

Water Quality Monitoring 2.0

Finding what we've been missing using Non-Targeted Analyses

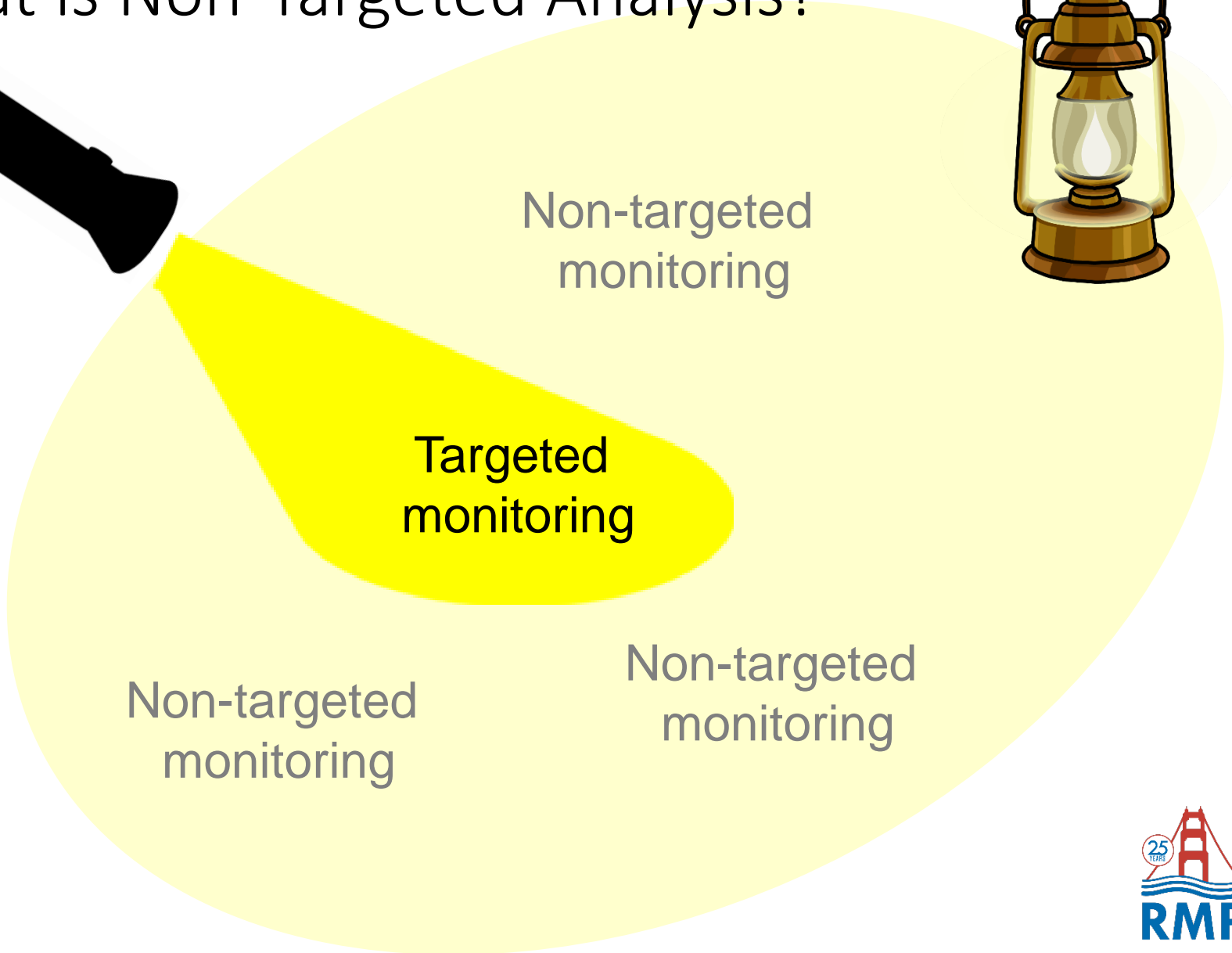
Jennifer Sun
Rebecca Sutton
San Francisco Estuary Institute

Lee Ferguson
Kirsten Overdahl
Duke University



2017

What is Non-Targeted Analysis?



Non-targeted monitoring

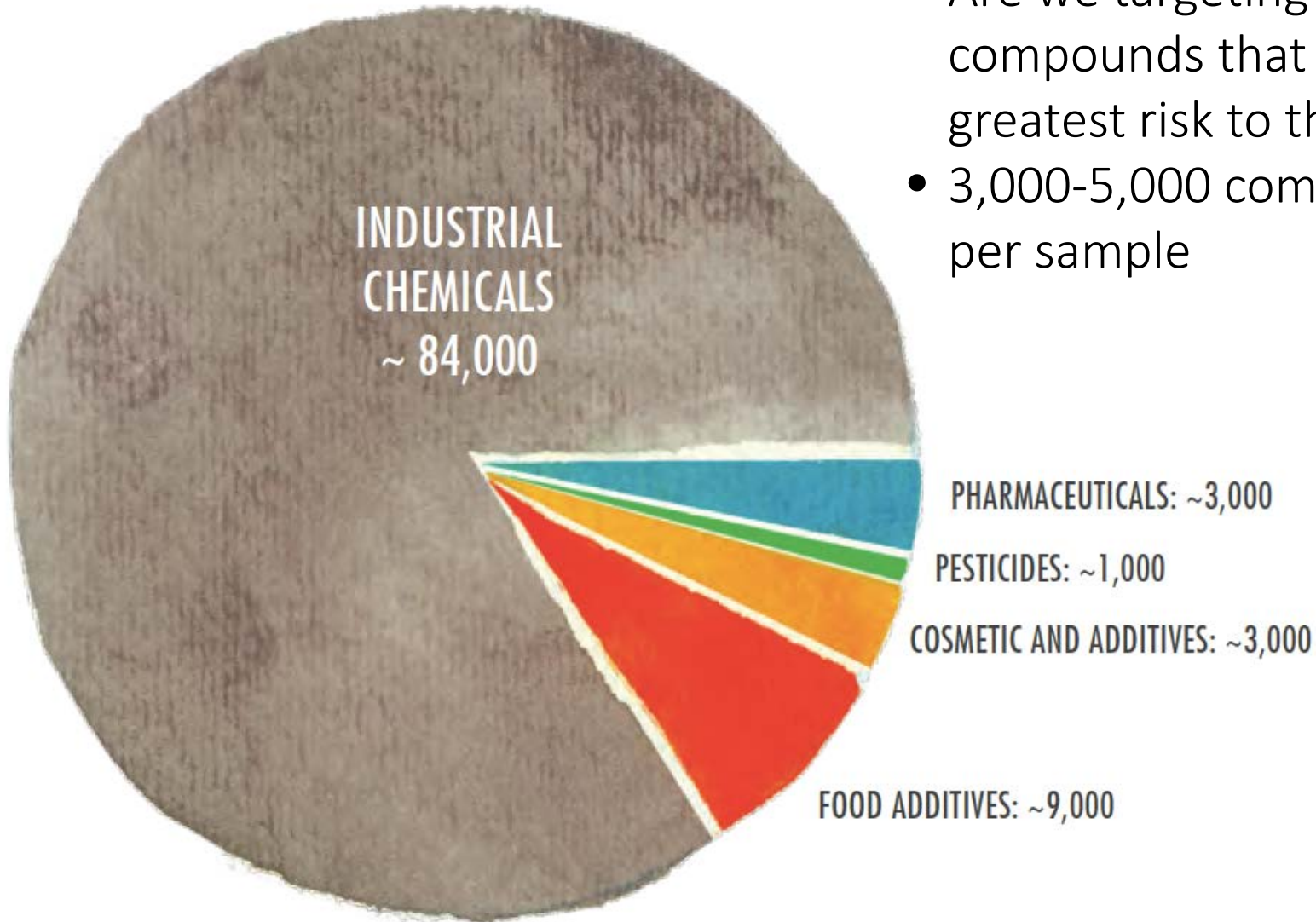
Targeted monitoring

Non-targeted monitoring

Non-targeted monitoring

Why do we need non-targeted analysis?

- Are we targeting the right compounds that pose the greatest risk to the Bay?
- 3,000-5,000 compounds per sample



RMP Non-Targeted Analyses



Mussels



Harbor seals

Wildlife tissue



Water



Ambient Bay water

Wastewater effluent



Sediment

Sediment

★ **Napa River**
April 2016
Agriculture

Study Design

3 ambient Bay sites

- Grab (before/after)
- Passive Sampler (1 month)

4 WWTP effluents

24hr composites

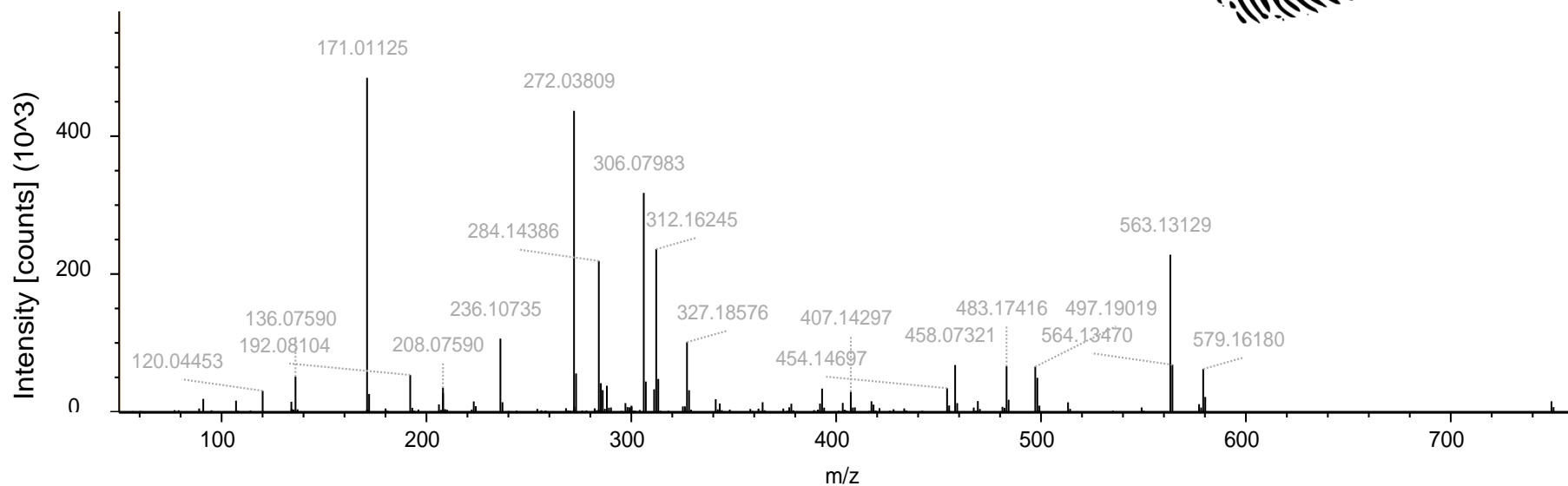
Passive sampler after a month
in San Leandro Bay
(polar organic contaminants)

★ **San Leandro Bay**
March 2016
Urban runoff

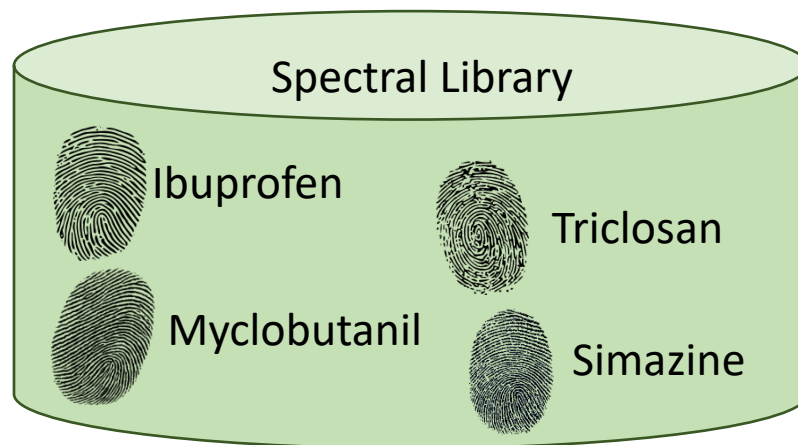
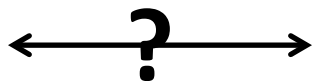
★ **Coyote Creek**
Aug/Sept 2016
WWTP



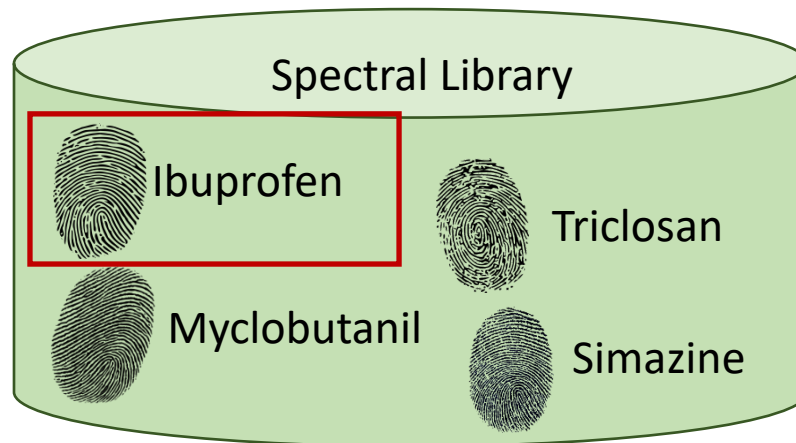
Chemical Identification



Chemical Identification

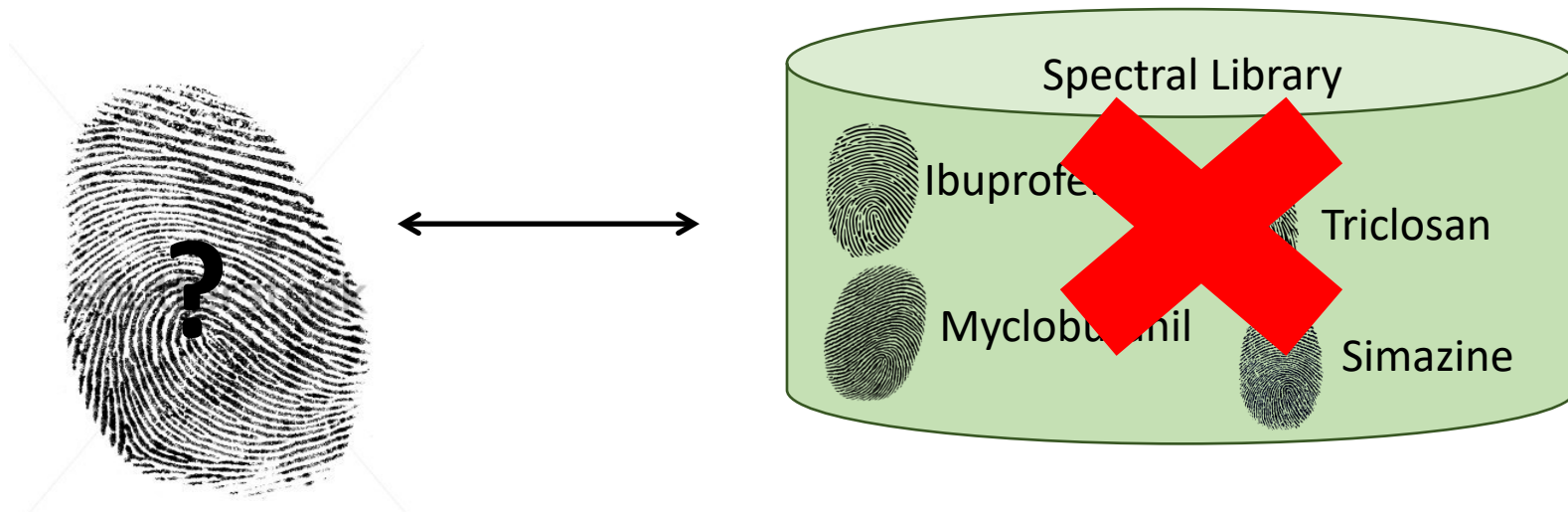


Chemical Identification

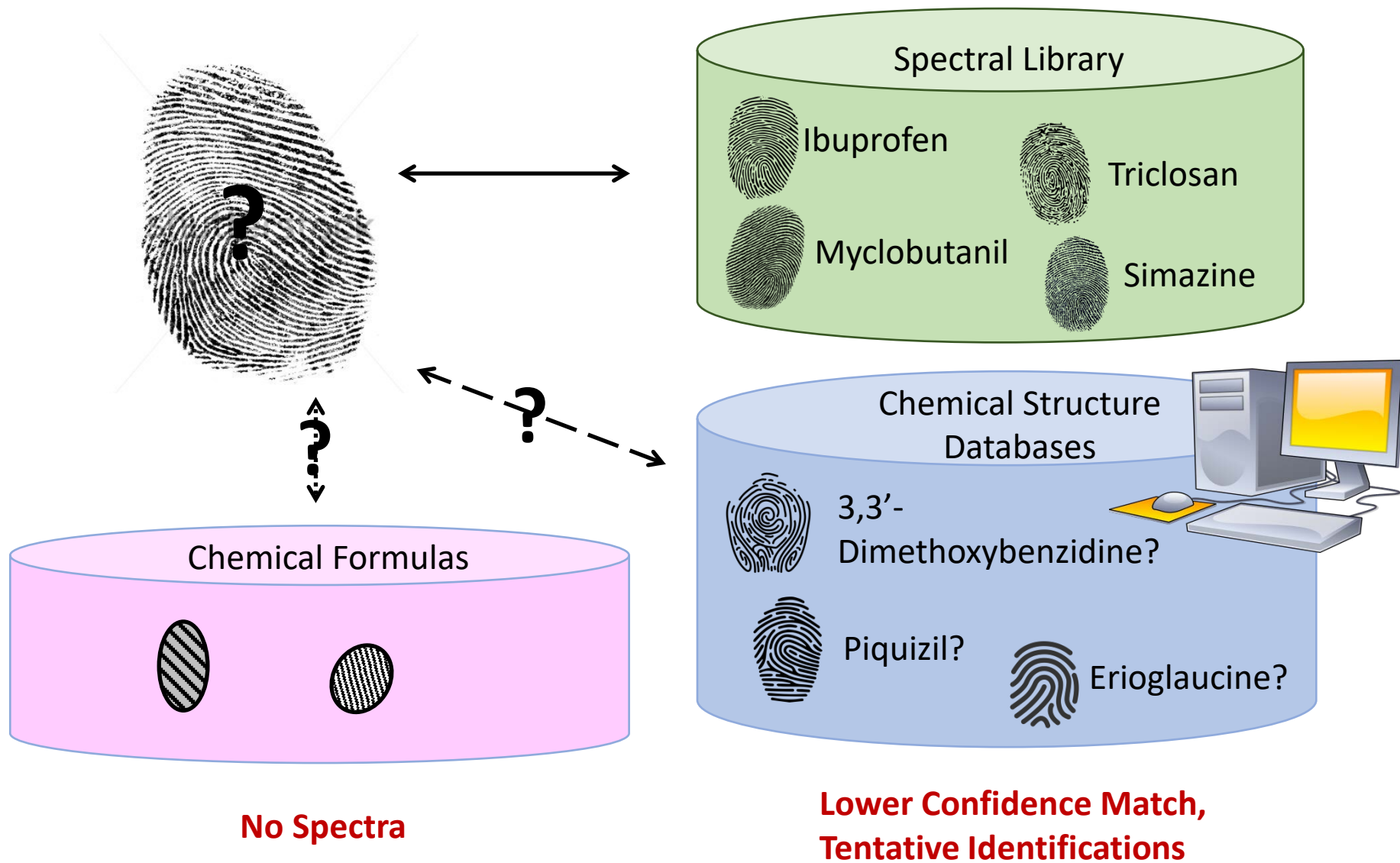


High Confidence Match

Chemical Identification



Chemical Identification



Chemical Identifications

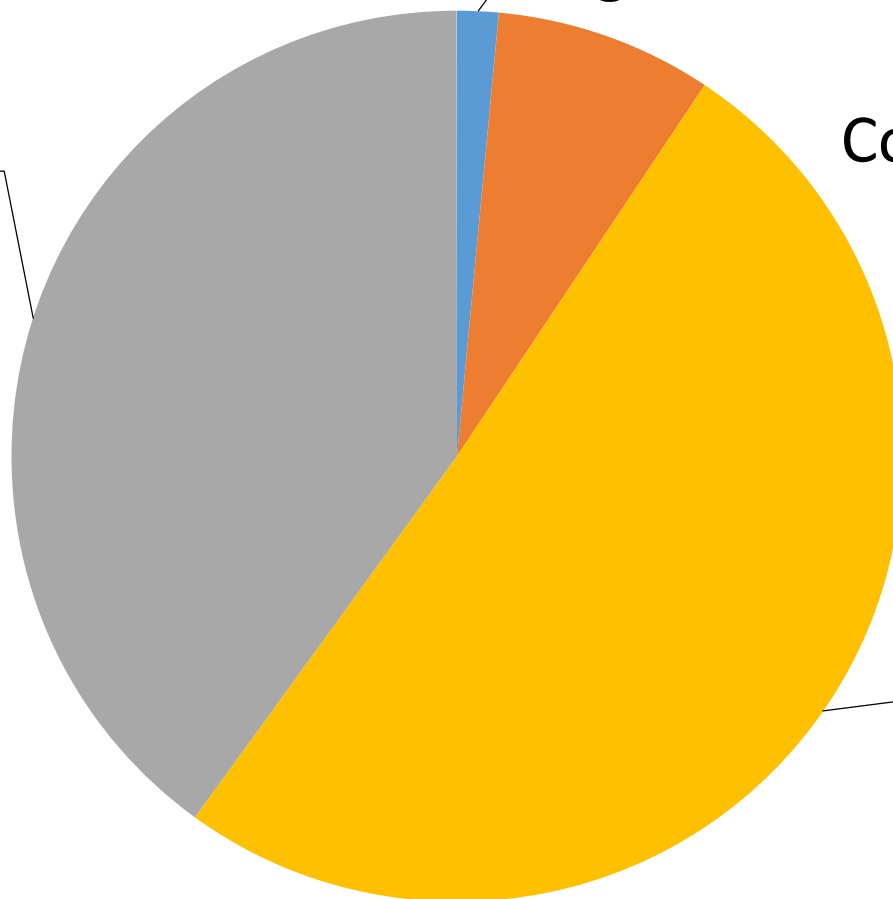
~5,000 compounds
observed

No Spectra

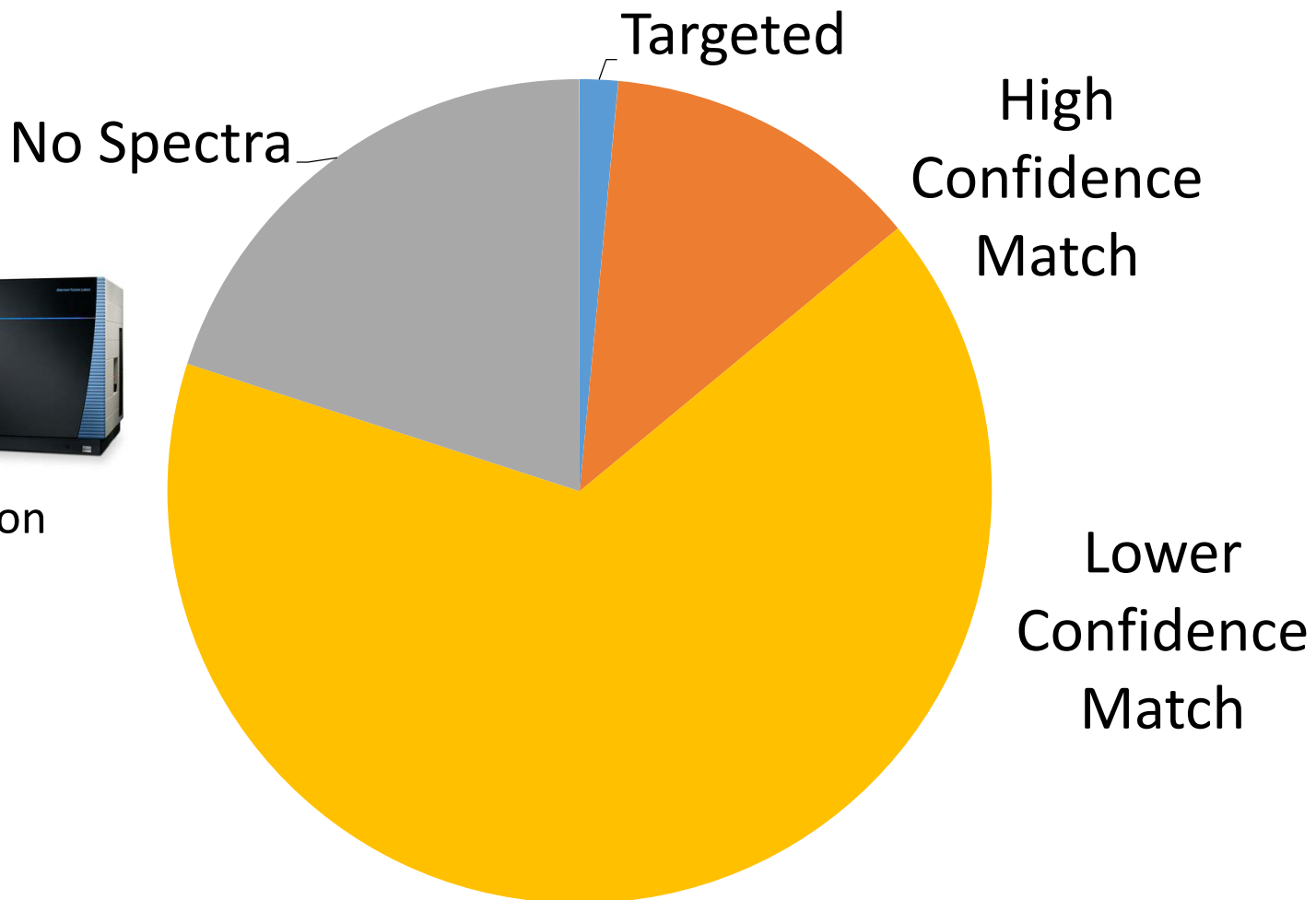
Targeted

High
Confidence
Match

Lower
Confidence
Match



Chemical Identifications



Orbitrap Fusion
Lumos MS

What have we been missing?



Coyote Creek



San Leandro Bay



Napa River

Coyote Creek



- South Bay focused monitoring
- Profile looks as expected: dilute WWTP effluent
- Pharmaceuticals
- Personal care products
- Some pesticides



Napa River

- Higher contaminant abundance during low tide
- Least contaminated site
- Pesticides, natural products
- Few identified synthetic chemicals

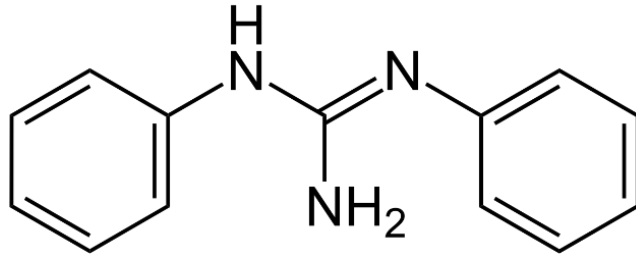


San Leandro Bay

- Most contaminated site
- Over 1,000 compounds found at higher levels here than in effluent
- Key compound groups highlight urban non-point sources

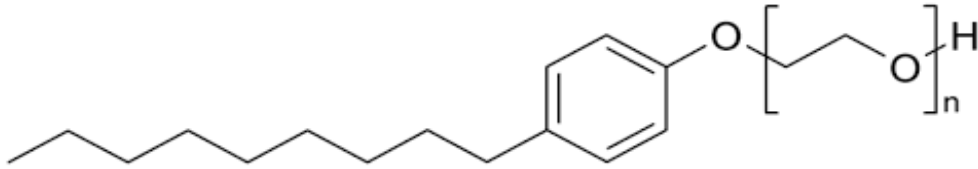


N,N'-Diphenylguanidine



- Rubber vulcanization – i.e. tire production
- Highly abundant compound detected in San Leandro Bay
- Slightly bioaccumulative
- Aquatic toxicity concern

Nonylphenol Ethoxylates (NPEs)



- Ingredient in detergents, cleaners, degreasers, emulsifiers
- Persistent, bioaccumulative, toxic, endocrine disruptors
- Previous studies measured and quantified short-chained NPEs, but not long-chained NPEs

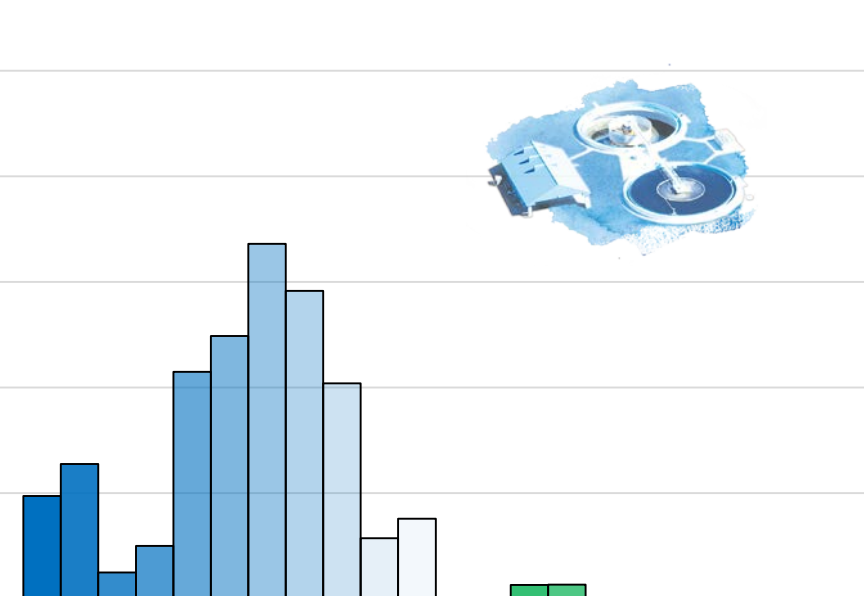
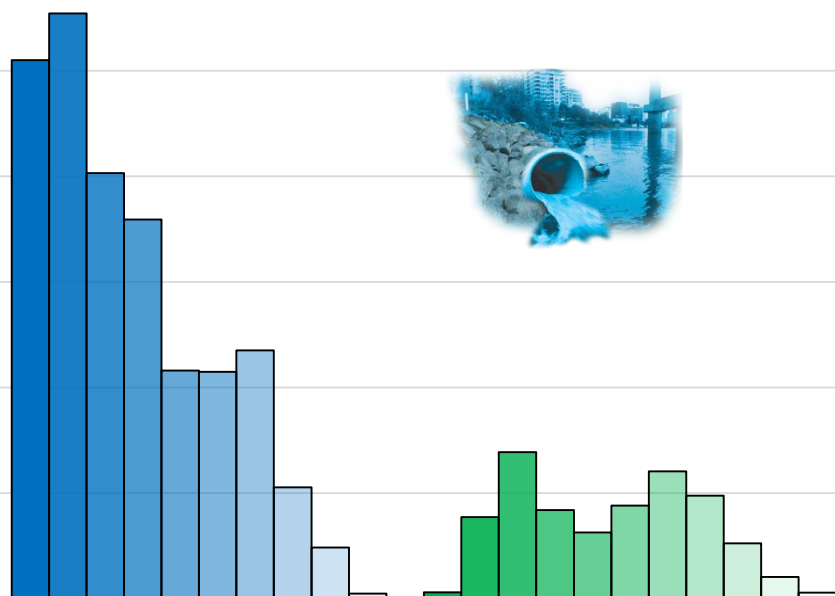
Urban stormwater runoff is a key pathway for NPEs



San Leandro Bay

Coyote Creek

Relative Abundance



Nonylphenol Ethoxylates

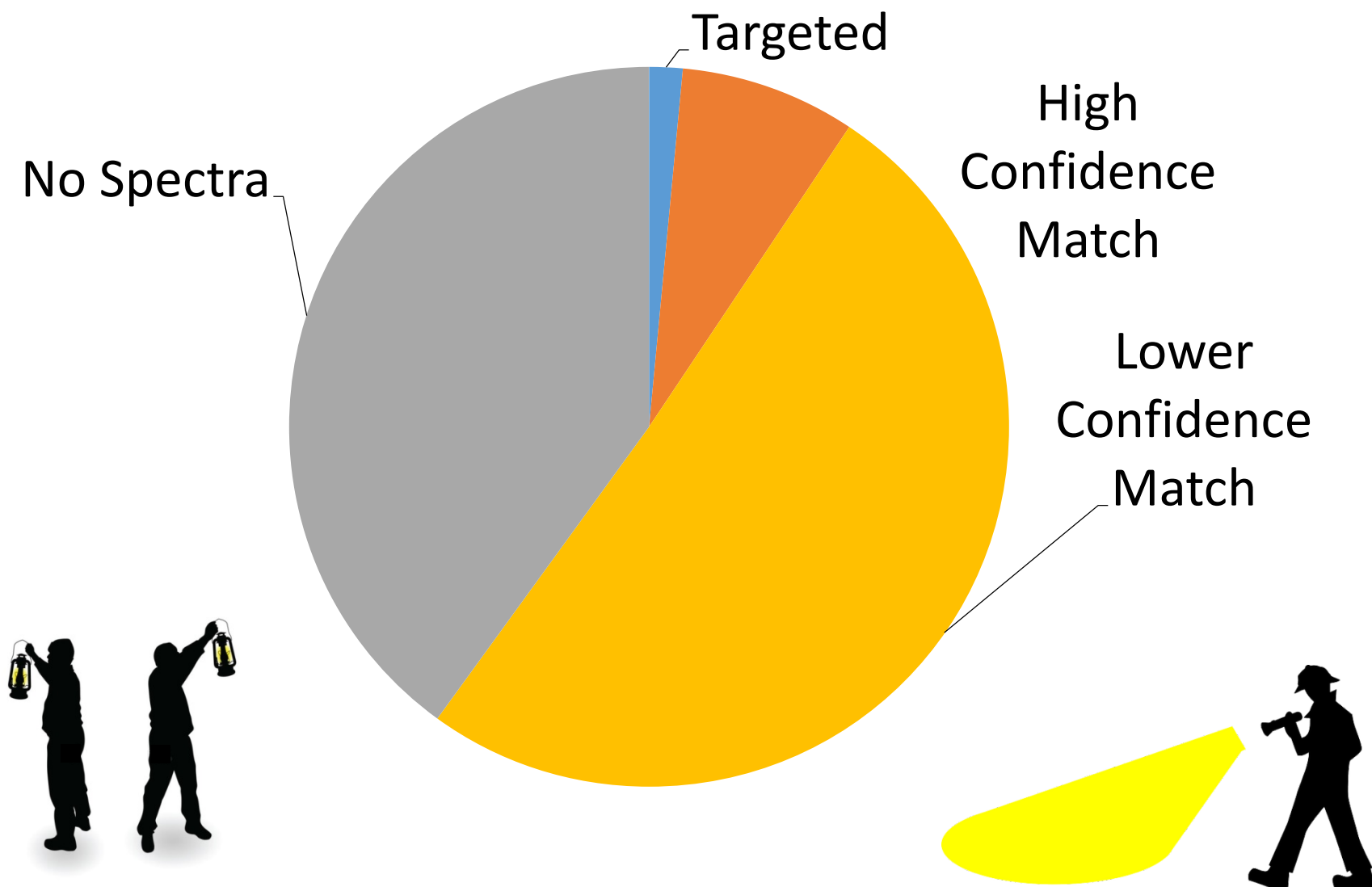
Octylphenol Ethoxylates

Nonylphenol Ethoxylates

Octylphenol Ethoxylates



What's Next?



What's Next?



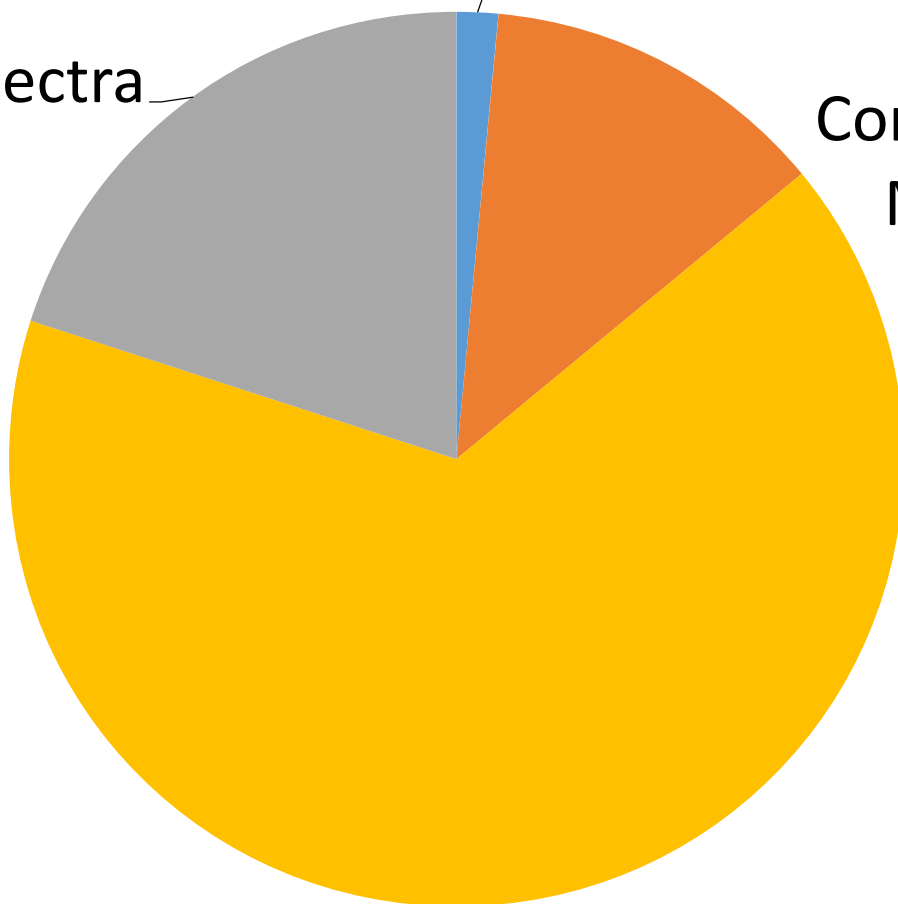
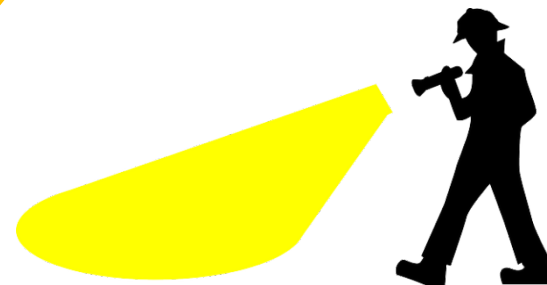
Orbitrap Fusion
Lumos MS

No Spectra

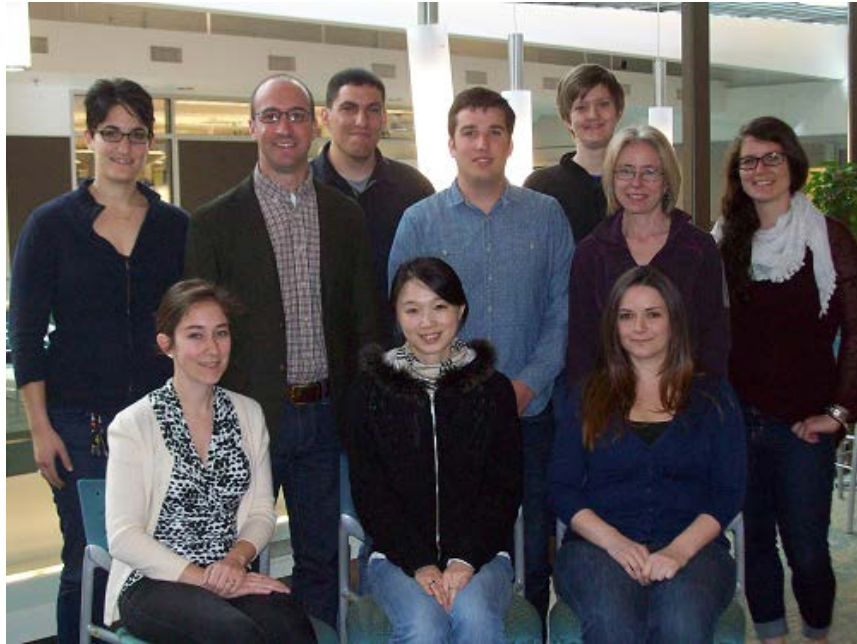
Targeted

High
Confidence
Match

Lower
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QUESTIONS?



Ferguson Lab Group

