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ENERGY | ENVIRONMENTAL | MEASUREMENT

Quaternary Ammonium Compounds (QACs)

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THE SCIENCE OF SURE®

Quaternary Ammonium Compounds

- Also know as quats.
- QAC compounds are among the most commonly used disinfectants (from household to hospital grade) .
- Their antimicrobial activity is more selective than that of other disinfectants, they are inactivated by organic soil, and they should not be diluted in hard water.
- QACs are, however, generally very effective against bacterial biofilms

Some background

- As the use of QACs has grown, so has their presence in wastewater treatment plant (WWTP) systems, often undetected until performance problems arise.

- Even at low concentrations, these compounds can severely disrupt biological treatment processes, leading to ammonia breakthrough, foaming, sludge instability, and noncompliance.

Some background

- Over the past years, the use of disinfectants and cleaning products has skyrocketed in our post COVID world.

- QACs are the active ingredient behind many of the 99.9% germ-free claims you see on cleaning products.

- They work great at disinfecting, but what happens when they go down the drain?
  - They don’t vanish…
  - They end up in your influent stream where they could wreck havoc on your biological treatment process.

Some background

- Operators have reported:
  - Sudden ammonia breakthrough despite healthy DO and alkalinity
  - Persistent foaming that defies traditional control methods.
  - Filamentous bulking and dewatering problems
  - Effluent toxicity exceedances and bio solid reuse issues.

Some background

- The pandemic is over, why are there still issues?
  - Disinfectants and sanitizers containing QACs have become standard across industries.
  - Food service, hospitals, manufacturing, and even households are sending a steady stream of these compounds down the drain.

What are QACs Chemically…

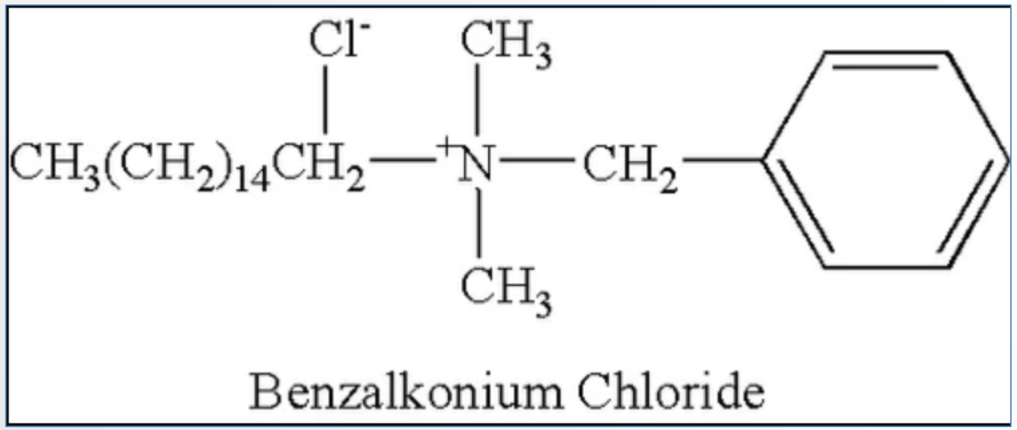
Chemically…

A quaternary ammonium compound (QAC) is a positively charged nitrogen compound in which a central nitrogen atom is bonded to four organic groups (alkyl or aryl groups), giving it a permanent positive charge.

Chemical Behavior

QACs	TMAH
Acts like a cationic surfactant	Not a surfactant
Binds to negatively charged microbial membranes	Chemically reactive due to hydroxide
Not a strong base	Acts like a strong base
Stable in neutral pH	Raises pH

Benzalkonium chloride (BAC)

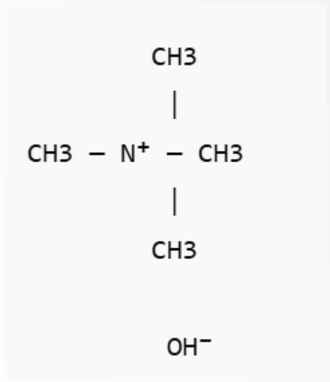


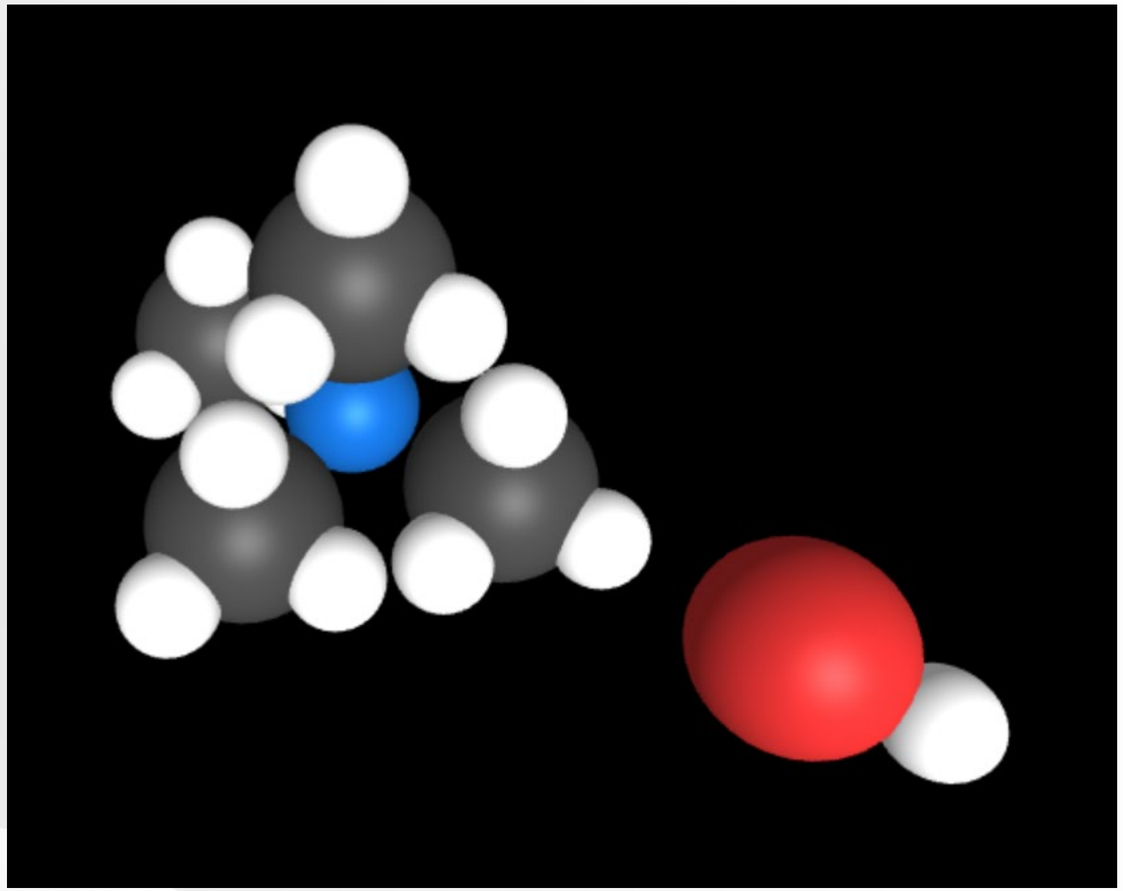
- General Chemical formula: $C_6H_5CH_2N(CH_3)_2R\ Cl$

- Consists of:
  - Benzyl group
  - Quaternary ammonium center
  - Alkyl chain
  - Chloride ion

Tetramethylammonium Hydroxide (TMAH)

- Chemical formula: $(CH_3)_4N^+ OH^-$
- Consists of:
  - Tetramethylammonium cation: $(CH_3)_4N^+$
  - Hydroxide anion: OH^-





Primary Function

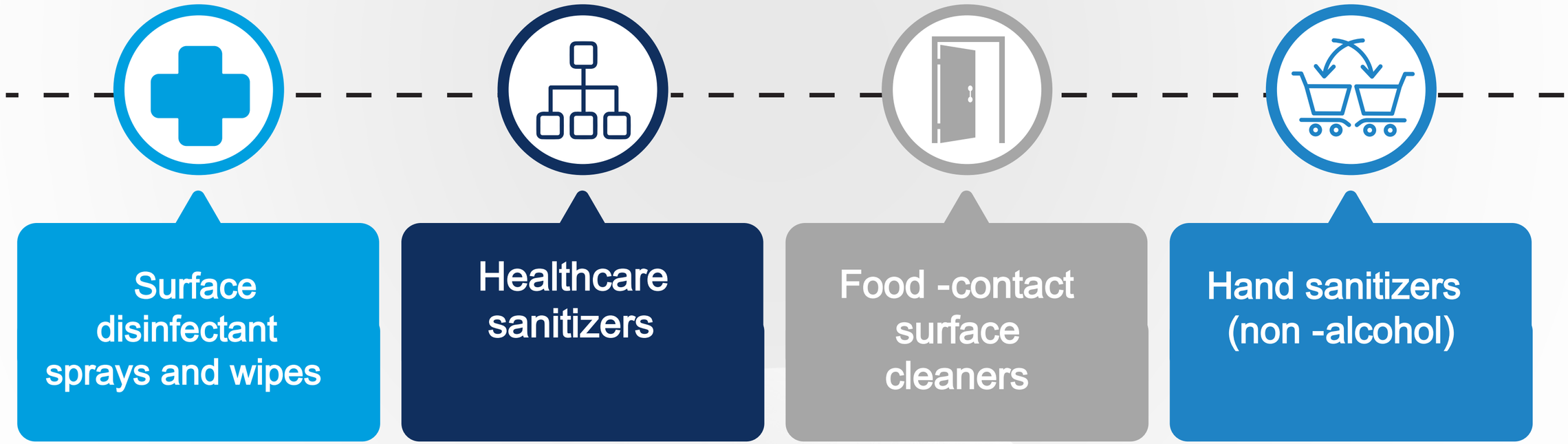
	QAC	TMAH
Main Role	Disinfectant / Surfactant	Strong base
Mechanism	Disrupt cell membranes	Provides hydroxide (raises pH)
Industrial Use	Cleaning and sanitizing	Semiconductor processing, photoresist developer

Benzalkonium Chloride (BAC)

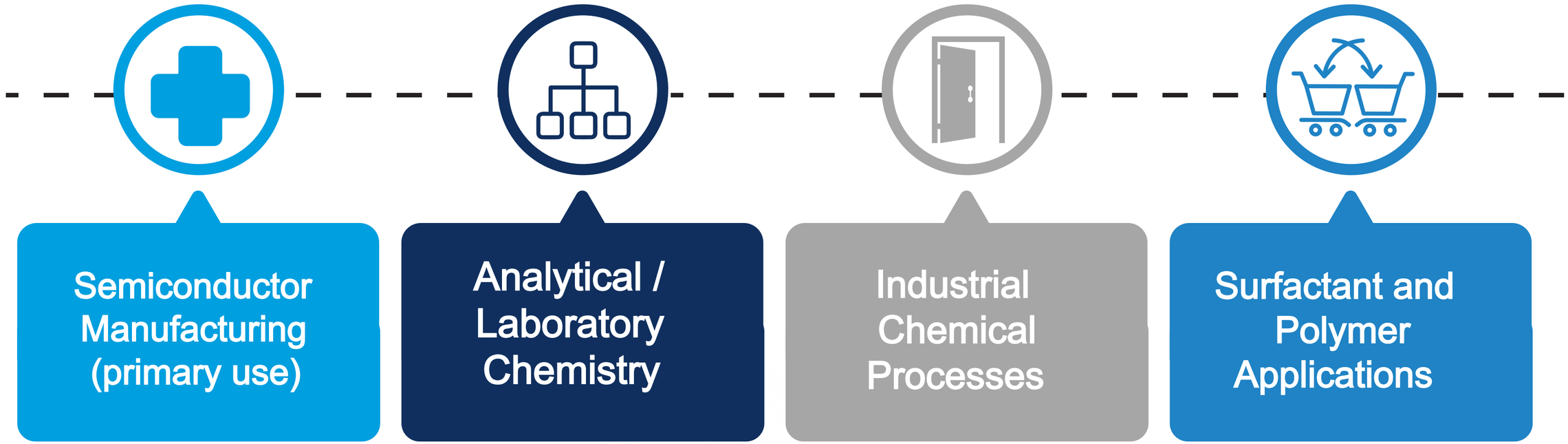
Effective against:

- Gram-positive bacteria
- Many Gram-negative bacteria
- Enveloped viruses

BAC is the most widely used QAC disinfectant



TMAH is a strong organic base used in high tech and analytical applications



How do they get into wastewater?

Sources of QACs

Household Products

Disinfectants, Cleaners

Healthcare Facilities

Disinfectants, Sanitizers

Laundry/Textile Processing

Softeners, Antistatic Agents

Industrial Use

Cleaners, Sanitizers

$C_2H_{25}^-$ — N^+ — Cl^-

Quaternary Ammonium Compounds (QACs):

$C_{12}H_{25}-N^+CH_3-Cl^-$

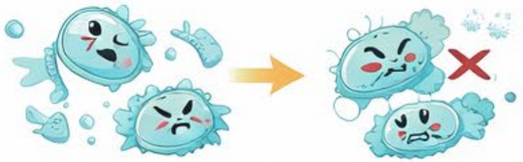
Wastewater Treatment Plant

QACs in Wastewater

Disinfectant residuals may enter treatment

Effluent

Inhibition of Microbes



Toxic to nitrifying bacteria, disrupts biological treatment

QACs accumulate in biosolids

Accumulation in Sludge

Foam Formation

Environmental Concerns

- Potential for antimicrobial resistance, environmental toxicity, & persistence

*QAC molecules accumulate in sediment & discharge can select for resistant microbes.

Entry into Wastewater

1. **Household Products**
   Disinfectants, cleaners, fabric softeners
2. **Healthcare facilities**
   Hospital surface disinfectants, hand sanitizers
3. **Industrial / institutional**
   Microchip fabrication, specialty chemical production, food processing, dairy, breweries, laboratories
4. **Laundry and textile processing**
   Softeners and antistatic agents
5. **Accidental or Improper Disposal**
   Spills, unauthorized discharge

In the environment and wastewater

- Ubiquitous cationic surfactants in wastewater.
- Toxic to microbes
- Treatment and monitoring are important, especially in industrial and hospital wastewater systems because you can’t fix what you can’t measure.

Negative Impacts of QACs

Environmental Concerns

QACs

- Antimicrobial resistance.
  - QACs in effluent may contribute to resistance microbial strains.
- Toxicity
  - Negative effects on aquatic organisms at relatively low concentrations.
- Persistence
  - Long-chain QACs accumulation in sediments.

TMAH, additional concerns

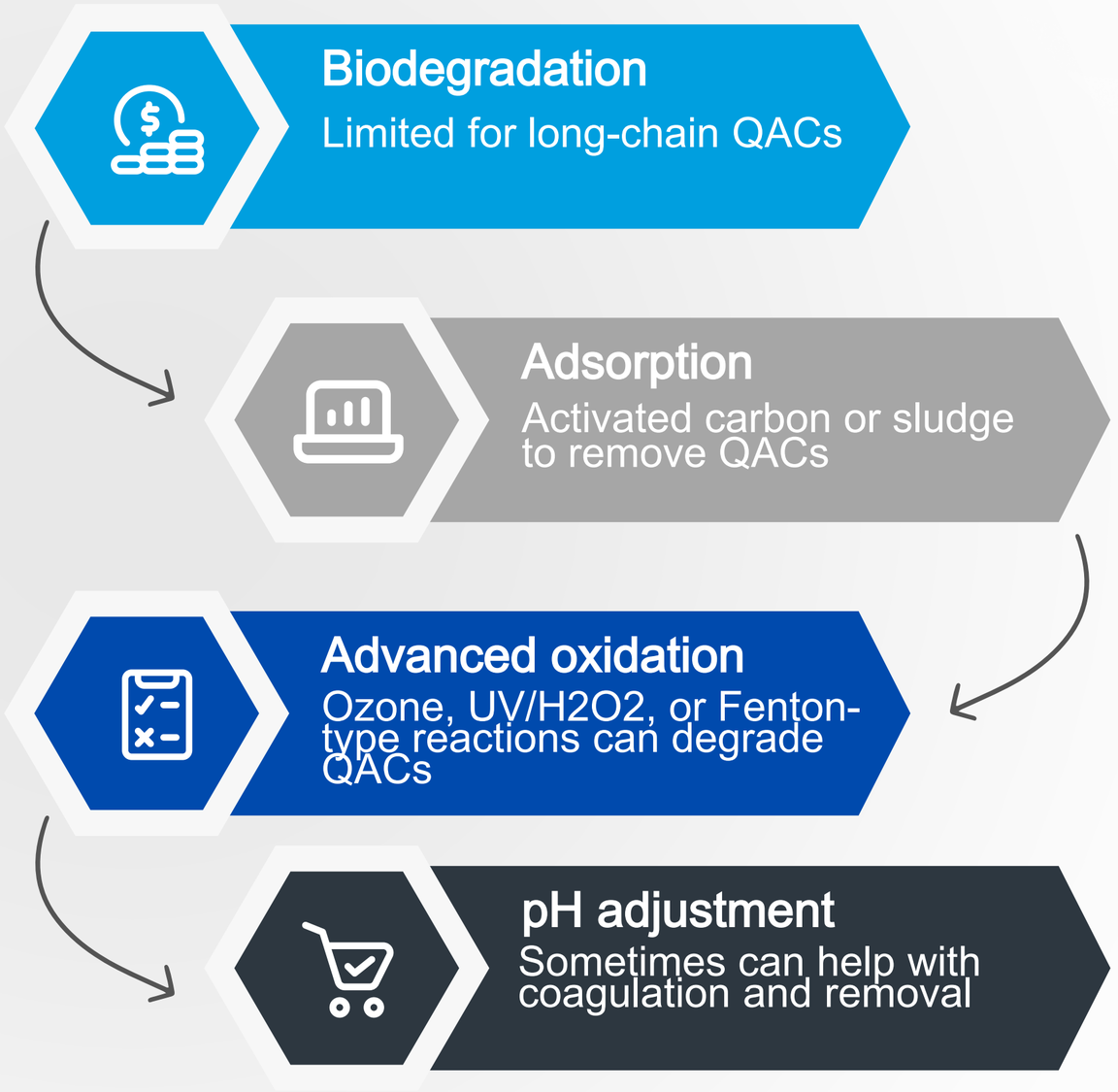
- Raises pH significantly
- Inhibition of biological treatment systems
- Quaternary ammonium toxicity

Wastewater compliance

QAC concerns:

- Inhibit Biological Activity
  - Suppress nitrifying bacteria, which can lead to ammonia breakthrough.
  - Disrupt anaerobic digestion, which reduces gas yield.
  - Interfere with BOD/COD removal, resulting in inefficient treatment and foaming.
- Trigger operational Challenges
  - Foaming and filamentous bulking in aeration basins
  - Solids carryover and poor sludge dewatering.
  - Increased risk of effluent toxicity or bio solids noncompliance.

Removal / Treatment Options

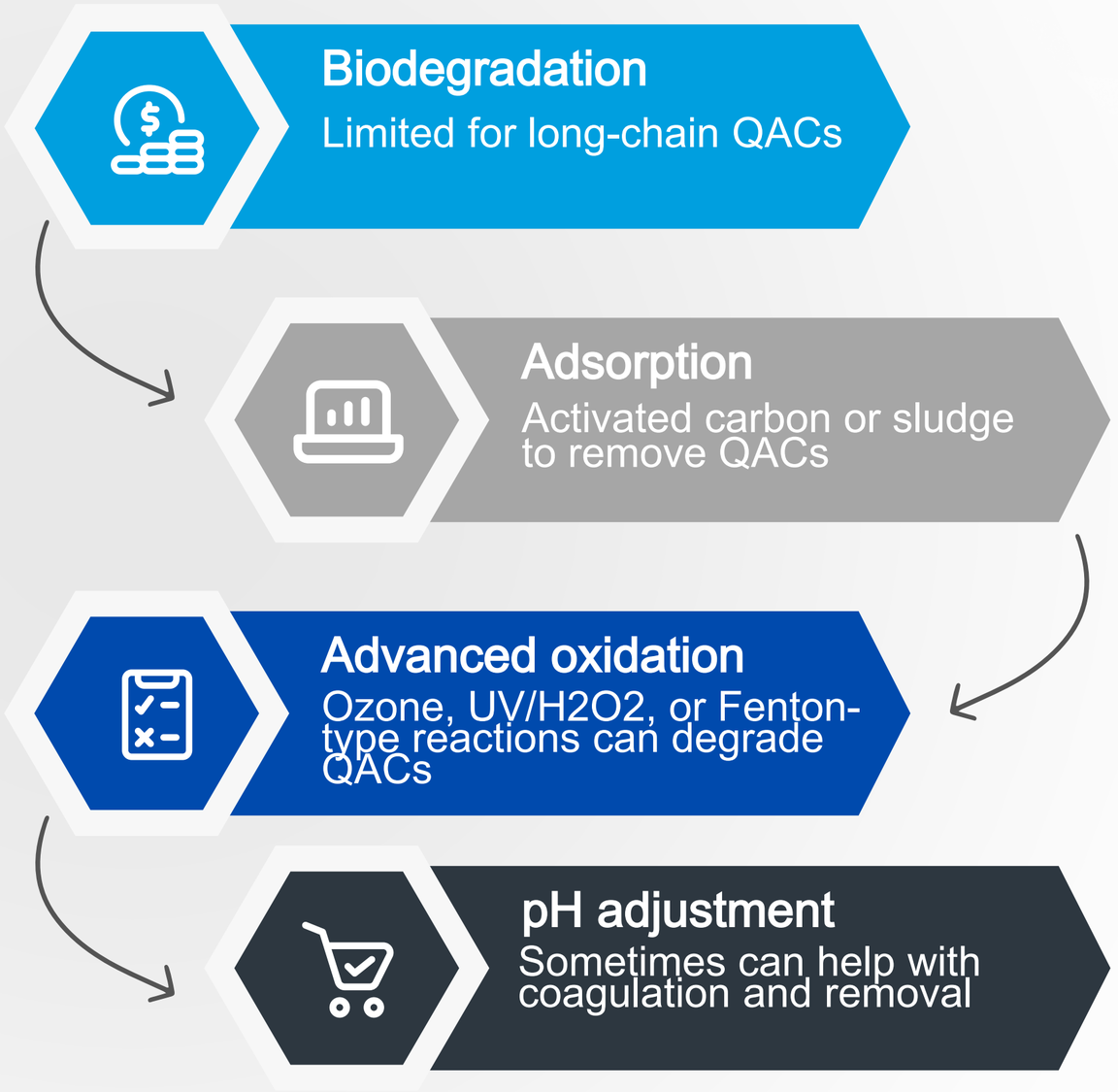


Wastewater compliance

Additional TMAH concerns:

- Slug loading events
- pH excursions (contributes high pH and strong alkalinity)
- Nitrification inhibition
- Toxicity to activated sludge biomass

Removal / Treatment Options



QAC Analytical Testing

How do we measure?

Analytical issues

Wet chemistry methods targeting organic nitrogen tend to overestimate QAC concentrations

QACs are not amenable to traditional GC or GC/MS analysis

HPLC using traditional detectors are subject to significant interference that can result in overestimating QAC

SPL's analytical solution

- SPL developed methods for extraction and analysis for QAC that using the best sample preparation and analysis technology available that produce defensible results that withstand regulatory and legal scrutiny.

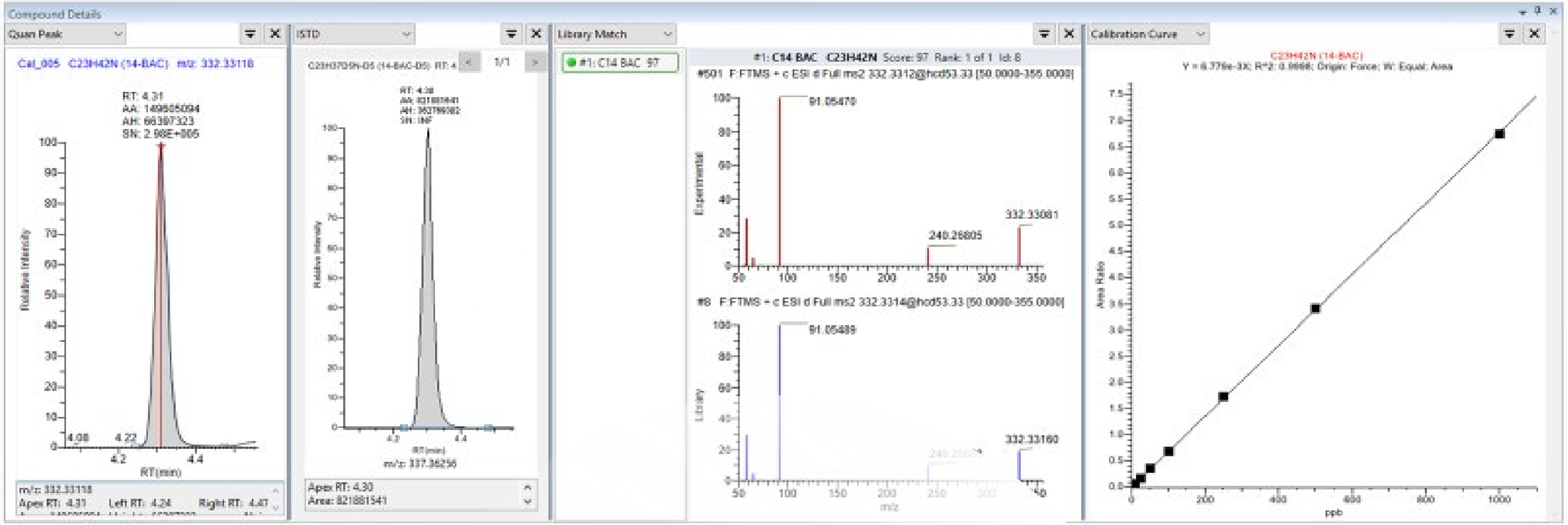
- SPL offers the latest technology (LC-MSMS) for analysis at ppb levels for accurate identification and quantitation of QACs in both solid and liquid matrices.

SPL's analytical solution

Unlike colorimetric methods, LC-HRMS/MS detects individual QAC species with high sensitivity and minimizes matrix interference.

Quaternary amines	Compound Formula	Abbreviation	CAS Number of Chloride Salt	mg/L	MQL
Tetramethylammonium	C4H12N	TMA	75-57-0	mg/L	0.01
Tetrapropylammonium	C12H28N	TPA	5810-42-4	mg/L	0.01
Benzyldimethyloctylammonium	C17H30N	C8 BAC	959-55-77	mg/L	0.01
Benzyldimethyldecylammonium	C19H34N	C10 BAC	965-32-2	mg/L	0.01
Benzyldimethyldodecylammonium	C21H34N	C12 BAC	147228-80-6	mg/L	0.01
Benzyldimethyltetradecylammonium	C23H42N	C14 BAC	139-08-2	mg/L	0.01
Benzyldimethylhexadecylammonium	C25H46N	C16 BAC	122-18-9	mg/L	0.01
Benzyldimethyloctadecylammonium	C27H50N	C18 BAC	122-19-0	mg/L	0.01
Dioctyldimethylammonium	C18H40N	C8C8 DADMA	5538-94-3	mg/L	0.01
Octyldecyldimethylammonium	C20H44N	C8C10 DADMA	32426-11-2	mg/L	0.05
Didecyldimethylammonium	C22H48N	C10C10 DADMA	7143-51-5	mg/L	0.01
Didodecyldimethylammonium	C26H56N	C12C12 DADMA	3401-74-9	mg/L	0.01
Ditetradecyldimethylammonium	C30H64N	C14C14 DADMA	10108-91-5	mg/L	0.01
Dihexadecyldimethylammonium	C34H72N	C16C16 DADMA	1812-53-9	mg/L	0.01
Dioctadecyldimethylammonium	C38H80N	C18C18 DADMA	107-64-2	mg/L	0.01
Cetylpyridinium	C21H38N	C16 PYR	123-03-5	mg/L	0.01

High resolution LC -MSMS Identification and Quantitation



Analytical problems / solutions

TMAH

QAC Library TF5.1

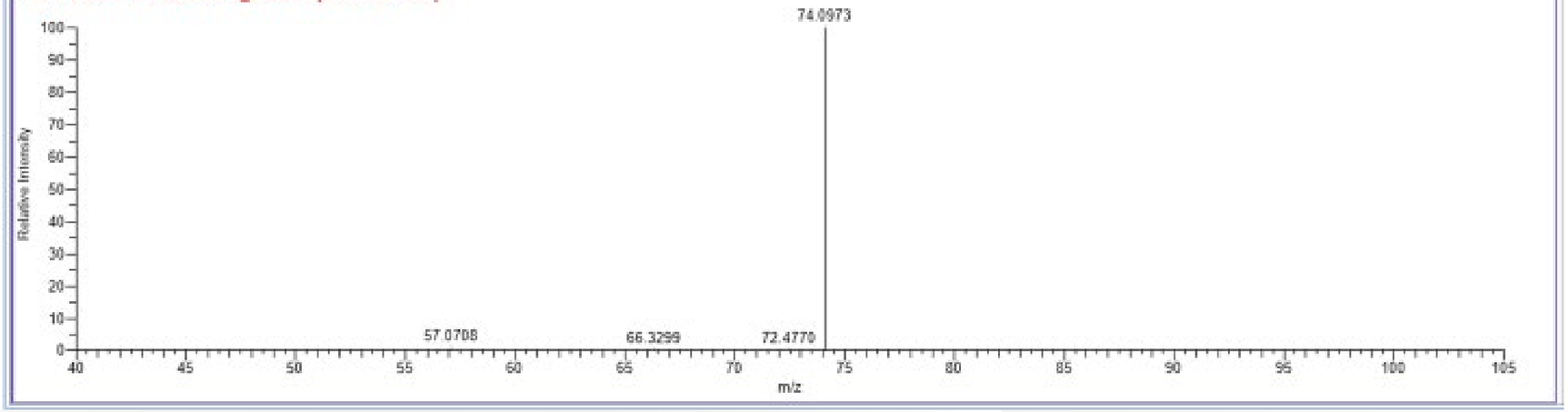
Compound List

Entry No	Compound	Synonyms	Formula	CAS ID	InChi Key	Compound Class	ChemSpider ID	HMDB ID	KEGG
6	C12 BAC		C21H38N						
7	C16 Cetylpyridium		C21H38N						
8	C14 BAC		C23H42N						
10	C16 BAC		C25H46N						
13	C36 DADMAC		C38H80N						
14	C32 DADMAC		C34H72N						
15	C28 DADMAC		C30H64N						
16	TMAH		C4H12N						
18	C20 DADMAC		C22H48N						
19	C24 DADMAC		C26H56N						
20	d25 DADMAC Surrogate		C26H31D25N						
22	C18 BAC		C27H50N						
23	C18 DADMAC		C28H44N						

Library Spectrum

Cal6_003.raw Scan: 80 RT: 0.60 NL: 2.93e06

FTMS + c ESI d Full ms2 74.0971@hcd53.33 [50.0000-95.0000]



SPL's analytical solution

- Identifies even low level impacts at ug/L (ppb) concentrations.

- Provides data for trouble-shooting, industrial enforcement, and long-term planning.

  - Enabling you to establish a QAC baseline.
  - Helps you understand what is "normal" for your plant.
  - Early warning protection before QACs disrupt biological treatment.
  - Pretreatment support with lab-backed evidence of industrial contributions

THANK YOU!

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