Tackling the selectivity issues in low-cost VOC sensors

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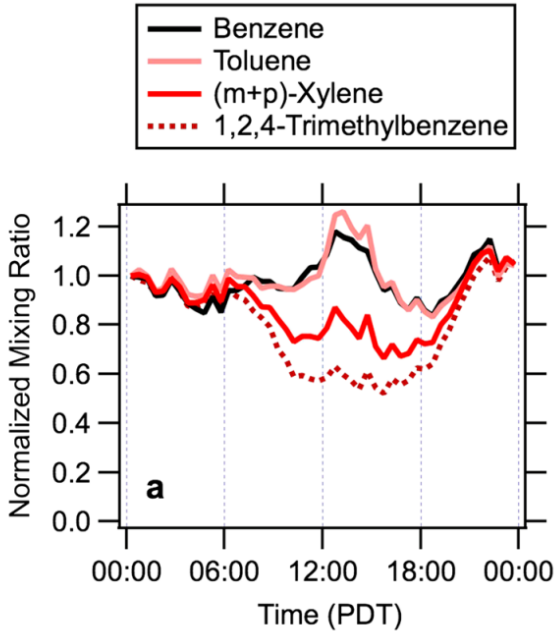
Volatile organic compounds may be:

Variable on spatial scales of meters

SCAQMD mobile lab

Variable on time scales of minutes



de Gouw et al., JGR, 2018

Harmful at ppt-ppb concentrations

Pollutant	Risk threshold (ppt)	
	Noncancer	*Cancer*[!]
Acrolein*	9	--
1,3-Butadiene*	900	14
Styrene*	230,000	--
Benzene*	9000	140
Toluene*	1,300,000	--
Xylenes*	23,000	--
Hexane	170,000	--
Naphthalene	560	--
Methyl methacrylate	170,000	--
Propylene oxide	12,000	110

[!]based on a risk threshold of 10^{-6}
*measured hourly at stationary field site

Examples from IRIS

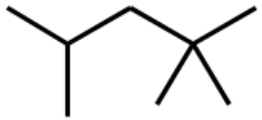
Let’s frame the complexity of VOCs:

- Every breath of air contains thousands of different organic gases
- Many of these gases differ by only slight changes in structure or chemistry
- Slight changes in structure can impact physicochemical properties
- Slight changes in structure does impact toxicity

Take for example regulated Hazardous Air Pollutants:

154 are organic molecules

Highly isomer-specific



Regulated HAP

Not classified as a HAP

Likely co-exist with molecularly similar non-HAPs

Measurement requirements

To pick out one molecule or one class of molecules out of a soup of chemically similar molecules:

Instrument ***needs***:

- Isomer-resolved (unambiguous ID)
- Sensitive (~ppb)
- Time-resolved (minutely to hourly)
- Portable

Instrument ***wants***:

- Cheap
- Flexible target (i.e., universal)

Current tools are insufficient

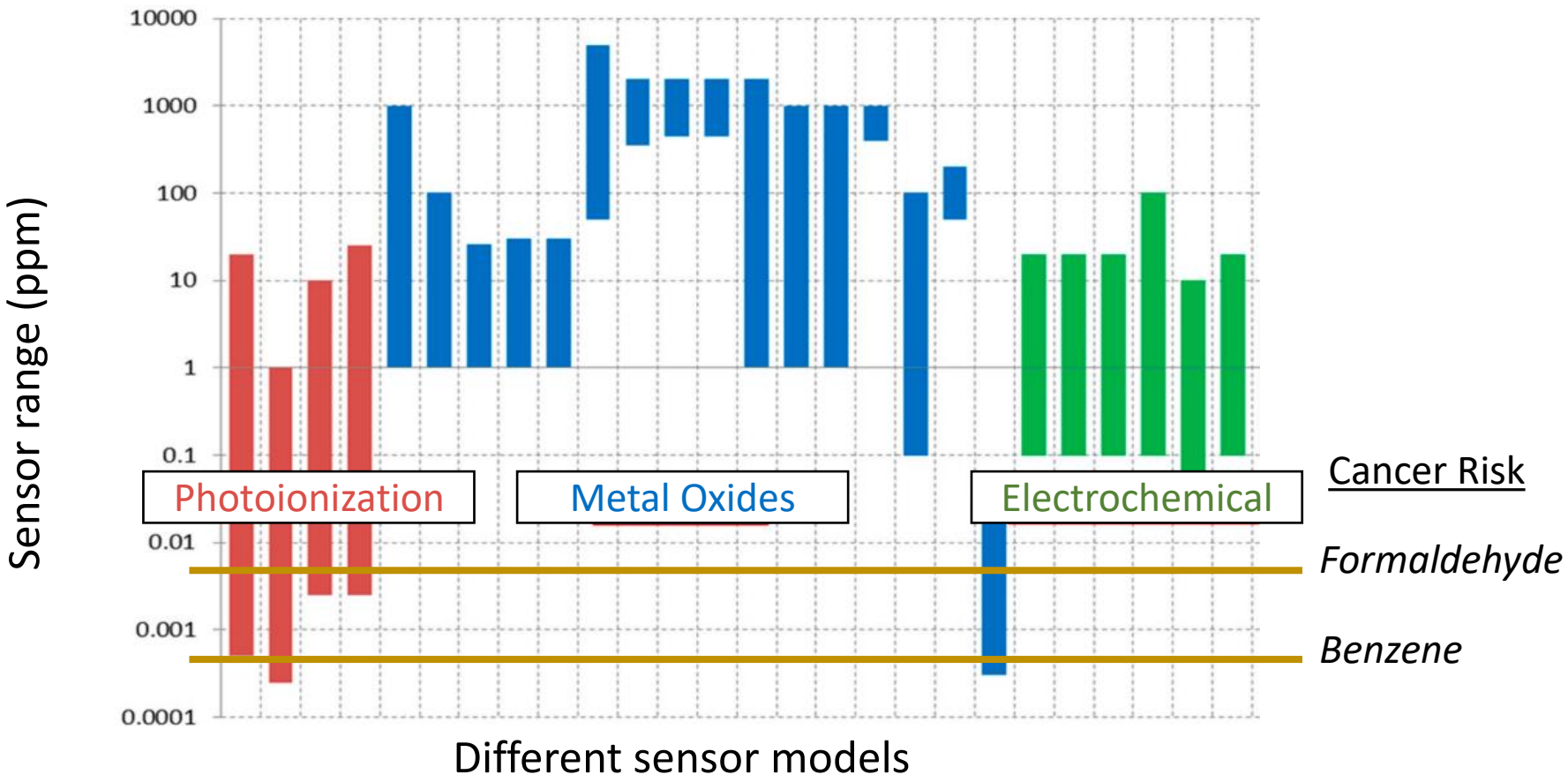
Stationary/semi-mobile options:

- Choose between chemical ID (e.g., gas chromatography) **or** time resolution (e.g., chemical ionization mass spec)
- Expensive (>$100,000) and bulky

Low cost/portable options (e.g., low-cost sensors):

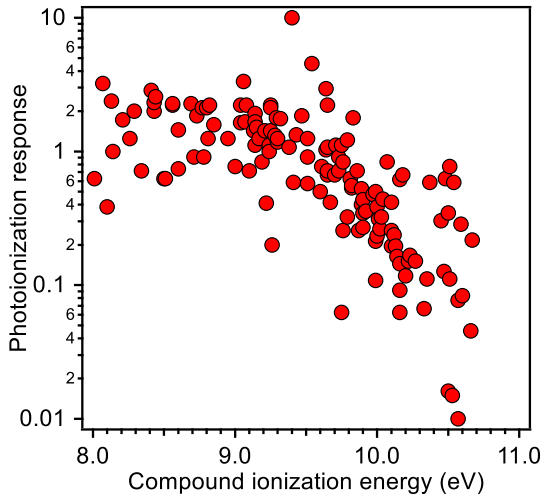
The reason we are here today!

Many low-cost sensors are not sensitive enough



Spinelle et al., Sensors, 2017

Universal response is a blessing and a curse



Data from RAE Systems

Few, if any, low-cost sensors have truly universal response

Sensitivity may vary by a factor of 10

*Change in signal means change in concentration **OR** in composition!*

Low-cost sensors as total VOC measurement

Variable response likely converges to similar average for complex mixtures

and

Sum of VOCs in air is likely above thresholds for sensitivity

therefore

Low-cost sensors can provide a reasonable total VOC measurement

However!

Total VOCs is very difficult to interpret either scientifically or toxicologically!

An indoor TVOC measurement can't tell the difference between baking chocolate chip cookies and painting your nails, but health effects are probably different!

Low-cost sensors as total VOC measurement

An indoor TVOC measurement can't tell the difference between baking chocolate chip cookies and painting your nails,

But if you are in a nail salon, it is probably the latter.

Total VOCs can be meaningful, but context is important and composition should be confirmed

Current tools are insufficient

Stationary/semi-mobile options:

+ Sensitive (~ppb)
+ Flexible target (i.e., universal)
○ Isomer-resolved (unambiguous ID)
○ Time-resolved (minutely to hourly)
- Portable
- Cheap

Low cost/portable options :
(e.g., low-cost sensors)

+ Portable
+ Cheap
+ Time-resolved (minutely to hourly)
○ Flexible target (i.e., universal)
- Isomer-resolved (unambiguous ID)
- Sensitive (~ppb)

Understanding varying sensor response

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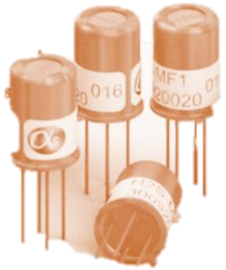
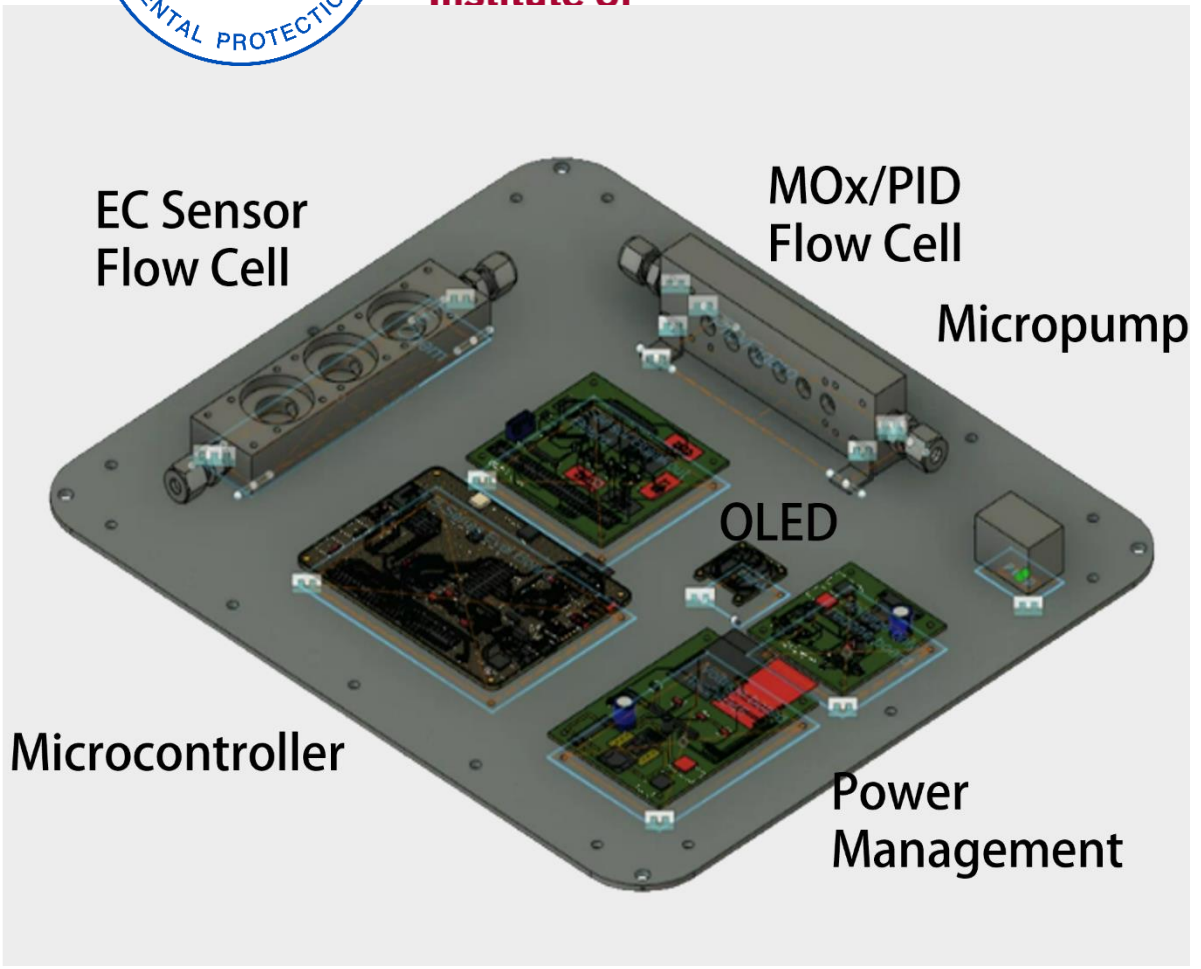


Metal Oxide (MOx)
Operating temperature

Photo-Ionization Detector (PID)
Lamp energy

Electrochemical (EC)
Applied bias voltage



Sensor response to different compounds

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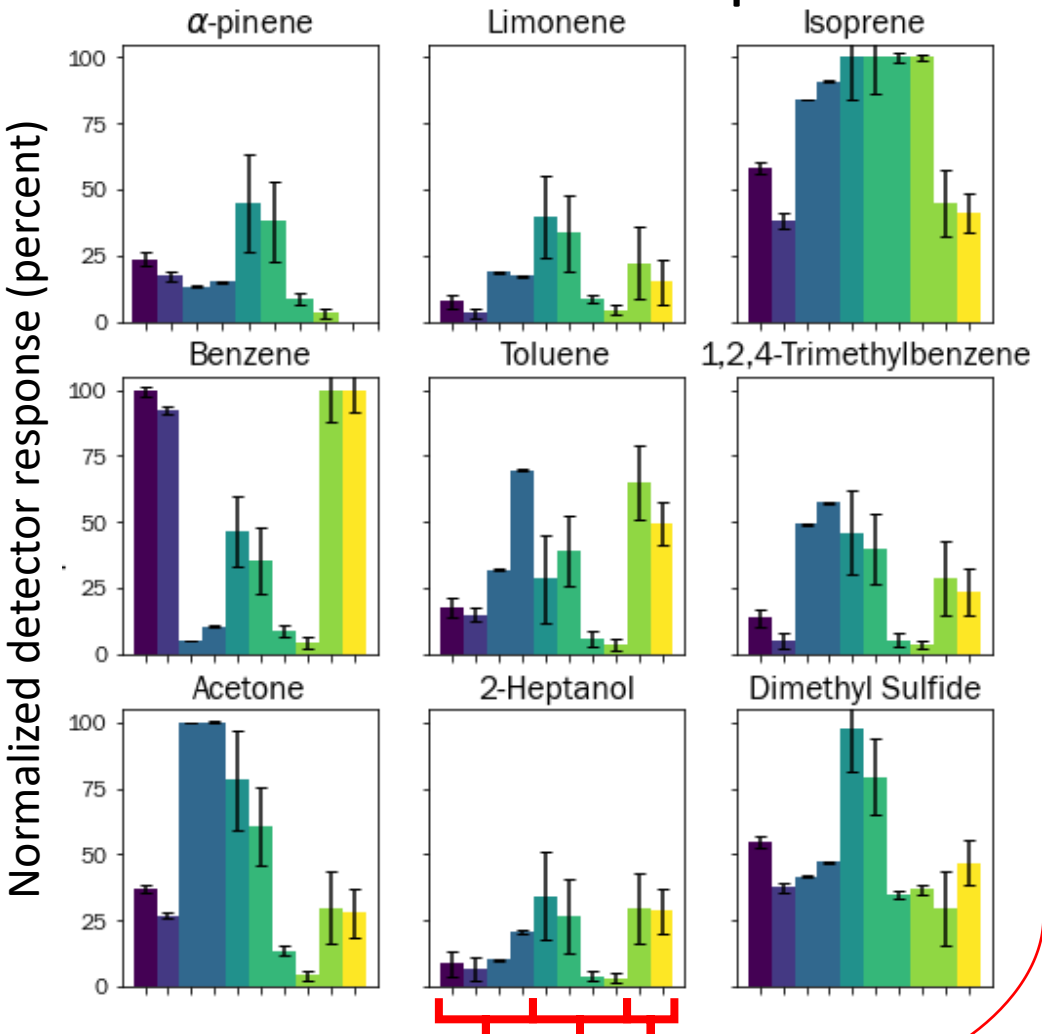
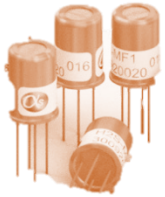


Multisensor array provides a "sensor fingerprint" for each compound



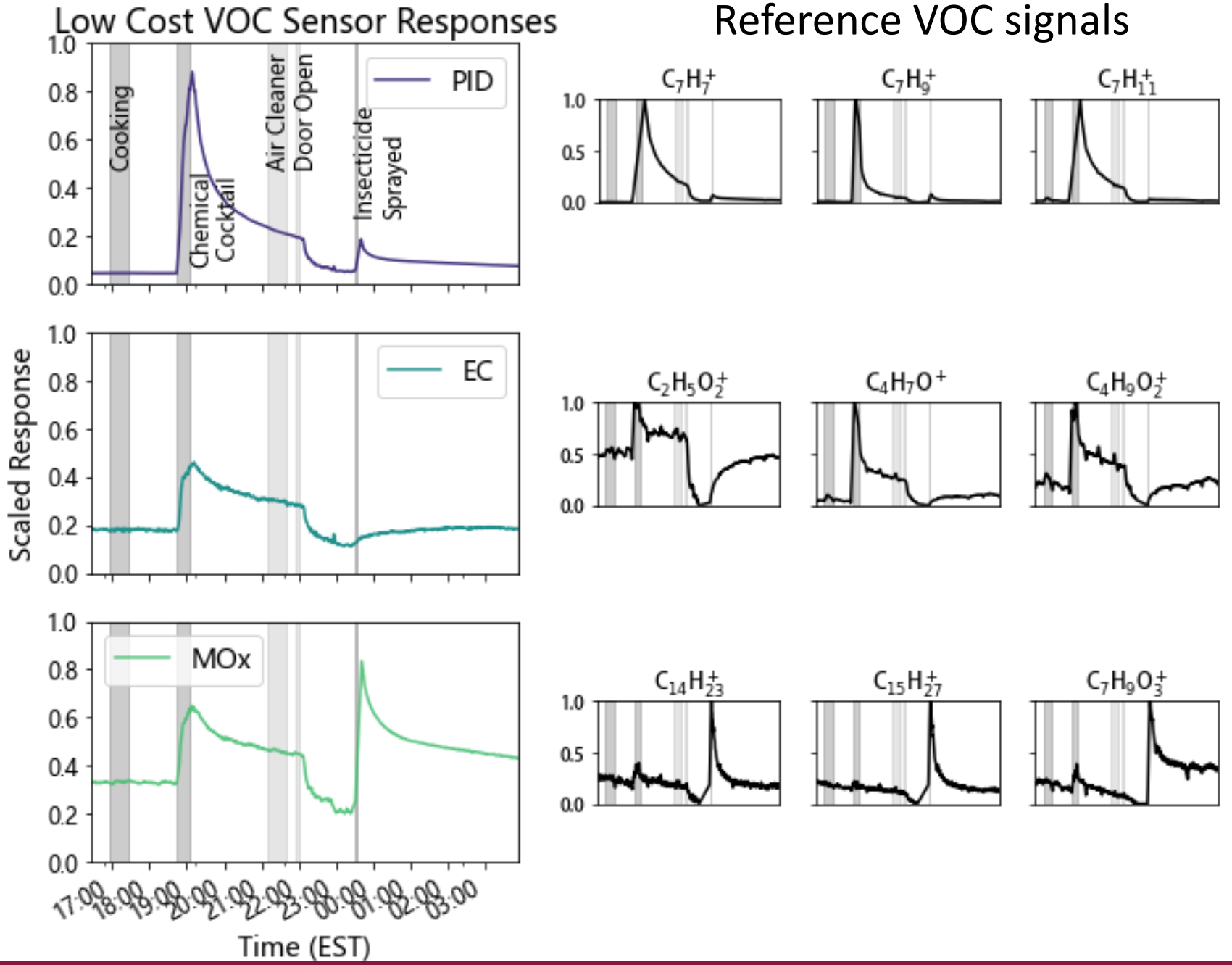
Metal Oxide (MOx)
Operating temperature

Electrochemical (EC)
Applied bias voltage

Photo-Ionization Detector (PID)
Lamp energy

Sensor array comparison

VOC sensors are consistent with reference data



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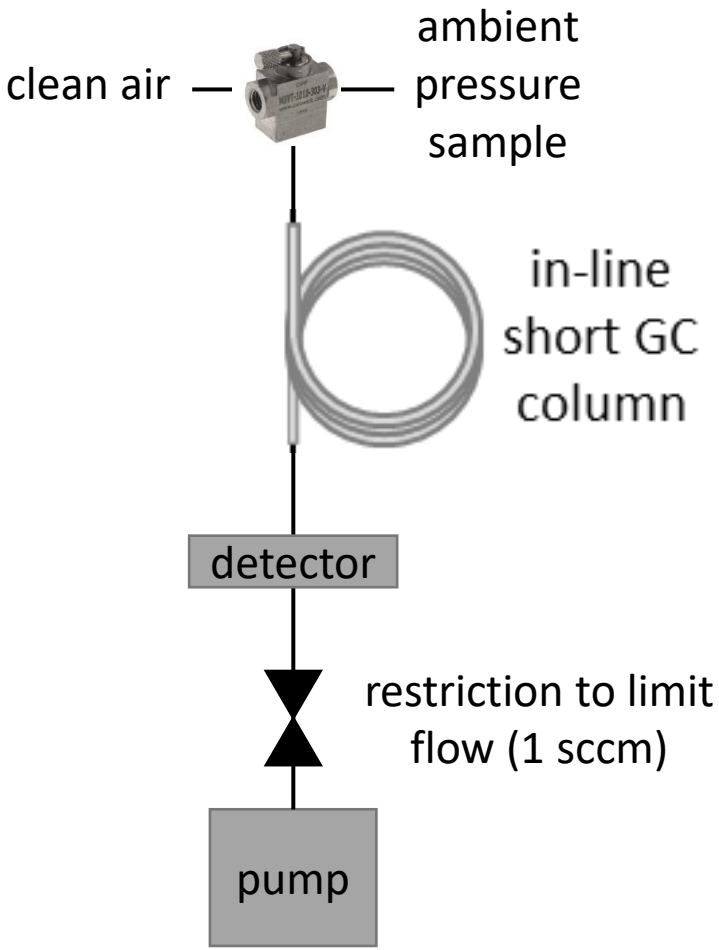
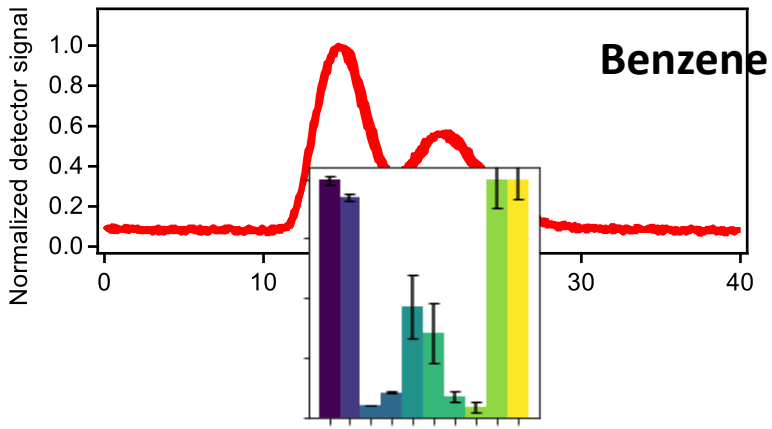
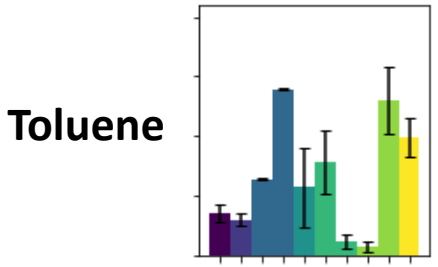
Example approach for separation before sensors







*"Multidimensional fingerprint" based on **both** sensor array and retention*

Take-home points

It is hard to be universal and selective!

Current low-cost sensing tools cannot provide enough selectivity for monitoring or measuring individual gases of concern

Total VOC measurements may be accurate but are difficult to interpret and are highly contextual (one tool in an arsenal)

We need to be thinking creatively about axes of separation to build targeted sensing tools

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