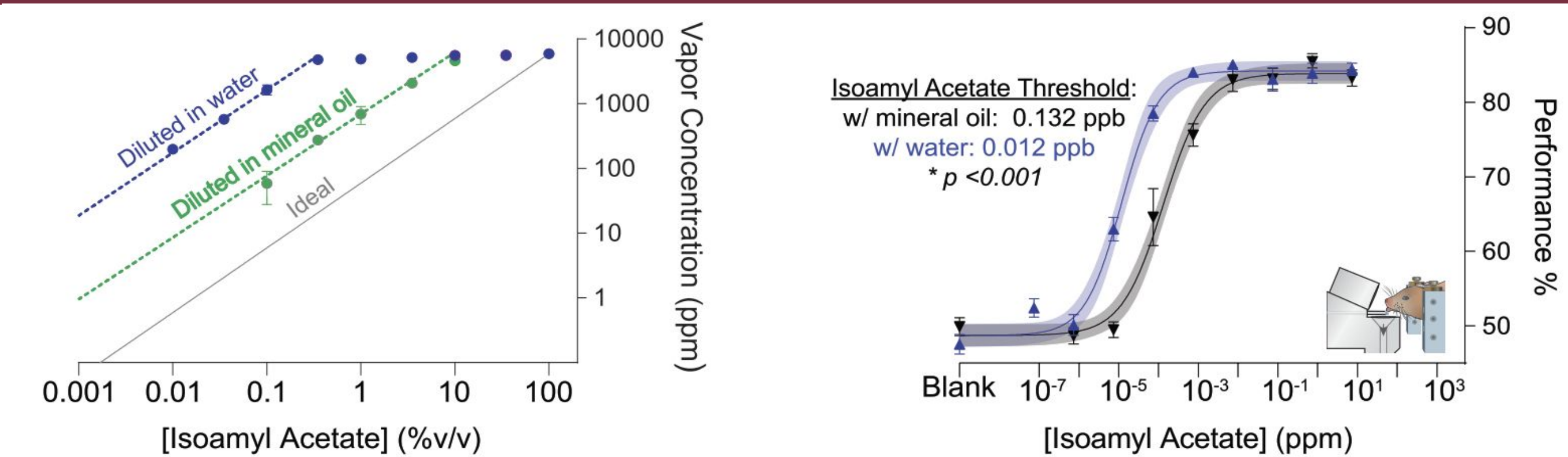Department of Psychology and Program of Neuroscience, Florida State University

Introduction

- Olfactory research often relies on liquid dilutions to manipulate the vapor-phase concentrations of volatile odorants.
- **Goal**: assess the relationship between liquid and vapor-phase concentrations of alkylbenzenes using our photoionization detector (PID) based method (Jennings et al., 2022).
- PID collects and exposes a vapor sample to a high intensity ultraviolet light that ionizes the volatile molecules, creating a current that is proportional to the vapor concentration.
- **Significance**: The liquid-/vapor-phase equilibrium equations can be used by other researchers to obtain accurate vapor-phase alkylbenzene concentrations.

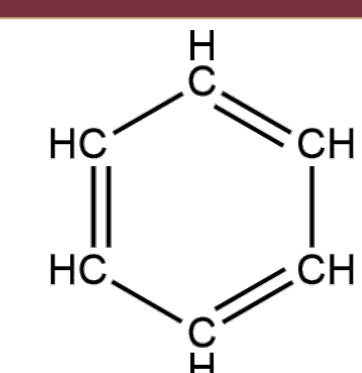## Odorants Infrequently Align with Laws of Proportionality

Raoult's Law for Ideal Solutions
The headspace above a liquid is proportional to its molar fraction.

Henry's Law for Ideal Dilute Solutions
At infinite dilutions, the headspace above a non-ideal solution is proportional to its molar fraction.

Odorants often deviate from the laws of proportionality resulting in higher than expected vapor-phase concentrations.

The Vapor Phase Concentration is Dependent Upon the Solvent

Isoamyl Acetate Threshold:
w/ mineral oil: 0.132 ppb
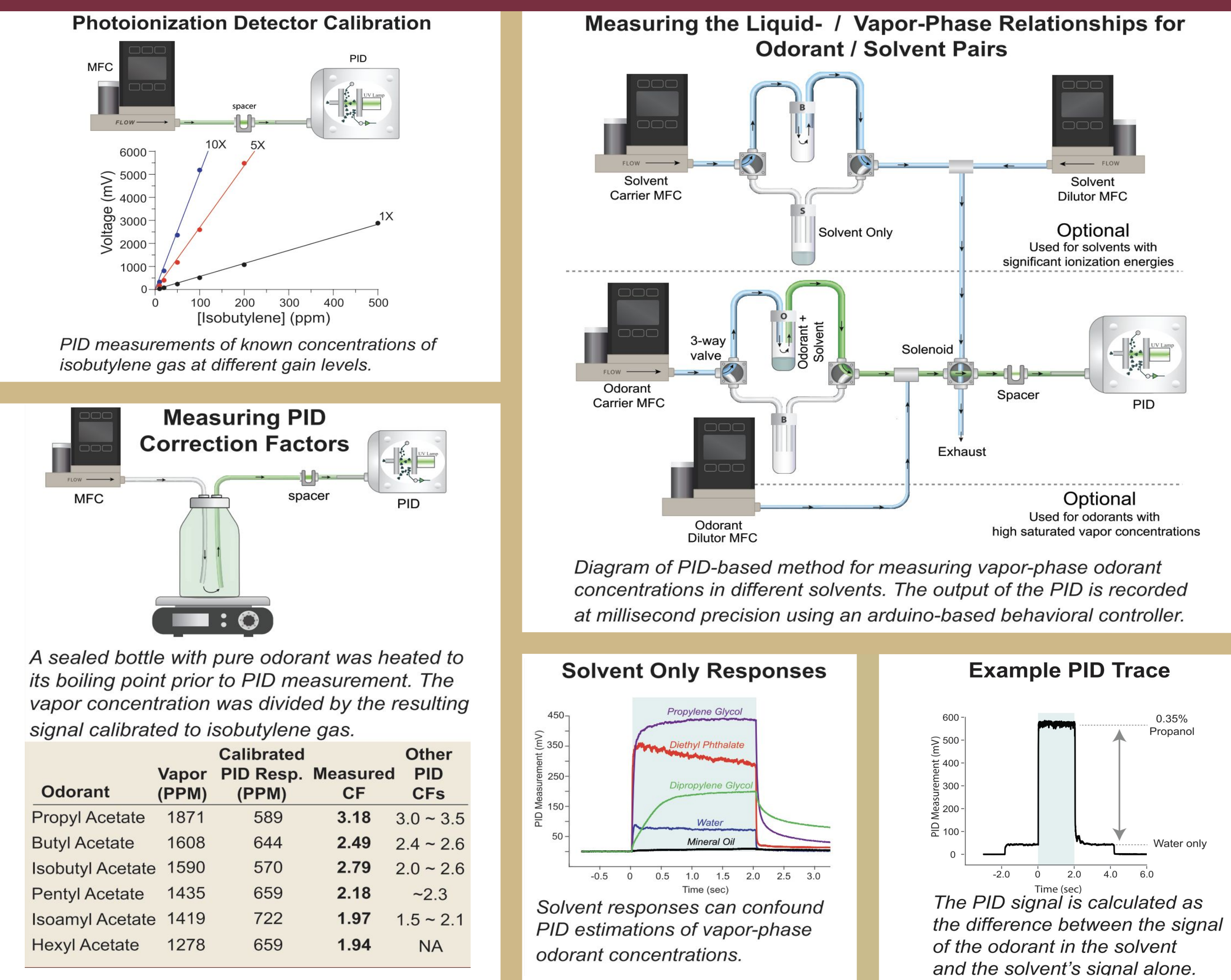w/ water: 0.012 ppb
* p <0.001

The vapor-phase concentration of an odorant can be influenced by its solvent and thus has the potential to confound the interpretation of functional experiments. For more details on our behavioral approach see Poster 150.

Alkylbenzene Odorants

- Alkylbenzenes are classified as aromatic hydrocarbons.
- Have "chemical" or "gasoline-like" odors.
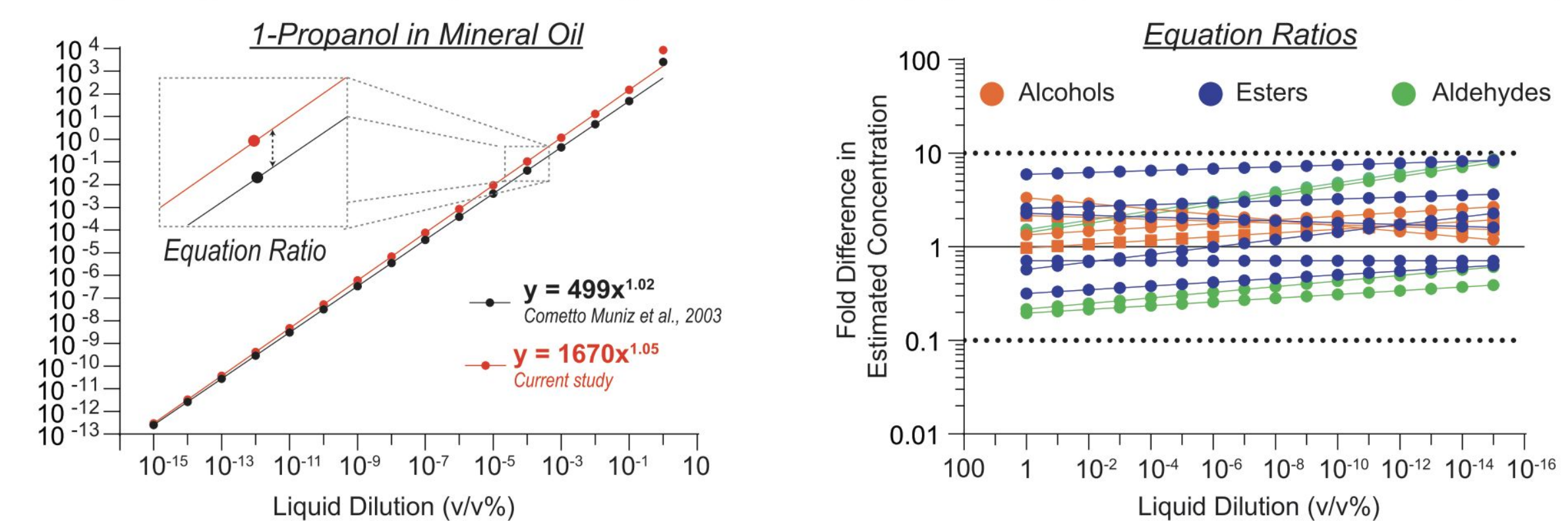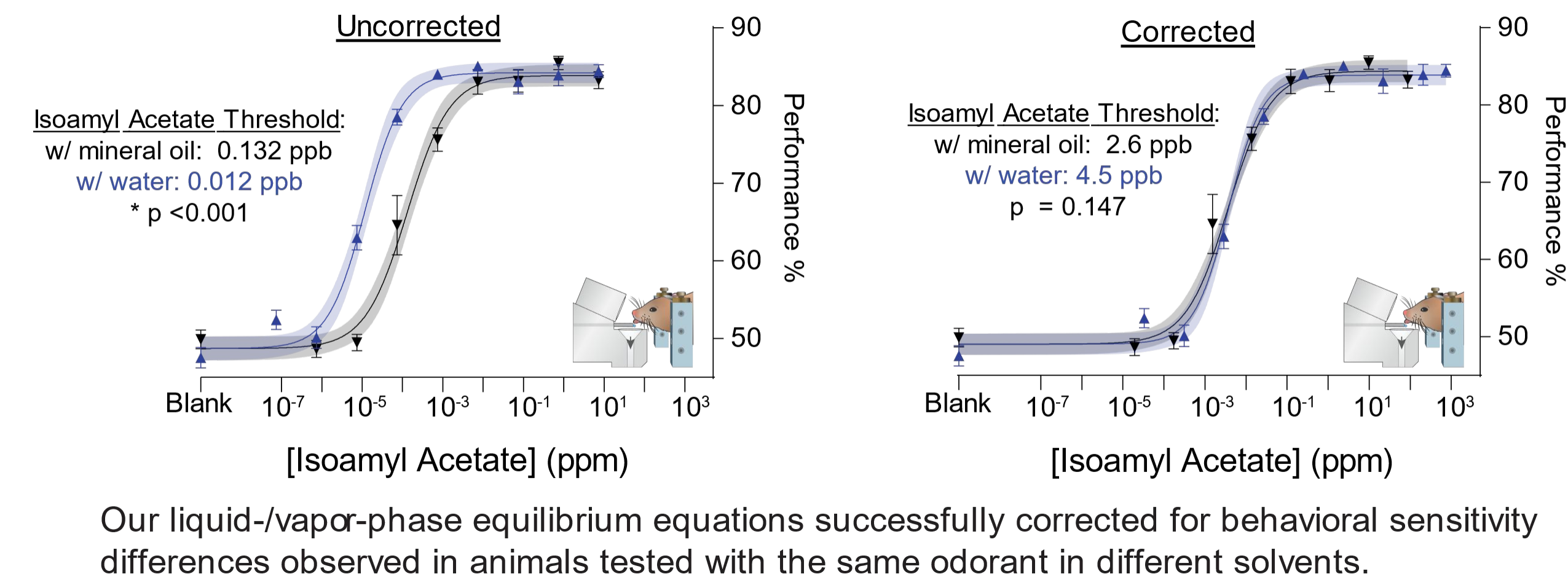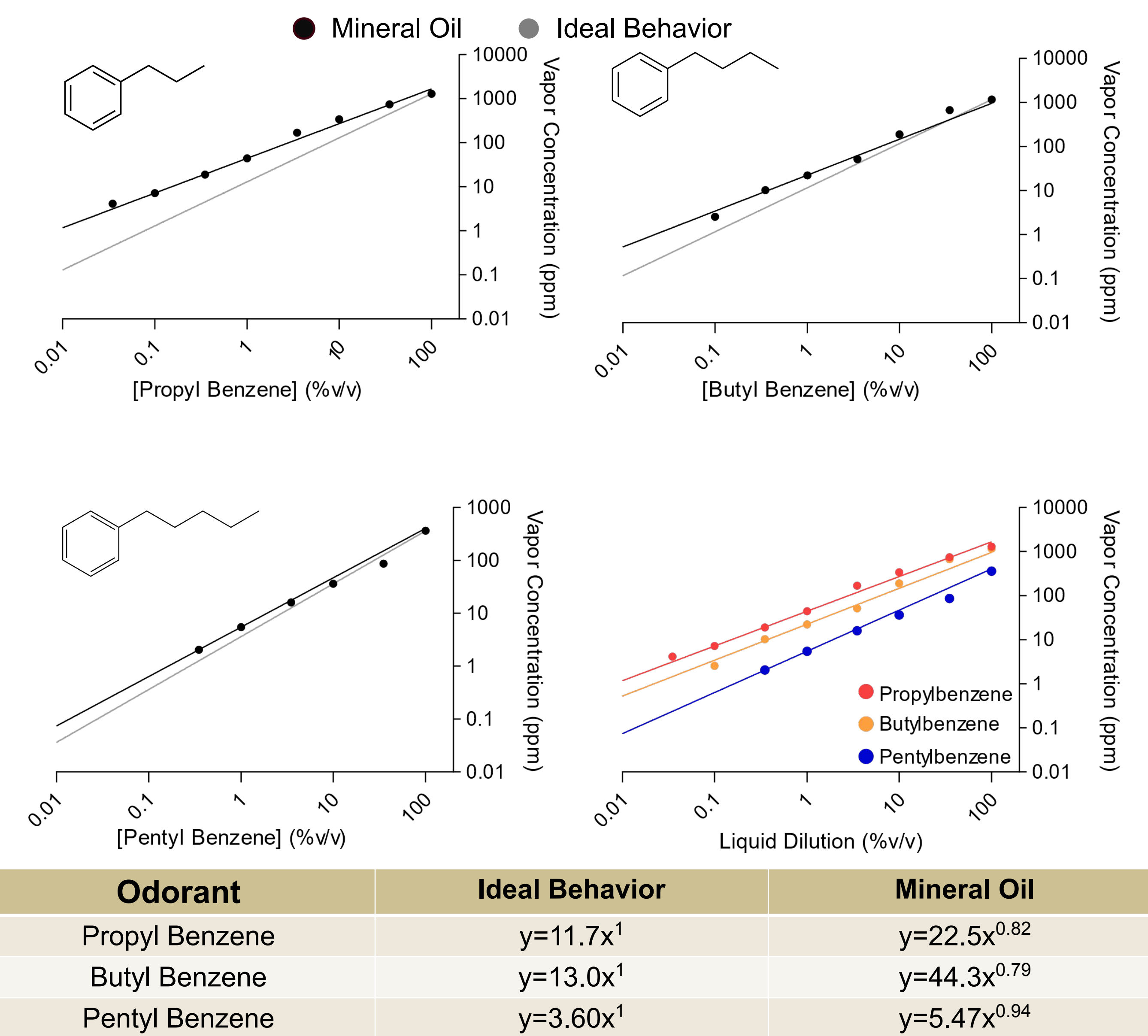- Low volatility
- Insoluble in water

Methods

Photoionization Detector Calibration

PID measurements of known concentrations of isobutylene gas at different gain levels.

Measuring PID Correction Factors

A sealed bottle with pure odorant was heated to its boiling point prior to PID measurement. The vapor concentration was divided by the resulting signal calibrated to isobutylene gas.

Odorant	Vapor (PPM)	Calibrated PID Resp. (PPM)	Measured CF	Other PID CFs
Propyl Acetate	1871	589	3.18	3.0 – 3.5
Butyl Acetate	1608	644	2.49	2.4 – 2.6
Isobutyl Acetate	1590	570	2.79	2.0 – 2.6
Pentyl Acetate	1435	659	2.18	~2.3
Isoamyl Acetate	1419	722	1.97	1.5 – 2.1
Hexyl Acetate	1278	659	1.94	NA

Measuring the Liquid- / Vapor-Phase Relationships for Odorant / Solvent Pairs

Diagram of PID-based method for measuring vapor-phase odorant concentrations in different solvents. The output of the PID is recorded at millisecond precision using an arduino-based behavioral controller.

Solvent Only Responses

Solvent responses can confound PID estimations of vapor-phase odorant concentrations.

Example PID Trace

The PID signal is calculated as the difference between the signal of the odorant in the solvent and the solvent's signal alone.

Validation of the Method

Comparing our data to a published gas chromatography study (Commetto-Muniz et al., 2003)

1-Propanol in Mineral Oil

Equation Ratio

y = 499x^1.02
Cometto Muniz et al., 2003

y = 1670x^1.05
Current study

Equation Ratios

Alcohols   Esters   Aldehydes

Our liquid-/vapor-phase equilibrium equations were reasonably similar to a previous study utilizing gas chromatography to estimate odorant concentrations in mineral oil.

Verifying this method using the mouse olfactory system

Uncorrected
Isoamyl Acetate Threshold:
w/ mineral oil: 0.132 ppb
w/ water: 0.012 ppb
* p <0.001

Corrected
Isoamyl Acetate Threshold:
w/ mineral oil: 2.6 ppb
w/ water: 4.5 ppb
p = 0.147

Our liquid-/vapor-phase equilibrium equations successfully corrected for behavioral sensitivity differences observed in animals tested with the same odorant in different solvents.

Results

Mineral Oil   Ideal Behavior

Propylbenzene   Butylbenzene   Pentylbenzene

Odorant	Ideal Behavior	Mineral Oil
Propyl Benzene	$y=11.7x^1$	$y=22.5x^{0.82}$
Butyl Benzene	$y=13.0x^1$	$y=44.3x^{0.79}$
Pentyl Benzene	$y=3.60x^1$	$y=5.47x^{0.94}$

Summary and Limitations

- Alkylbenzenes in mineral oil exhibit near ideal behavior.
- This data will be included in a practical archive of liquid / vapor-phase equilibrium equations of different odorants in various solvents.
- Although not as sensitive or accurate as gas chromatography, our approach is reasonably accurate at measuring liquid / vapor-phase equilibrium equations.
- Future experiments will analyze additional alkylbenzenes and utilize different solvents

References

- Cometto-Muñiz, J.E., Cain, W.S., and Abraham, M.H. 2003. Quantification of chemical vapors in chemosensory research. Chem Senses. 28:467–477.
- Jennings, L., Williams, E., Caton, S., Avlas, M., & Dewan, A. (2022). Estimating the relationship between liquid- and vapor-phase odorant concentrations using a photoionization detector (pid)-based approach. *Chemical Senses*, *48*. https://doi.org/10.1093/chemse/bjac038