



Monitoring of Emission Sources Using SIFT-MS

PRESENTER

Caleb Allpress PhD | Scientist | Syft Technologies



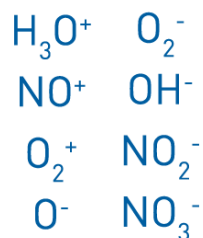
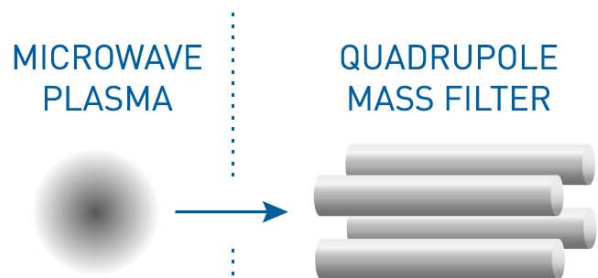
syft.com



An Introduction to SIFT-MS

SIFT-MS: How this soft chemical ionization technique works

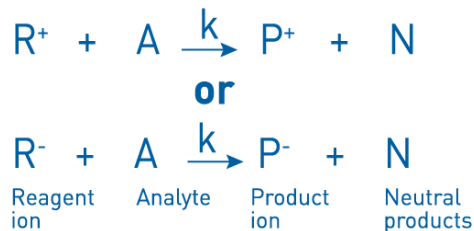
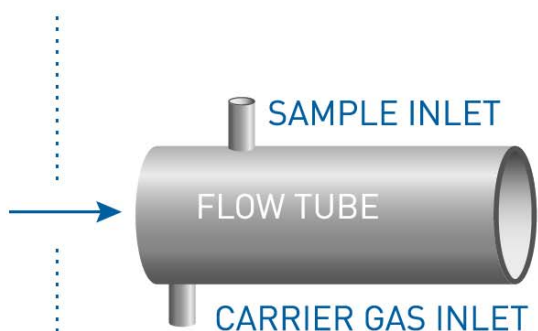
Reagent Ion Selection



Select **one**
 R^+ or R^-

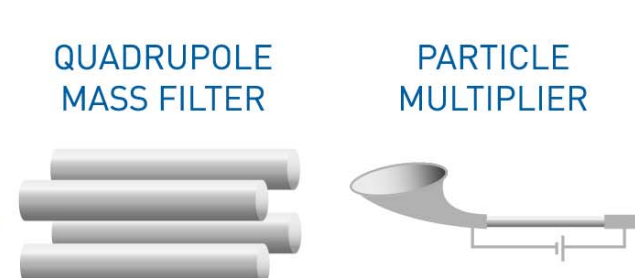
MULTIPLE
REAGENT IONS

Analyte Ionization



ULTRA-SOFT SAMPLE
IONIZATION

Analyte Quantitation

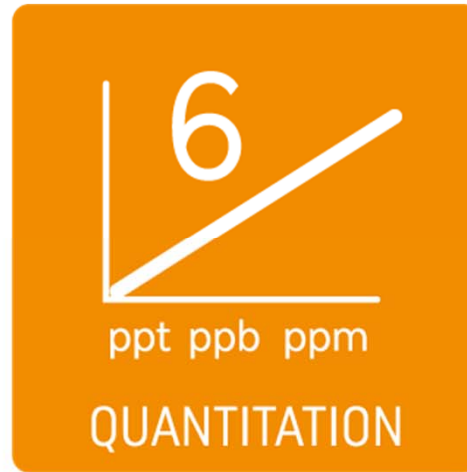


$$[\text{A}] = \gamma \frac{[\text{P}^+]}{[\text{R}^+]^k} \quad \text{or} \quad [\text{A}] = \gamma \frac{[\text{P}^-]}{[\text{R}^-]^k}$$

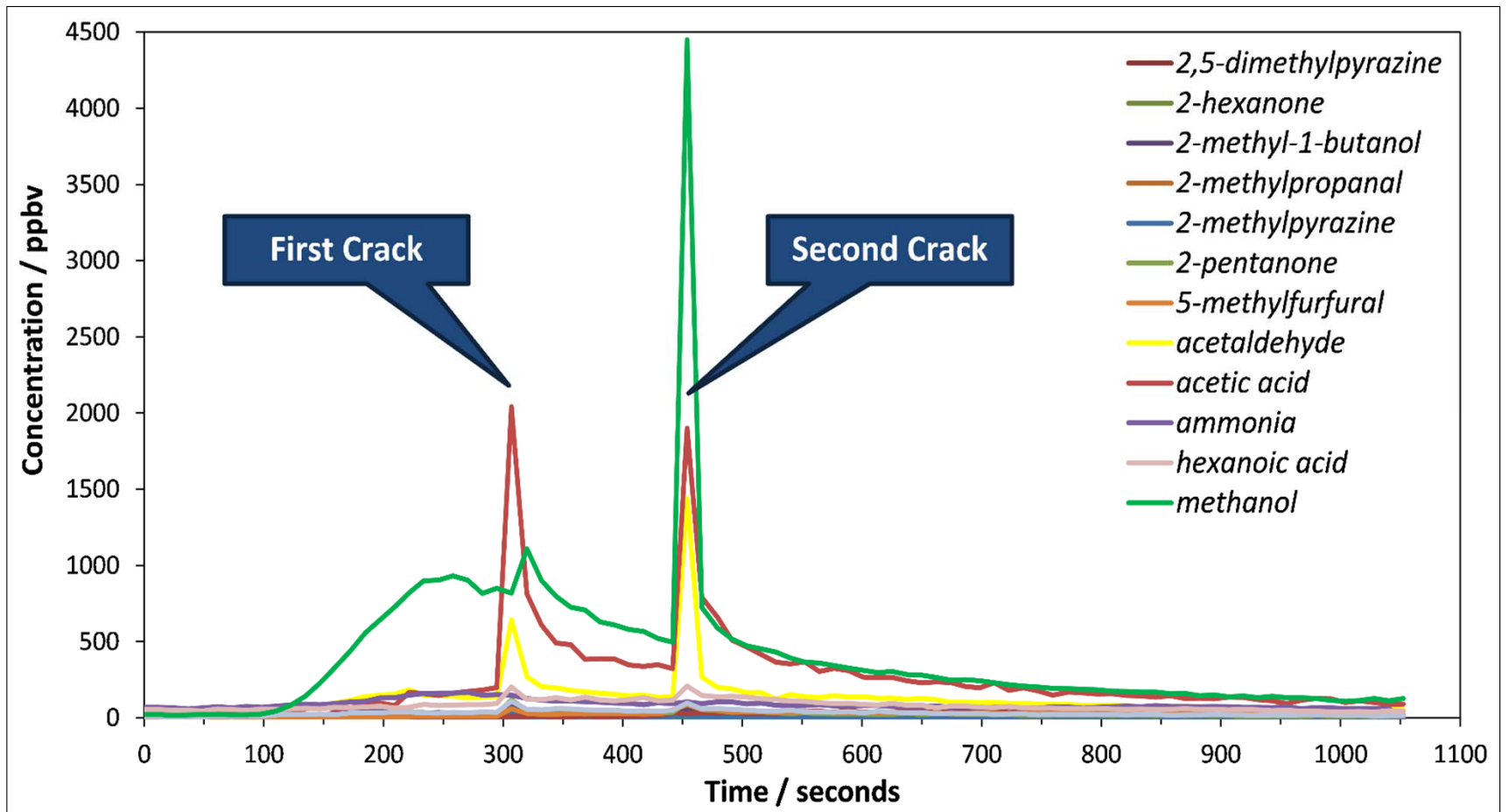
γ = instrument calibration factor

MASS
SPECTROMETER





SIFT-MS: Key benefits







Benefit 1: Real-time analysis



Benefit 2: Comprehensive analysis from application of **eight** reagent ions

 SPEED	hydrocarbons	alkanes, alkenes, aromatics, monoterpenes
 SELECTIVITY	oxygenates	alcohols, aldehydes (including formaldehyde), ketones, esters, ethers, carboxylic acids
	nitrogen compounds	amines, amides, nitriles, nitrated organics, nitrosamines
 QUANTITATION	sulfur compounds	mercaptans, thioethers, carbonyl sulfide
	halogenated compounds	aliphatic and aromatic fluorides, chlorides, bromides and iodides
 DIRECT ANALYSIS	inorganics	ammonia, hydrogen cyanide, hydrogen sulfide, nitrogen dioxide, phosphine, hydrogen chloride, hydrogen fluoride, carbon dioxide, sulfur dioxide, ozone

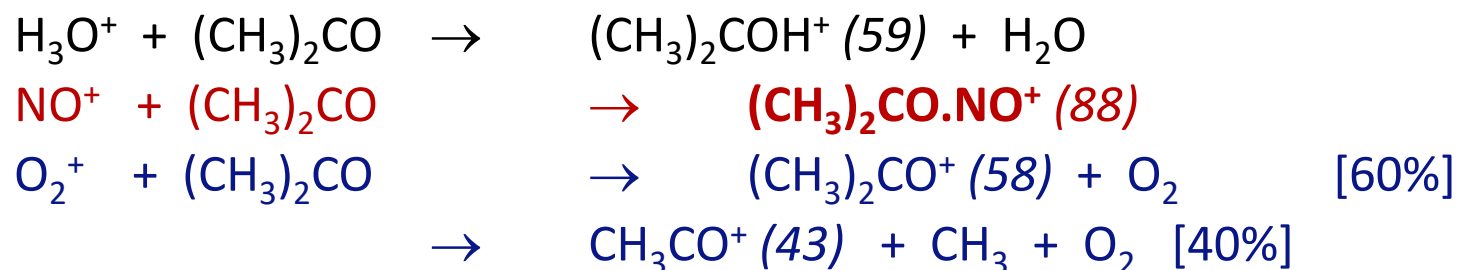
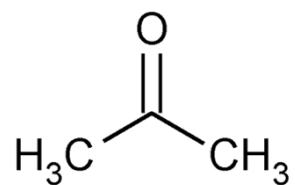
Benefit 2: Eight reagent ions coupled with MS also provides high selectivity

	Mechanism	H ₃ O ⁺	NO ⁺	O ₂ ⁺	OH ⁻	O ⁻	O ₂ ⁻	NO ₂ ⁻	NO ₃ ⁻
 SPEED	Proton transfer (PT)	✓	✗	✗					
	Electron transfer (ET)	✗	✓	✓	✗	✗	✓	✗	✗
 SELECTIVITY	Dissociative ET	✗	✓	✓					
	Hydride abstraction	✗	✓	✓					
 QUANTITATION	Association	✓	✓	✗	✓	✓	✓	✗	✗
	Proton abstraction				✓	✓	✓	✓	✓
	Hydrogen atom transfer				✗	✓	✗	✗	✗
 DIRECT ANALYSIS	Associative detachment				✓	✓	✓	✗	✗
	Displacement				✓	✓	✗	✗	✗
	Elimination				✓	✓	✗	✗	✗

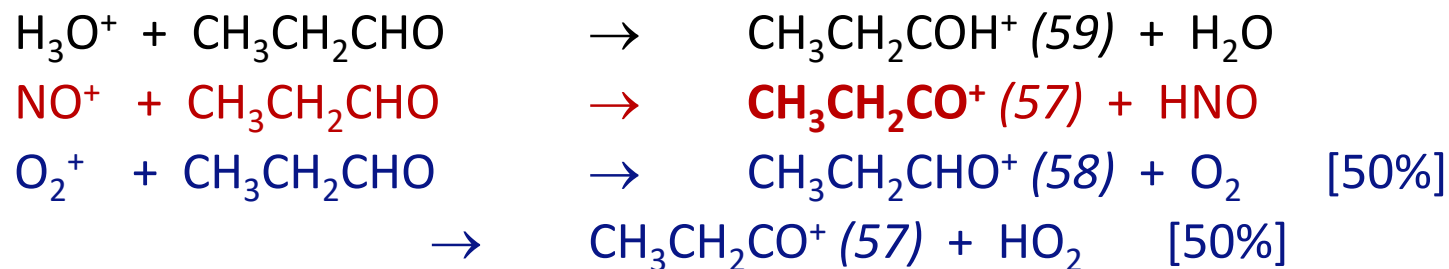
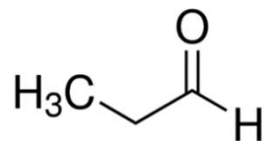
Benefit 2: Eight reagent ions coupled with MS also provides high selectivity

The multiple reagent ion system of SIFT-MS is able to resolve certain isobaric and isomeric compounds.

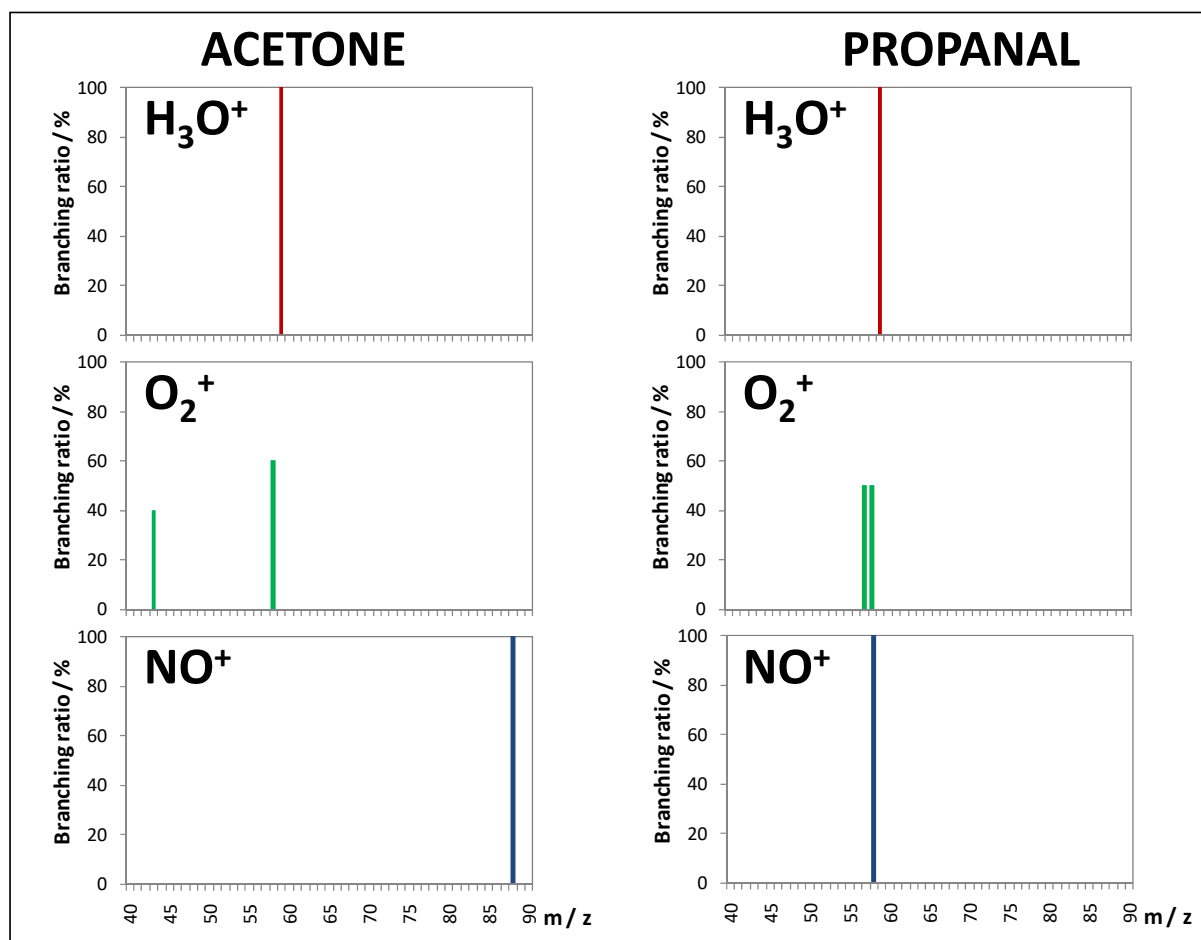
Acetone



Propanal

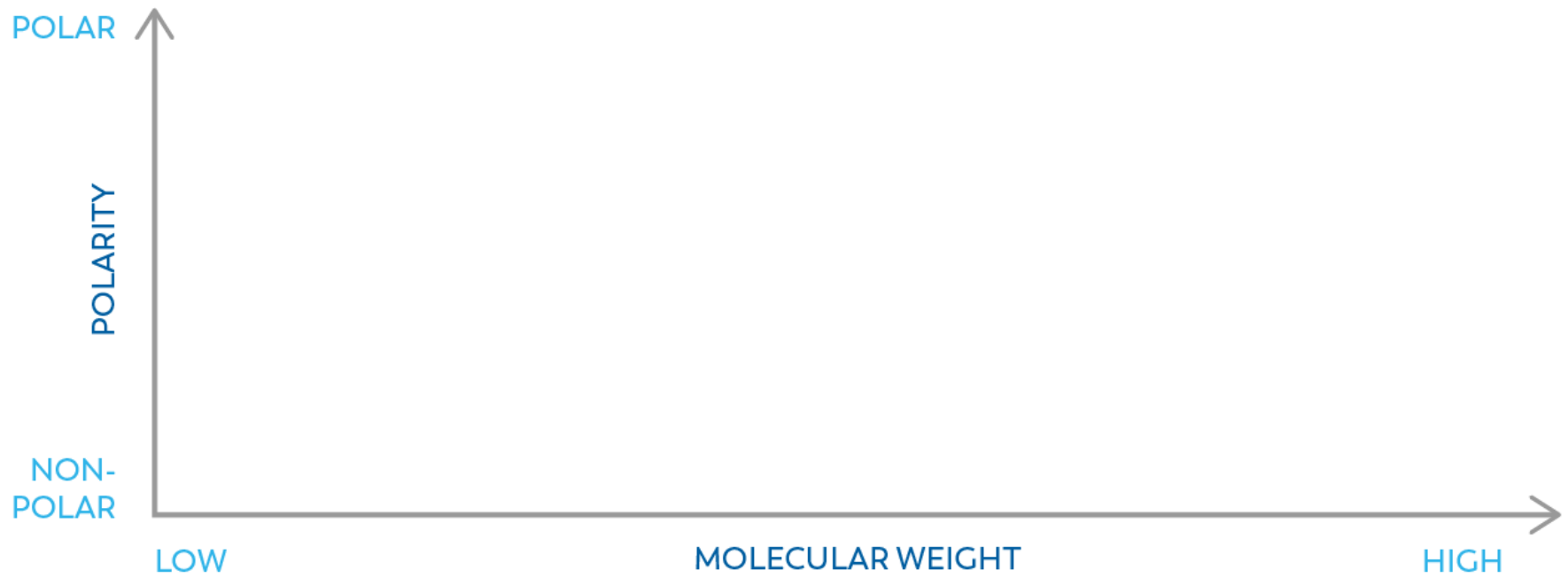


Benefit 2: Eight reagent ions coupled with MS also provides high selectivity



Reagent Ion	Ionization mechanism(s) (analyte-dependent)
H ₃ O ⁺	Proton transfer $\text{H}_3\text{O}^+ + \text{A} \rightarrow \text{A}.\text{H}^+ + \text{H}_2\text{O}$
O ₂ ⁺	Electron transfer (ET) $\text{O}_2^+ + \text{A} \rightarrow \text{A}^+ + \text{O}_2$ Dissociative ET $\text{O}_2^+ + \text{A} \rightarrow \text{Fragment}^+ + \dots$
NO ⁺	Association $\text{NO}^+ + \text{A} + \text{M} \rightarrow \text{A}.\text{NO}^+ + \text{M}$ Hydride abstraction $\text{NO}^+ + \text{A} \rightarrow [\text{A}-\text{H}]^+ + \text{HNO}$

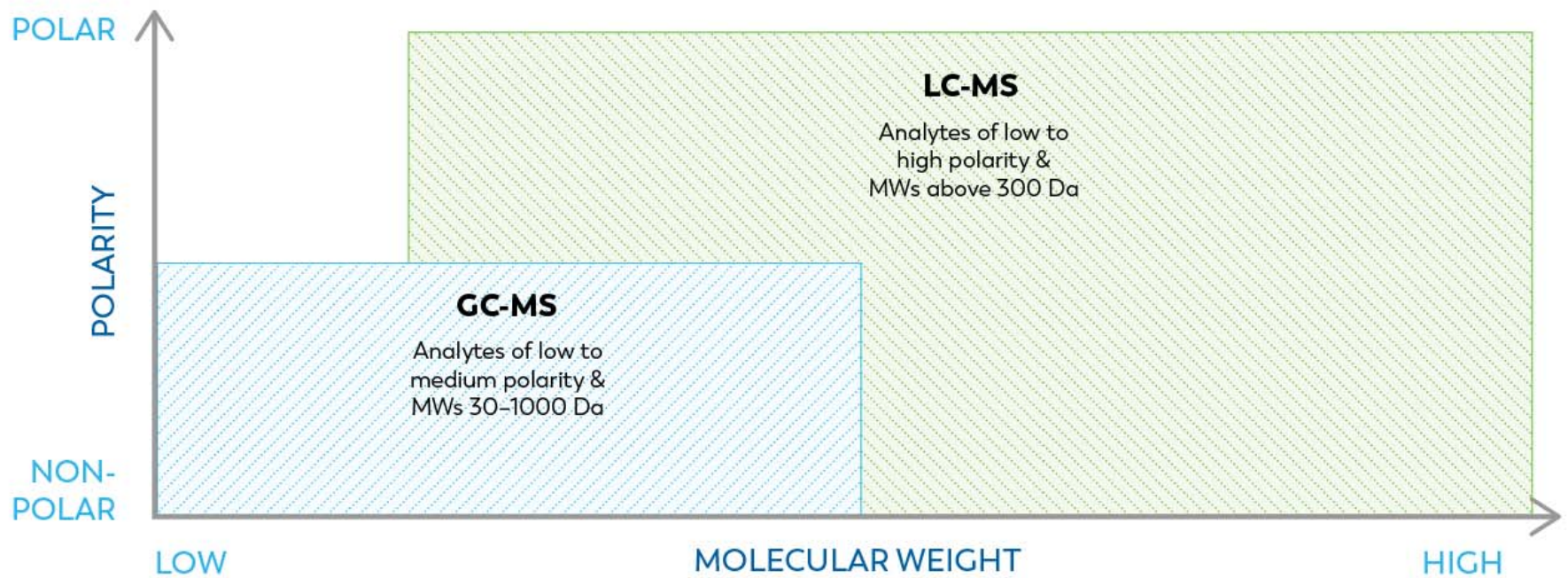
Finding the missing piece of the analytical puzzle...



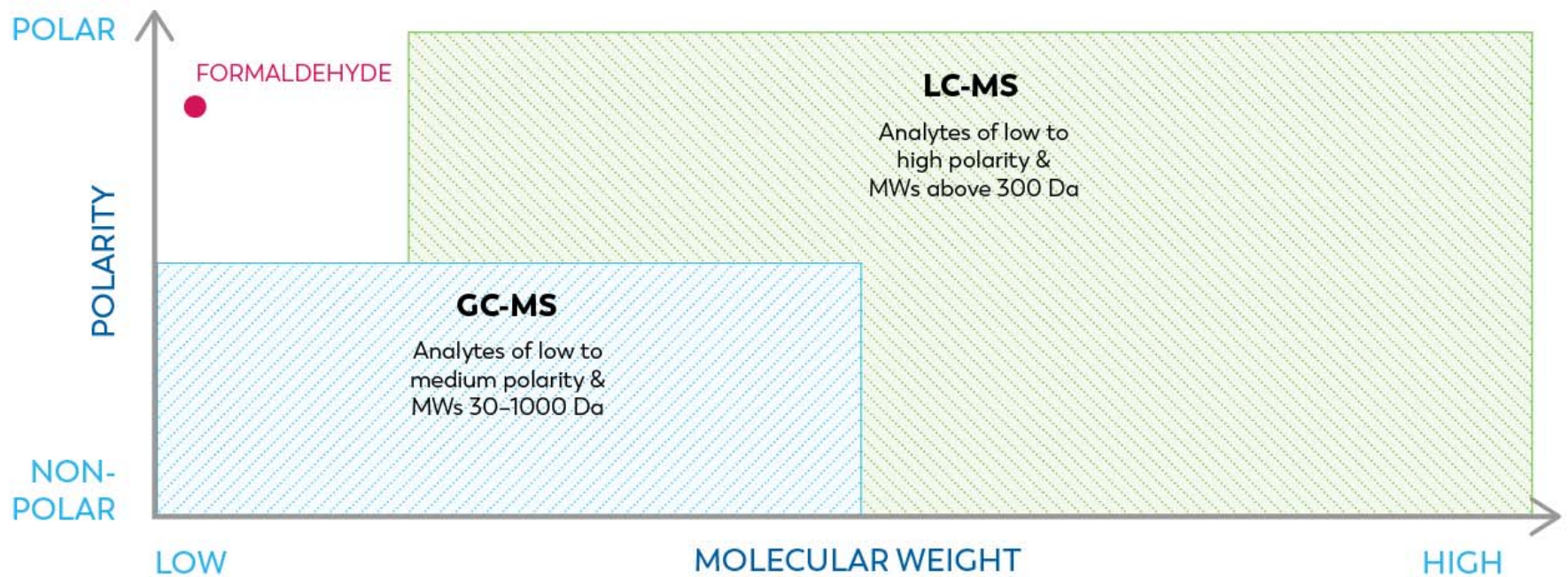
Finding the missing piece of the analytical puzzle...



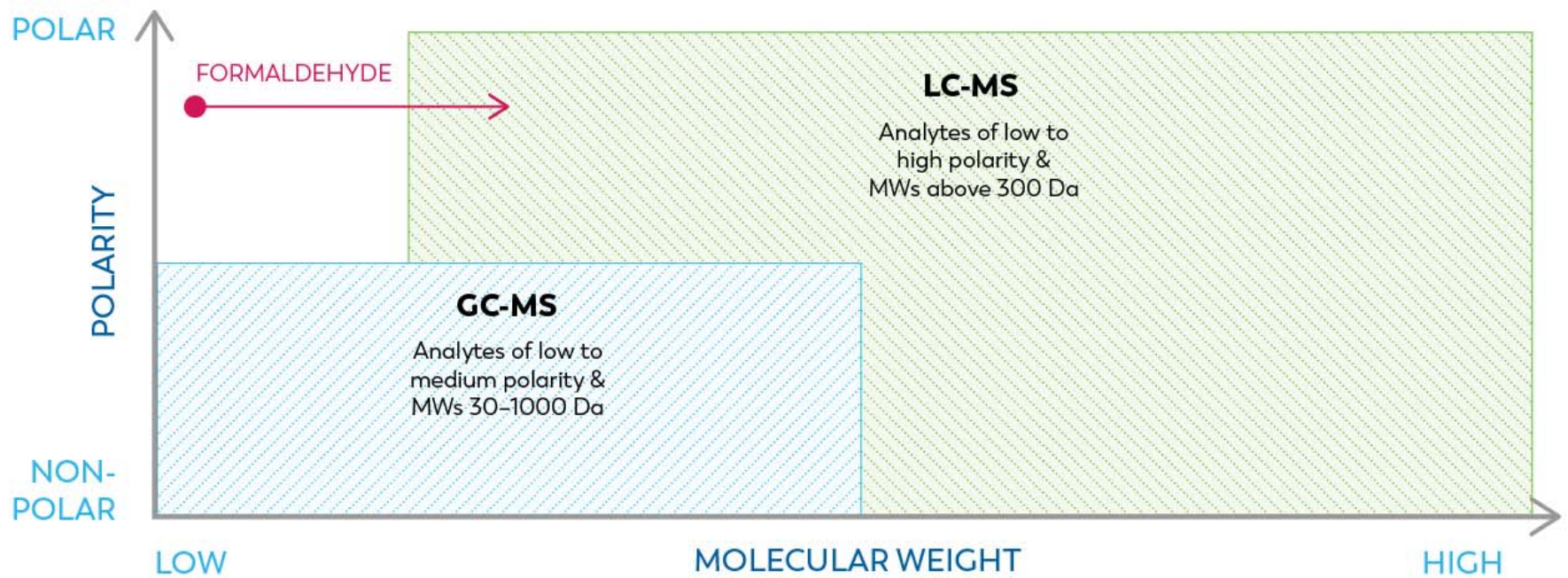
Finding the missing piece of the analytical puzzle...



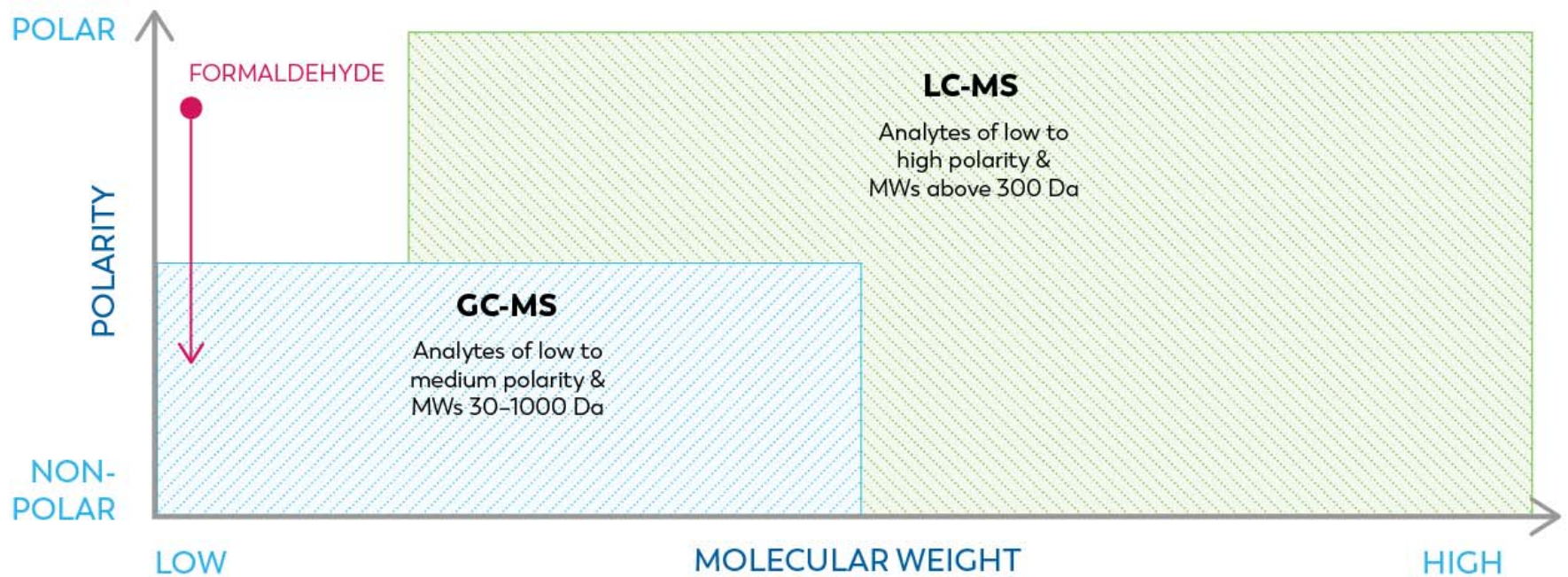
Finding the missing piece of the analytical puzzle...



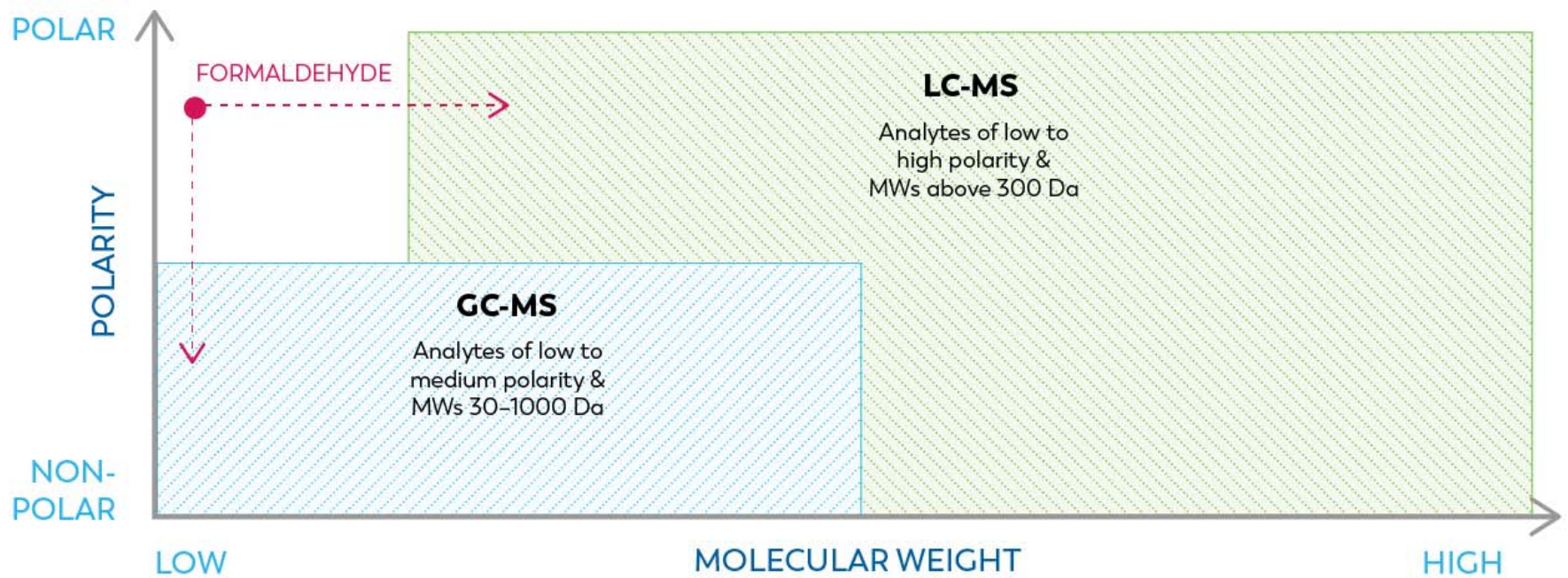
Finding the missing piece of the analytical puzzle...



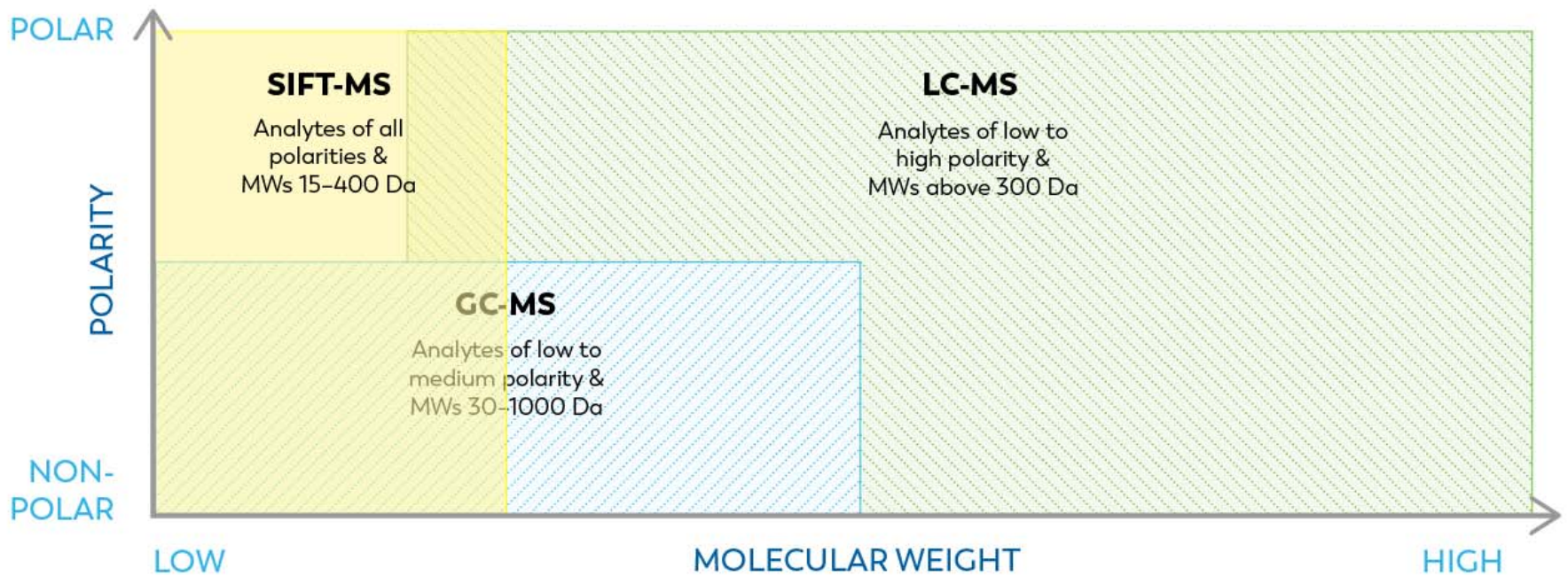
Finding the missing piece of the analytical puzzle...



Finding the missing piece of the analytical puzzle...

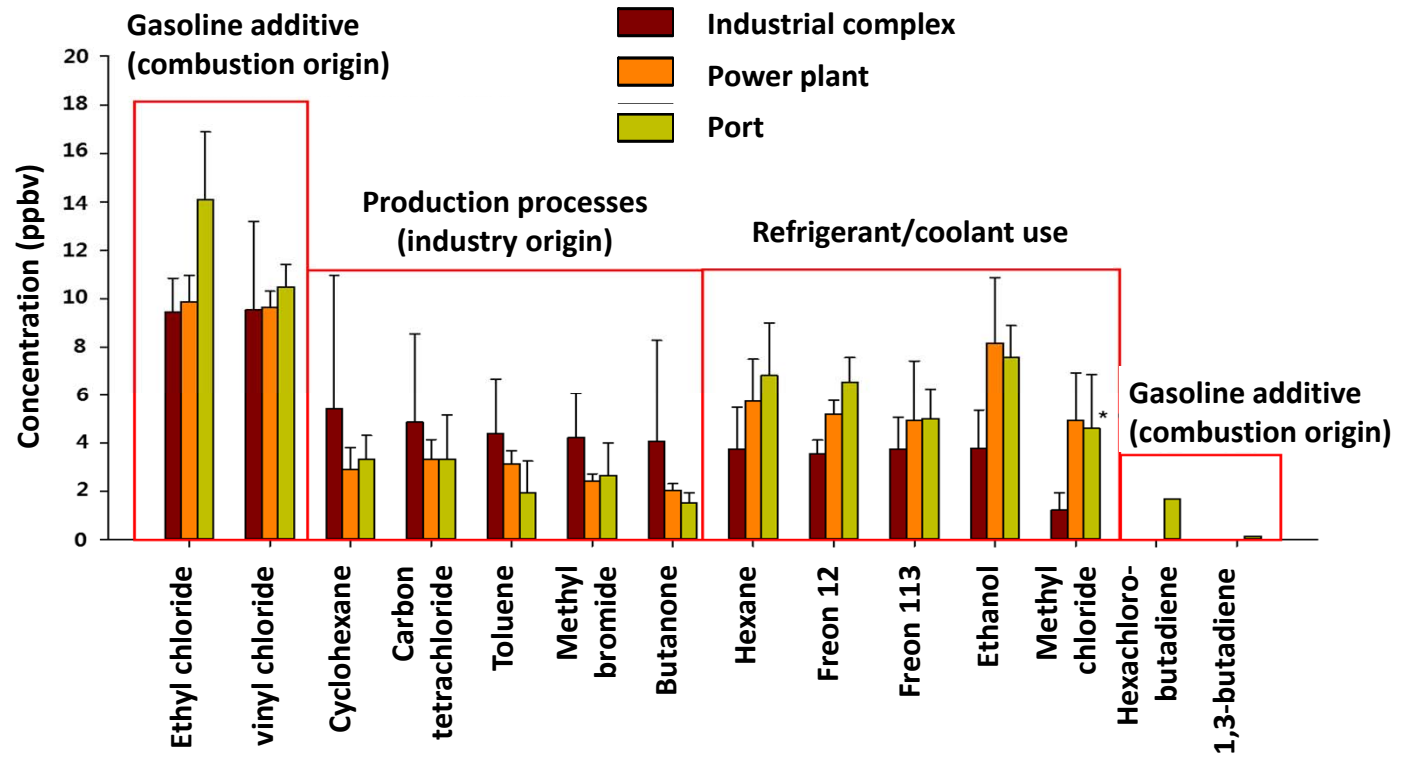
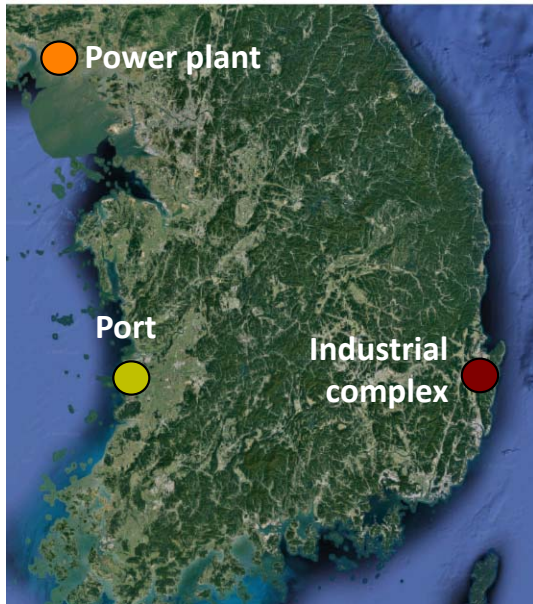


The missing piece of the analytical puzzle is SIFT-MS!



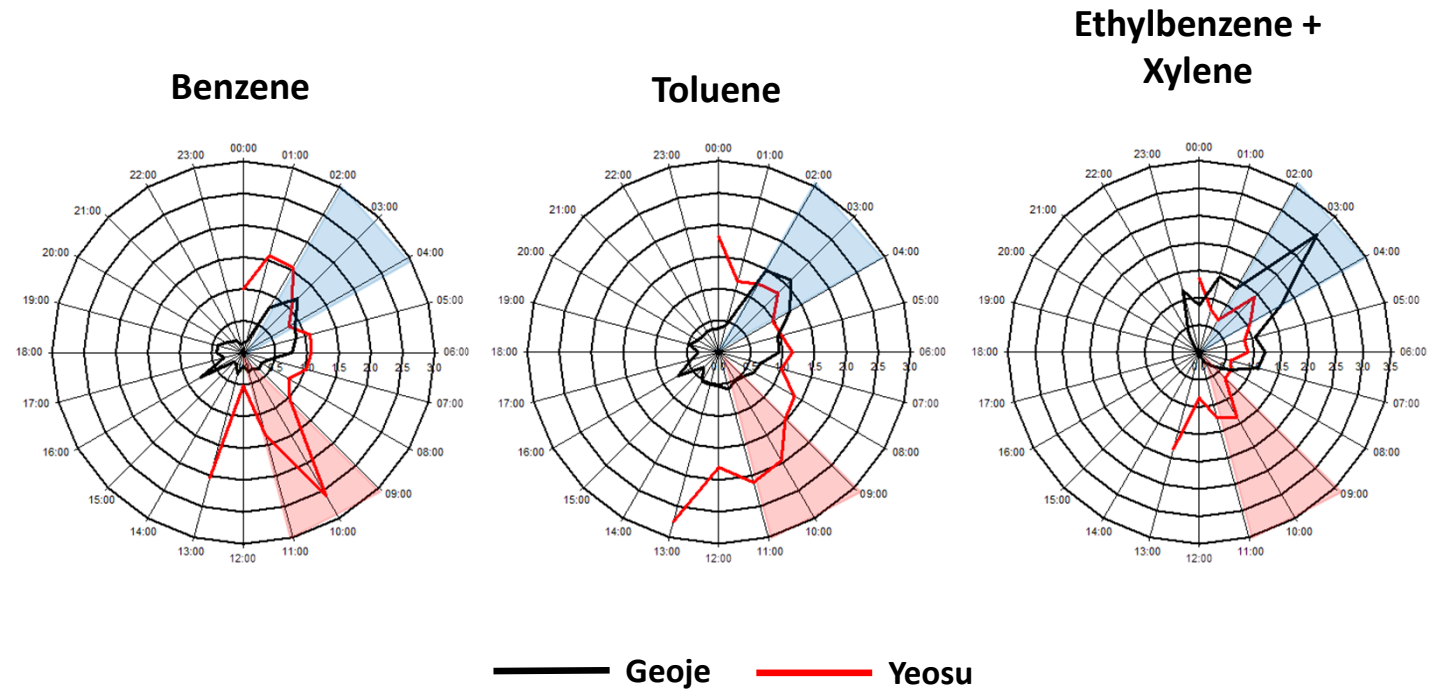
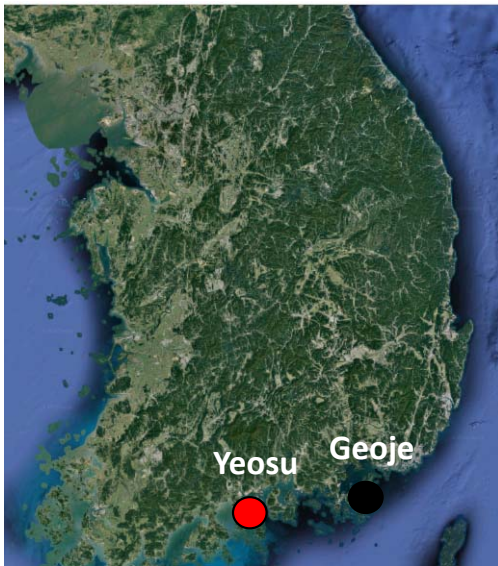
Site emission comparison on the Korean Peninsula: One-hour monitoring

Comparing the top 14 species for three facilities

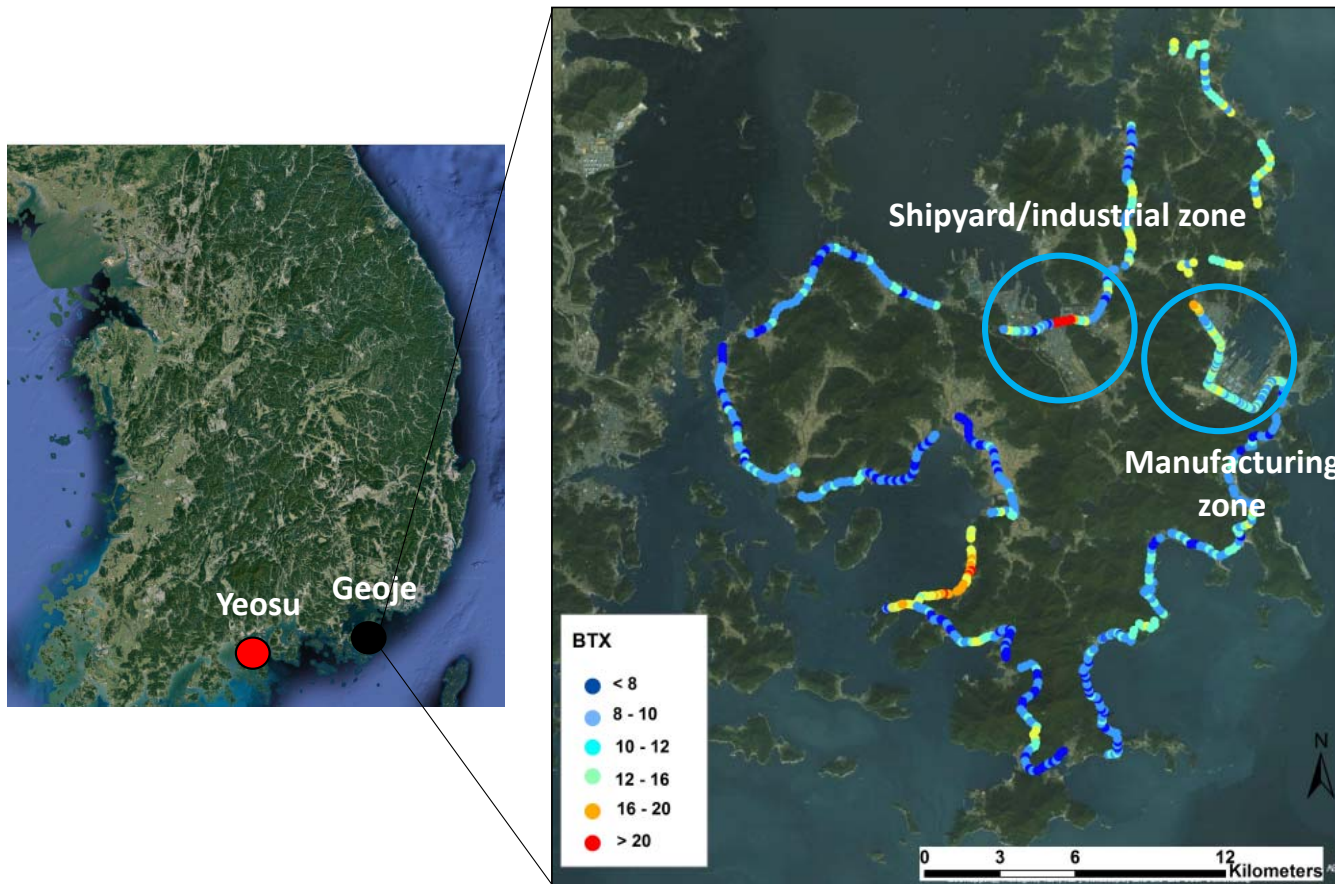


Site emission comparison on the Korean Peninsula: 24-hour monitoring

24-hour monitoring of two separate industrial zones



Mobile BTEX measurement on the Korean peninsular: Regional monitoring

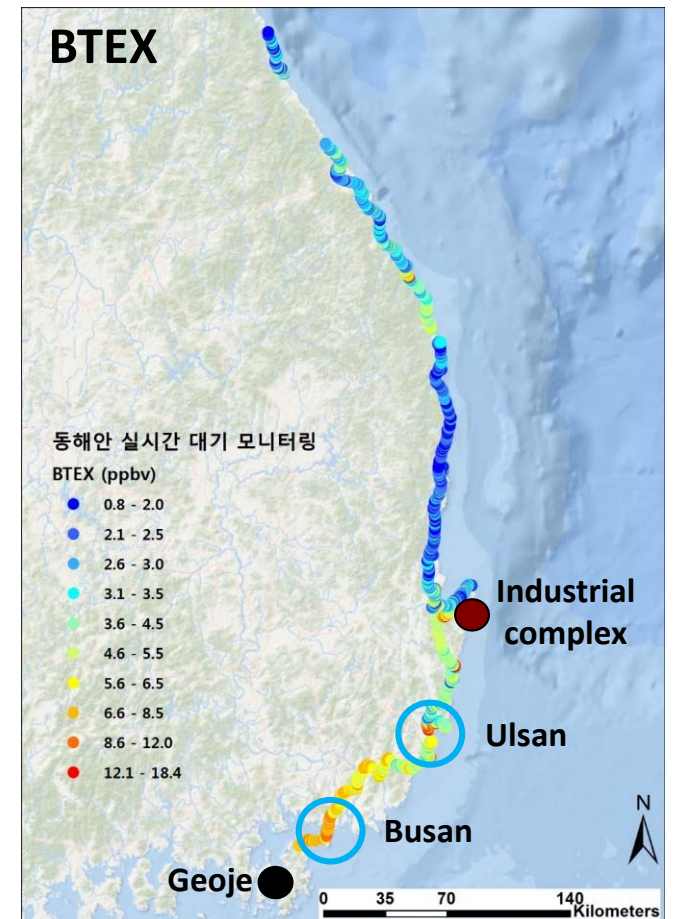
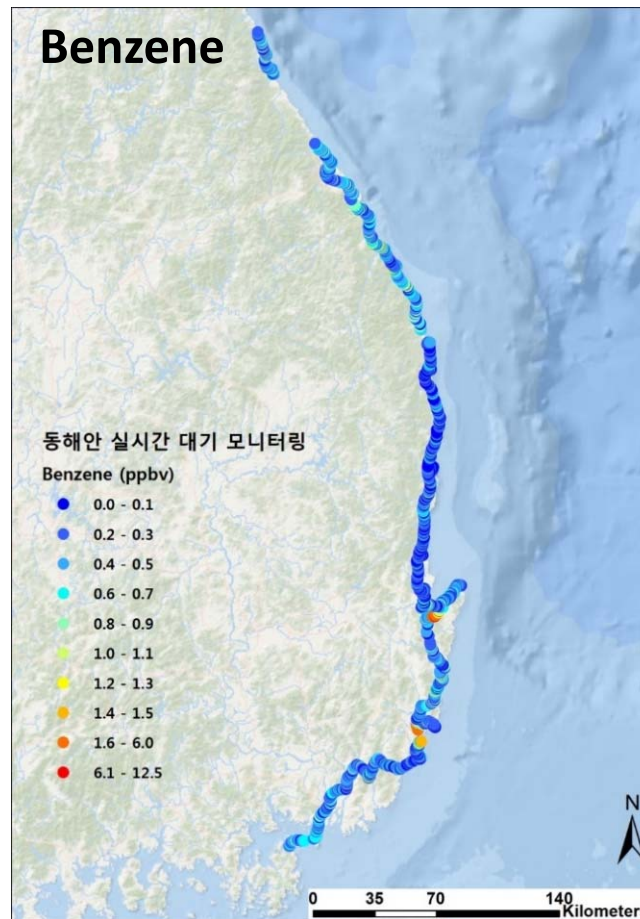
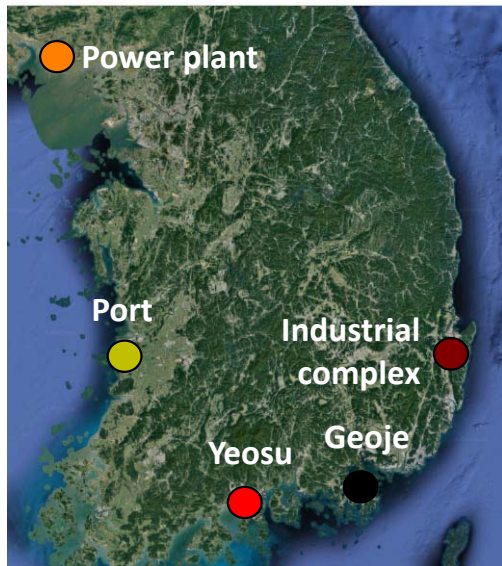


SIFT-MS data from moving van-mounted unit

Concentration and GPS data integrated for regional pollution mapping


Higher BTEX concentration for areas of greater industrial activity


Mobile BTEX measurement in the Korean peninsular: Regional monitoring





2020-06-22

 < 11

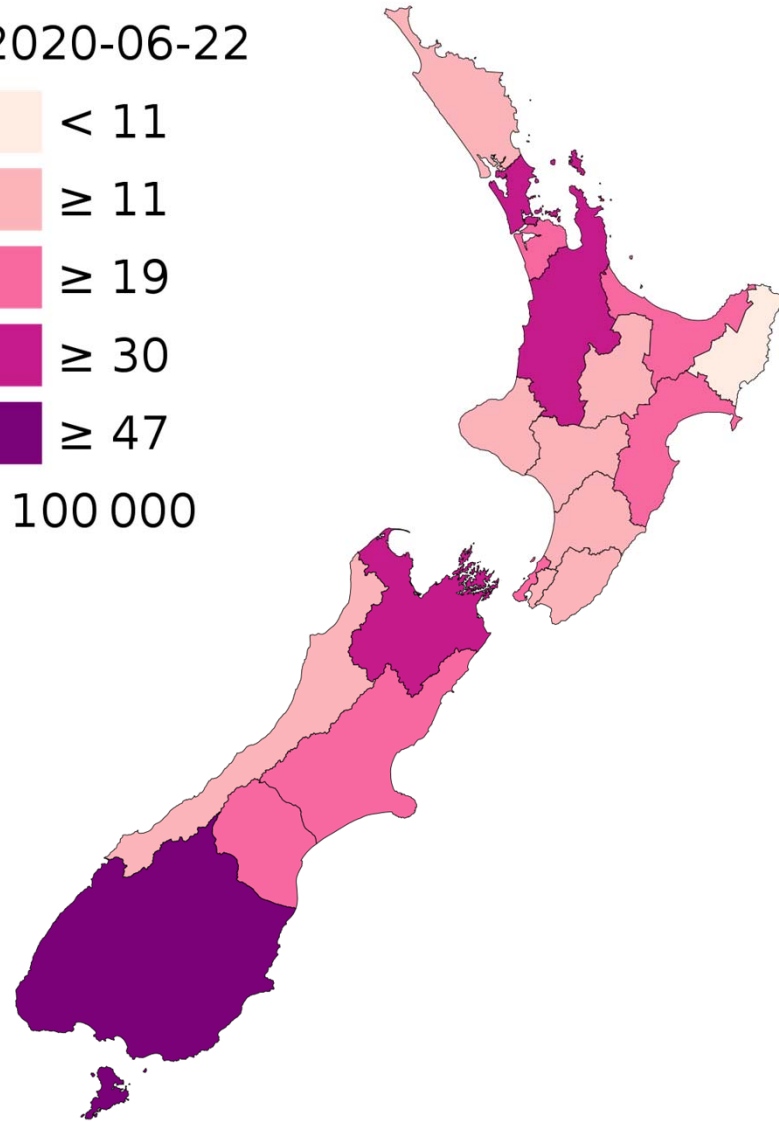
 ≥ 11

 ≥ 19

 ≥ 30

 ≥ 47

/ 100 000



Stages of alert

ALERT LEVEL ONE: PREPARE

Covid-19 in NZ, but contained

- Activate border measures
- Contact tracing
- Cancel mass gatherings of more than 500 people
- Stay at home if sick and report flu-like symptoms
- Intensive testing for Covid-19
- Physical distancing encouraged

ALERT LEVEL TWO: REDUCE

Contained but risk of community transmission growing

- Entry border measures maximised
- Further restrictions on mass gatherings
- Physical distancing on public transport
- Limit non-essential travel around country
- Employer to begin alternative ways of working if possible (shift work, working from home etc)
- Business contingency plans activated
- High risk people to remain at home (over 70s, people with existing conditions)

ALERT LEVEL THREE: RESTRICT

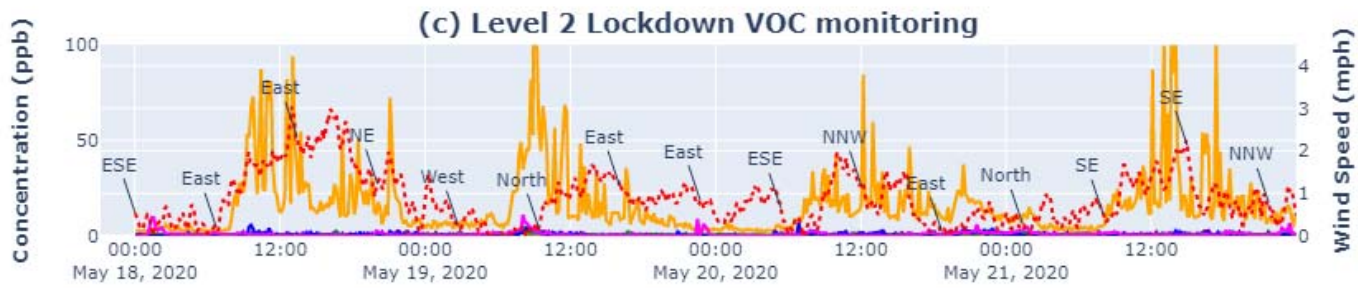
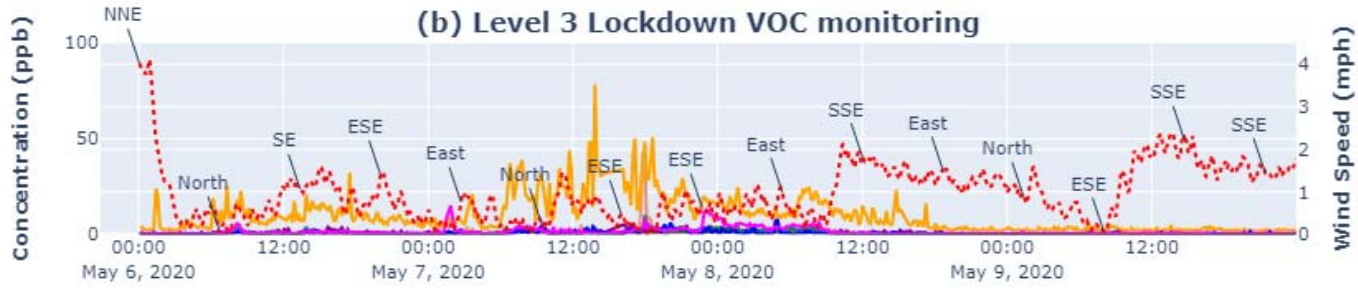
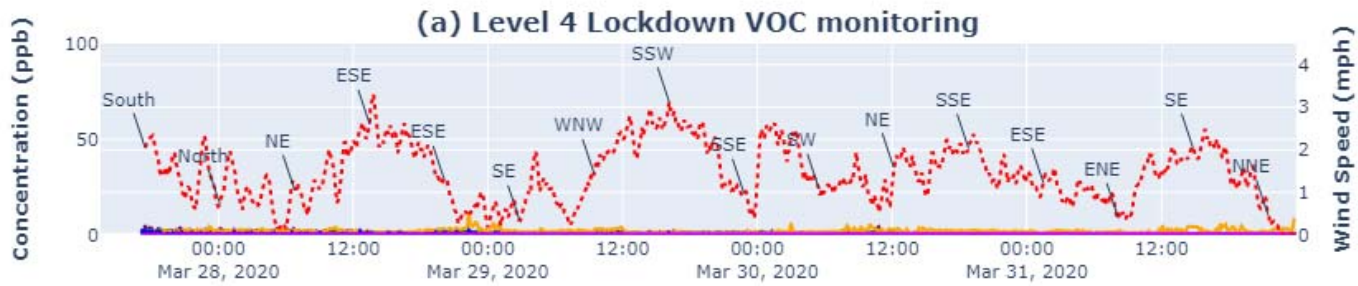
Heightened risk that disease not contained

- Travel in areas of community transmission limited
- Affected educational facilities closed
- Mass gatherings cancelled
- Public venues closed
- Alternative ways of working required and some non-essential businesses closed
- Non-face-to-face primary care consultations
- Elective surgeries and procedures deferred and healthcare staff reprioritised

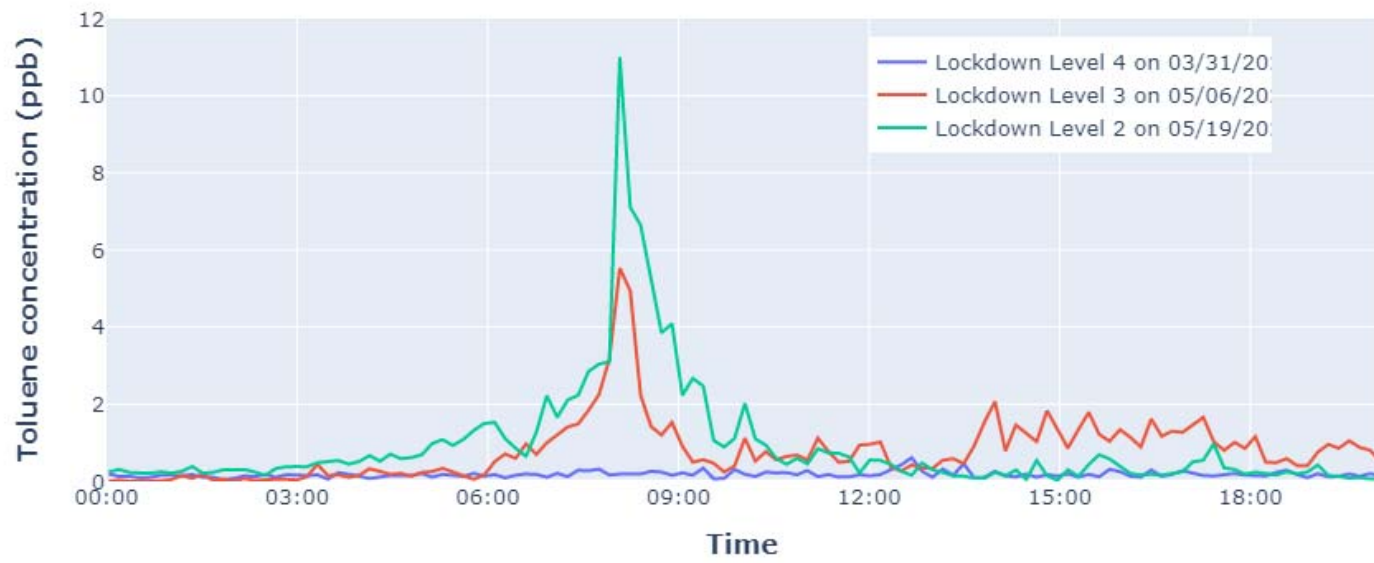
ALERT LEVEL FOUR: ELIMINATE

Likely that disease not contained

- People to stay at home
- Educational facilities closed
- All non-essential businesses closed
- Rationing of supplies and requisitioning of facilities
- Severe travel restrictions
- Major reprioritisation of healthcare services



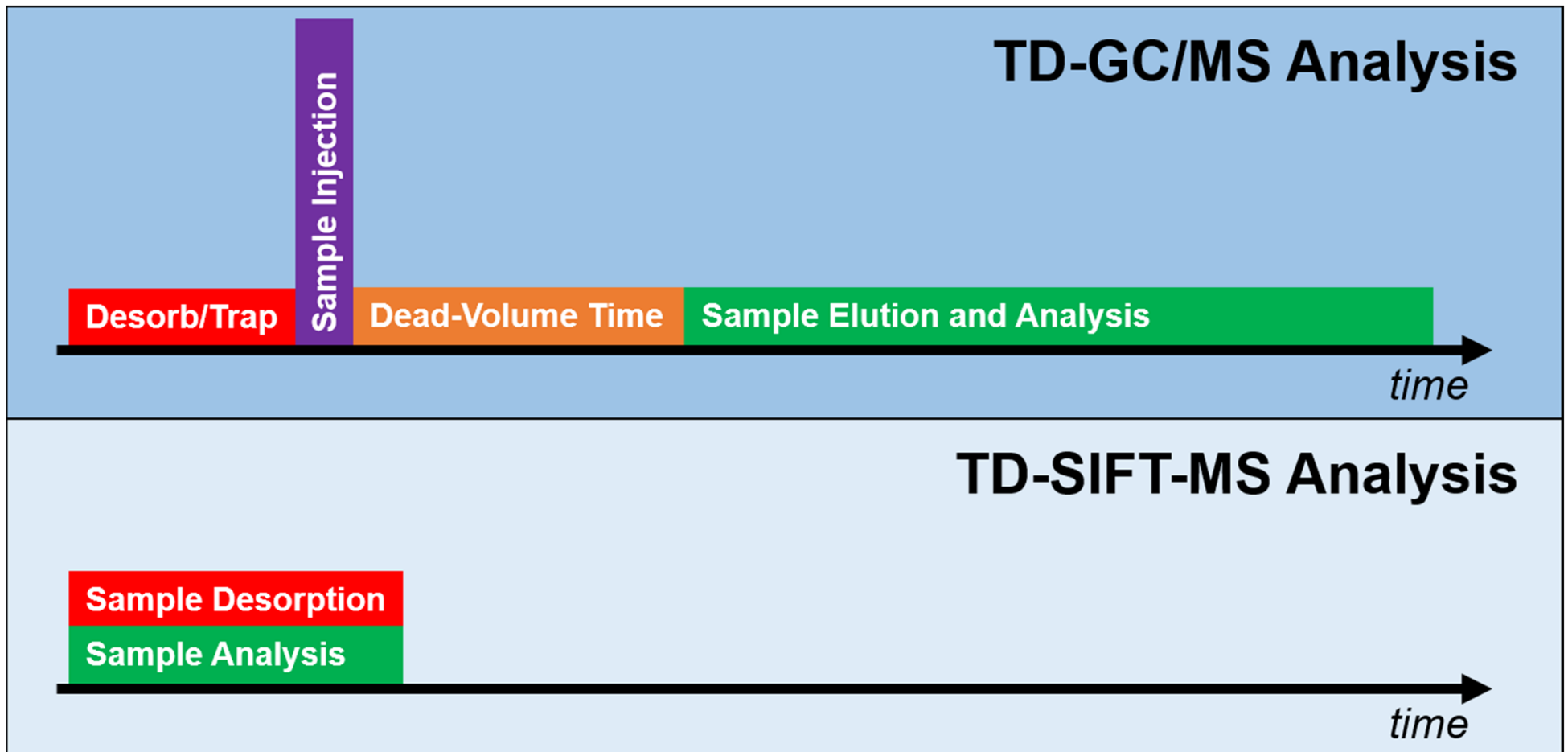
- Date**
- acetaldehyde (75-07-0)
 - acetone (67-64-1)
 - acrolein (107-02-8)
 - beta-pinene (127-91-3)
 - ethanol (64-17-5)
 - ethylbenzene+xylenes (100-41)
 - formaldehyde (50-00-0)
 - toluene (108-88-3)
 - ⋯ Wind speed (smoothed)



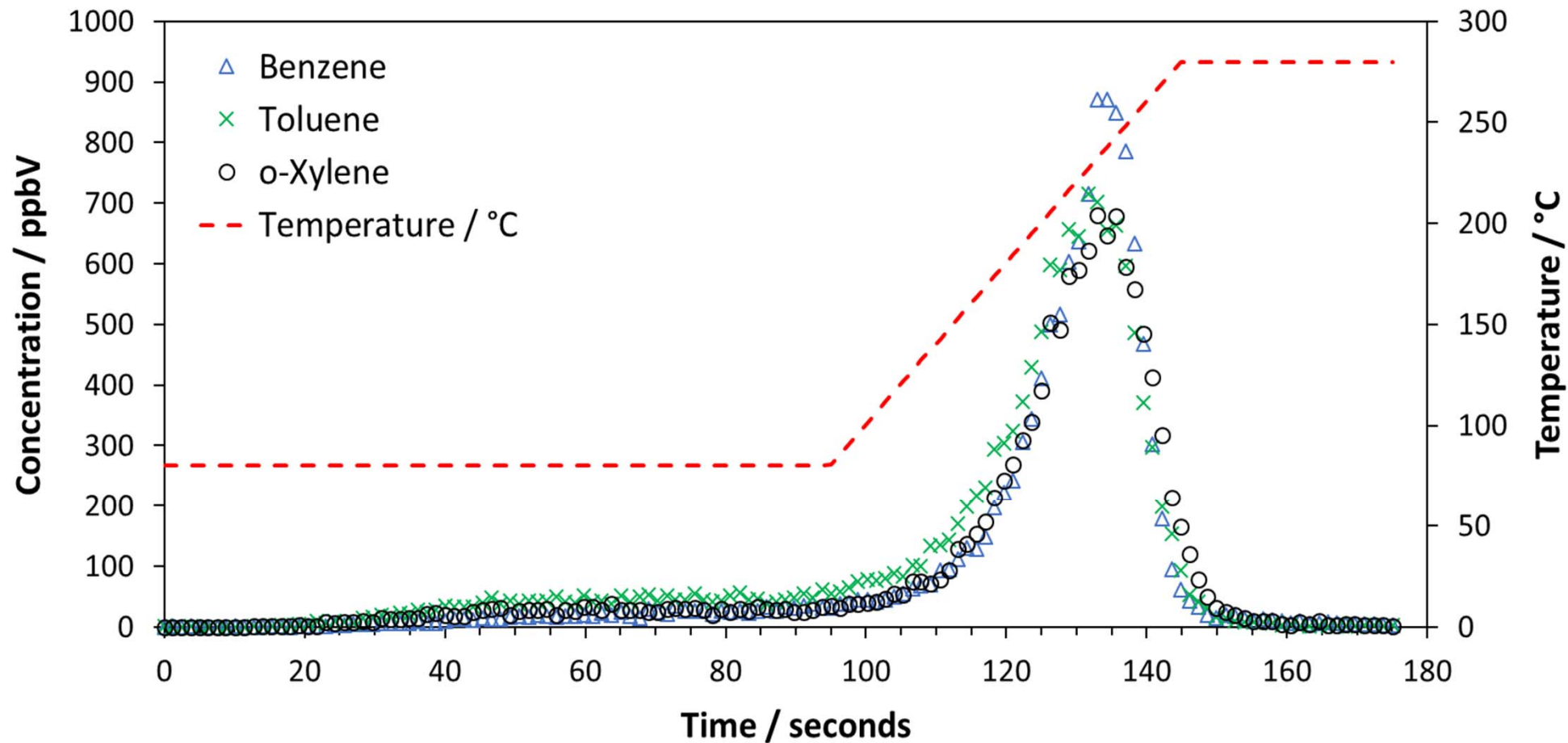


Thermal Desorption-SIFT-MS

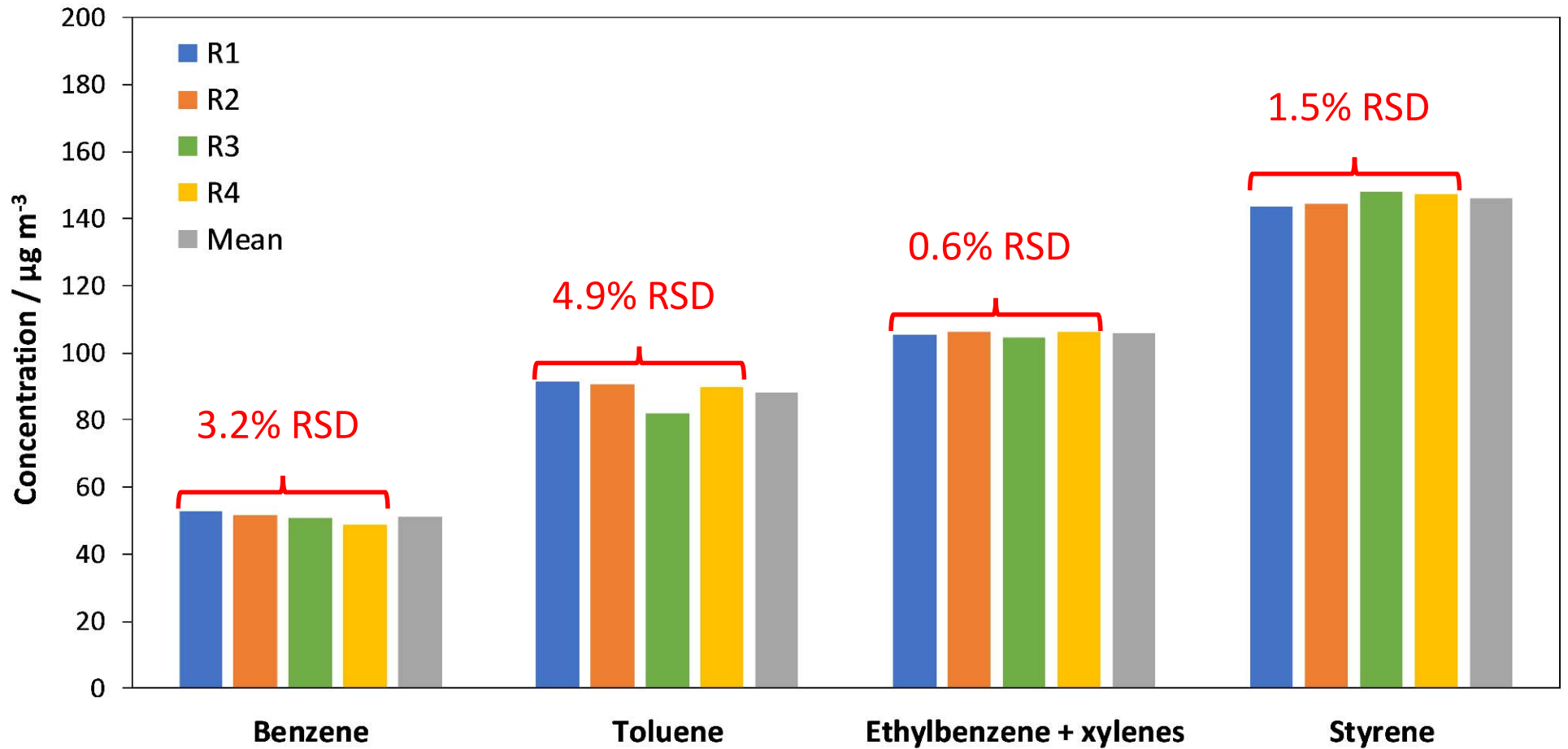
TD-GC/MS and TD-SIFT-MS analytical approaches are different!



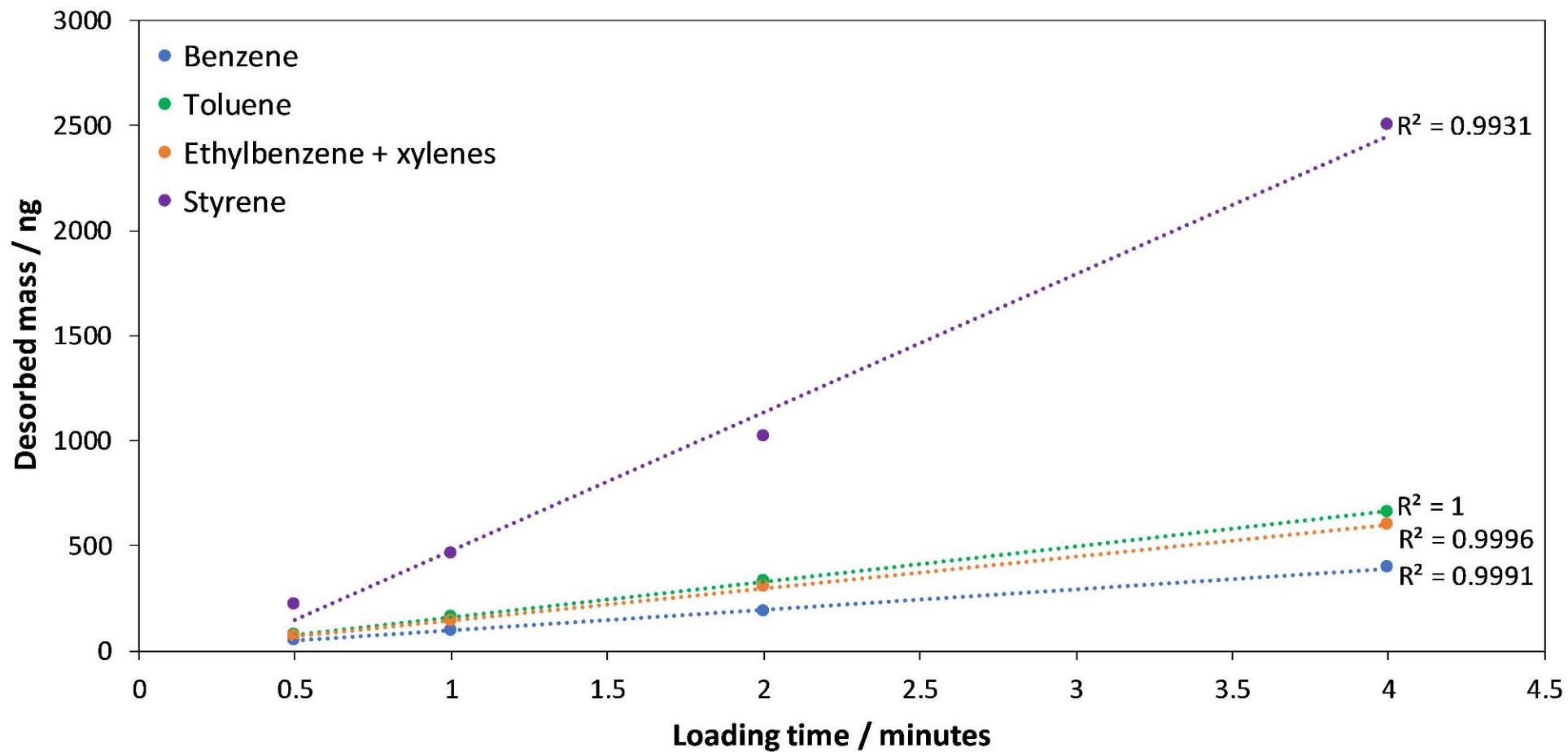
TD-SIFT-MS desorption profile



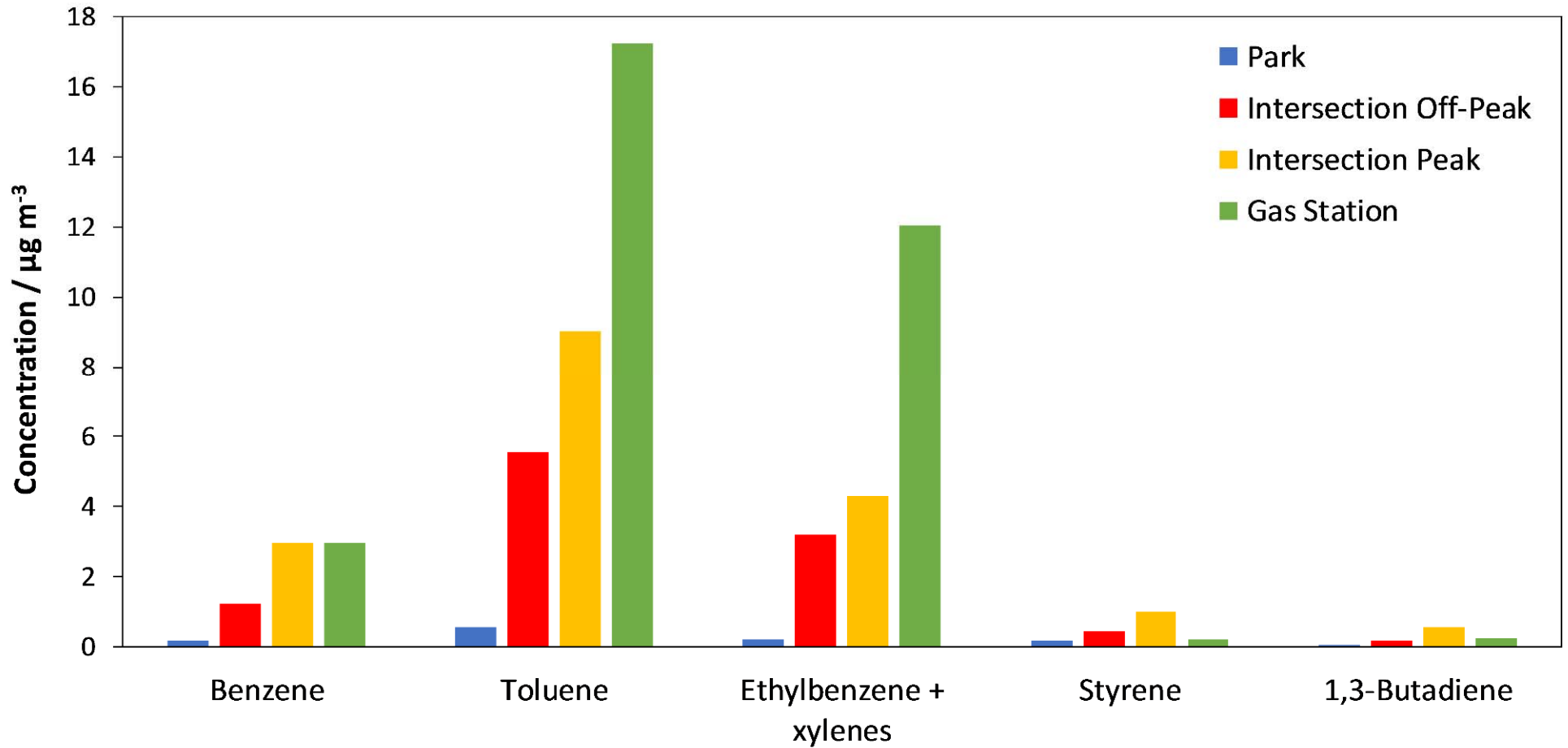
TD-SIFT-MS application: Rapid analysis of BTEX and styrene



TD-SIFT-MS loading and desorption linearity



TD-SIFT-MS application: Rapid analysis of environmental BTEX, etc.





**THANK YOU FOR YOUR ATTENTION!
QUESTIONS?**

Email: caleb.allpress@syft.com



syft.com