Inside Quaternary Ammonium Compounds: Innovation, Use and Regulatory Outlook

Speakers

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Outline

- Trends in Regulatory Activity
- DTSC Safer Consumer Products Program
- Quaternary Ammonium Compounds Applications
- Chemistry
  - Charges
  - Chain Length /MW & Charge Density
- Functional Uses
  - Betaines
  - Cationic Surfactants
  - Cationic Polymers
  - Organo-Clays
- Next Steps
- Q&A

Regulatory Trends, Industry Needs and Solutions

Trend:

- Increase in state regulations with heavy technical emphasis (Washington, California)

Needs:

- Early and increased cooperation between policy and science to prioritize issues, engage with appropriate PCPC committees/industry experts
- Flexible – not all regulations will require the same amount of effort
    - Establish *ad hoc* group to respond and engage with regulators as PCPC's Committees (Regulatory, SISComm) may not have the expertise and are too large to address issues in a timely manner.

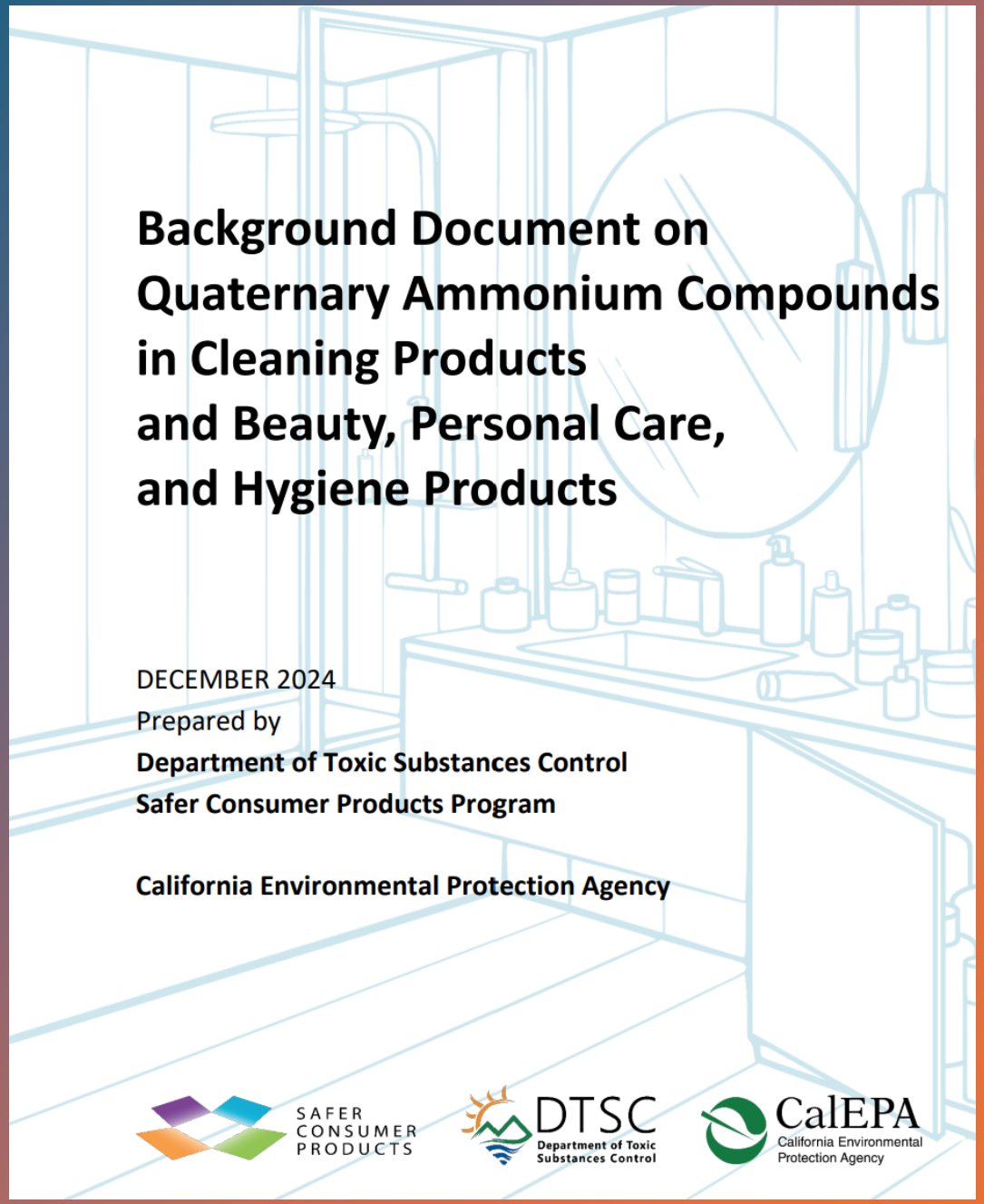
Solution:

- Establish Ingredient Defense group with technical expertise from PCPC science committees, coordinated with PCPC Regulatory and Legal staff
- Currently: 23 companies, 40 company experts
- You can join too!

Safer Consumer Products Program

- California statute requires that the program establish a prioritization system for its chemical regulation work that includes three considerations:
  - the volume of a chemical in commerce in CA;
  - the potential for exposure to the chemical in a consumer product; and
  - potential effects on sensitive subpopulations, including infants and children

DTSC
Department of Toxic Substances Control



DTSC Findings

- 263 unique quats in 78 product categories

- conditioner (89.6% of products),
- shampoo (83.9%),
- shower products, including body wash (78.6%),
- hair treatments (64.9%),
- liquid soap (62.7%),
- concealer (55.2%),
- hair styling products (53.7%),
- hair colorants (53.5%),
- nail color cosmetics (53.2%), and
- bleach/disinfectant (51.6%).

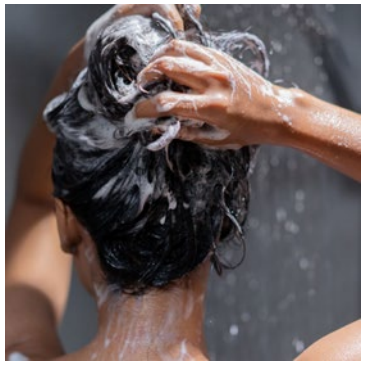
- Human exposure
  - Dermal, respiratory or immune effects
- Environmental persistence
  - Toxicity to algae, aquatic invertebrates and fish
- Potential adverse impacts to humans and the environment

Data Evaluation (2025 snapshot using US FDA RLD)

- Over 730,000 reported products to FDA
- 247 quat or quat-like ingredients in personal care and cosmetic products
- The DTSC identified ingredient with the current highest frequency in products is only in about 6.6% of reported products

Ingredients Essential to Healthy Life

Chemical Ingredients in Personal Care



Cleansing:
Healthy Skin & Hair

Prevention:
Hair Breakage
Color Fade
Skin Aging

Chemicals:
Surfactant
Polymers
…..

Protect:
Skin Hydration
Hair Hydration
Nail Strength

Beautification:
Self-Expression
Colorful Creation

Repairing:
Damaged Hair
Damaged Skin

Where are Quats Used?

Everywhere

Quats Applications

Laundry & Cleaning

Textile auxiliaries

Fabric Softeners

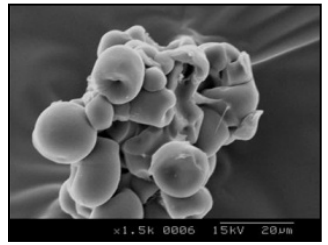
Cleaning (I&I)

Agriculture & Paper

Metal & Mining

Corrosion Inhibitors

Phase Transfer Catalysts



Oil & Roads

Asphalt Emulsifiers

Water Treatment

Algaecide

Flocculating Agents

Personal Care

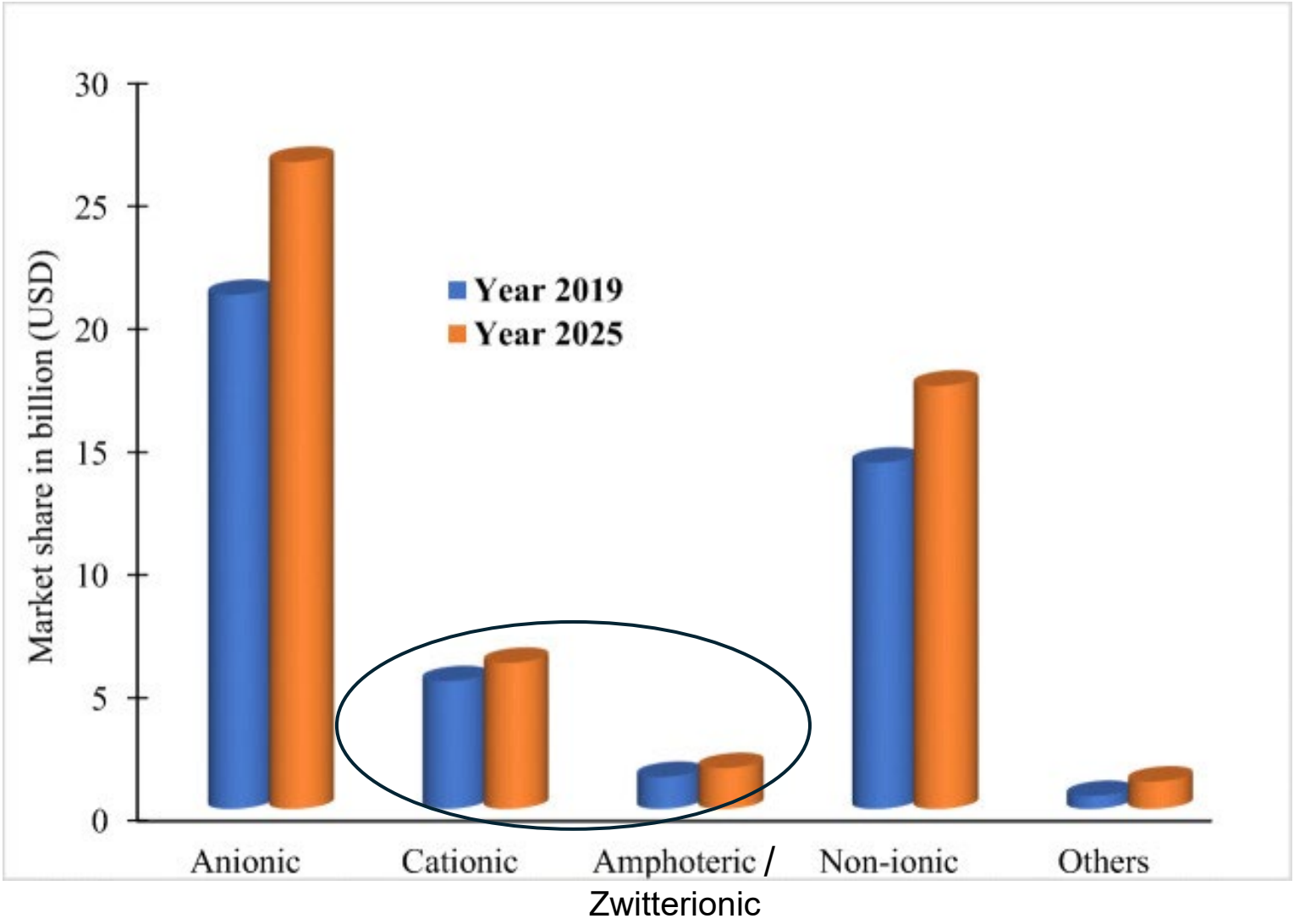
Hair

Nail

Skin

Global Market Shares - Surfactants

Quats use volume in personal care products is a small portion of the overall usage.

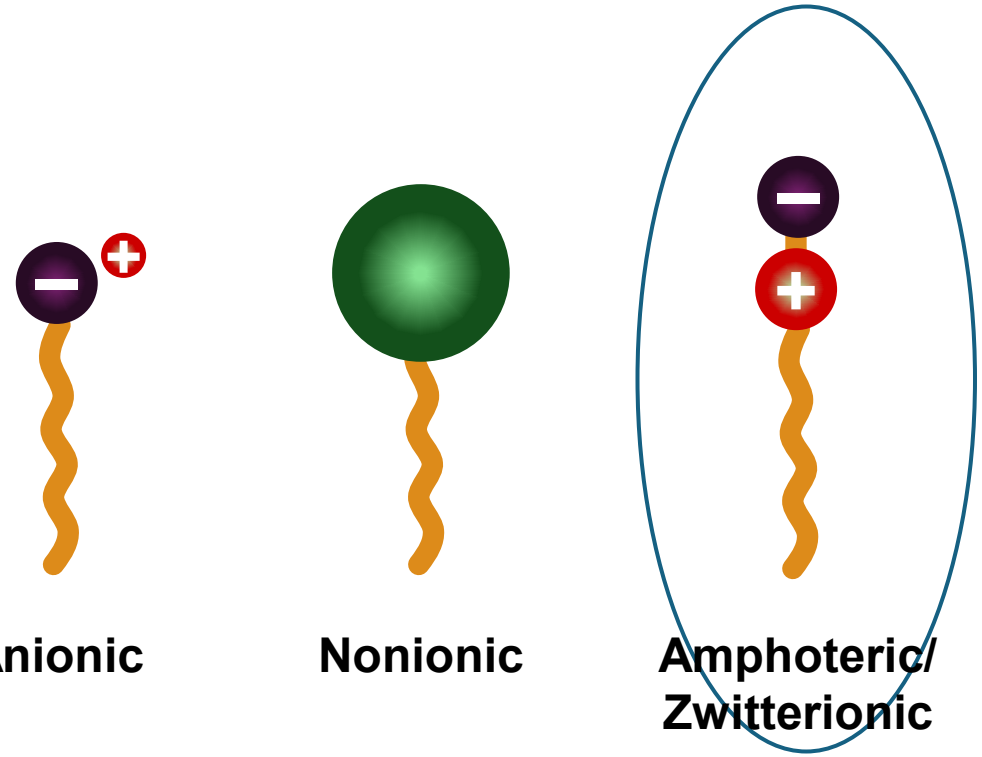


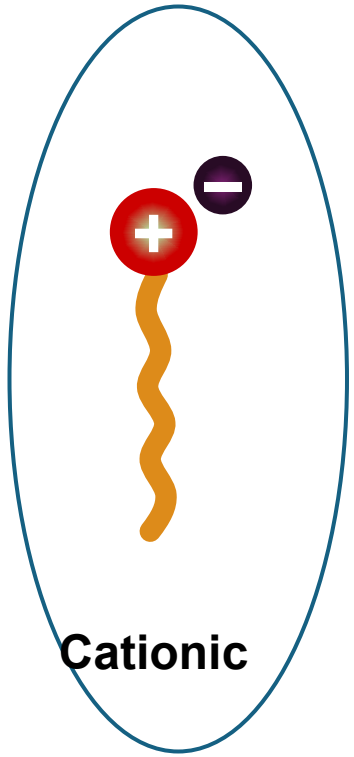
The recent and projected global market of surfactant types
(Sources: marketsandmarkets.com and alliedmarketresearch.com)

Chemistry

Charge, Molecular Weight/Alkyl Chain Length impact on Cationic Charge Benefits

Chemistry – Charge

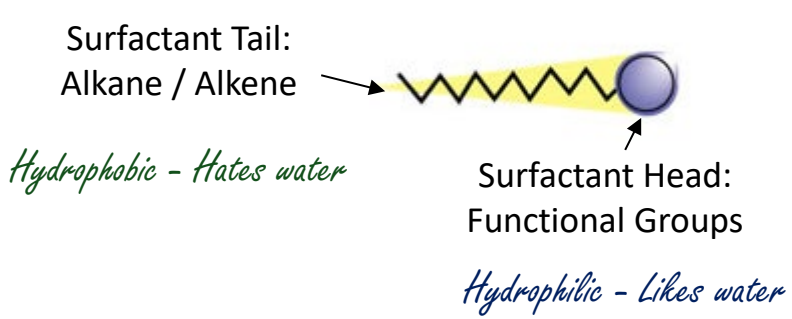


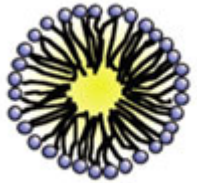


Cleansing/Detergency and Dispersion

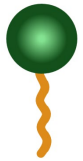
Softening, Conditioning and Suspending

Surfactants/ Polymers



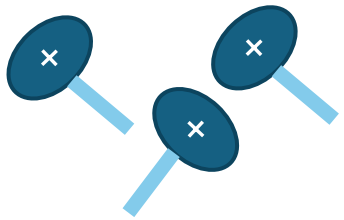


Micelle

Surfactant/Polymer	Characteristics	Ingredient Type
Nonionic	No charge groups in its head 	Polysorbate/EO/PO-Alcohols /Glycerine Esters Fatty amines/Amido Amines /Polyamines/Alkylpolyglucosides/Polymers
Anionic	Negative charge group in its head 	Alkyl ether sulphate/Carboxylated Phosphoric Esters/Polymers
Cationic	Positive charge group in its head 	Quaternary Ammonium Chloride/Cationic Phospholipids/Esterquats/Polymers
Zwitterionic/ Amphoteric	Two oppositely charged groups 	Betaines Amine Oxides

Chain Length/MW and Solubility

INCREASING MOLECULAR WEIGHT



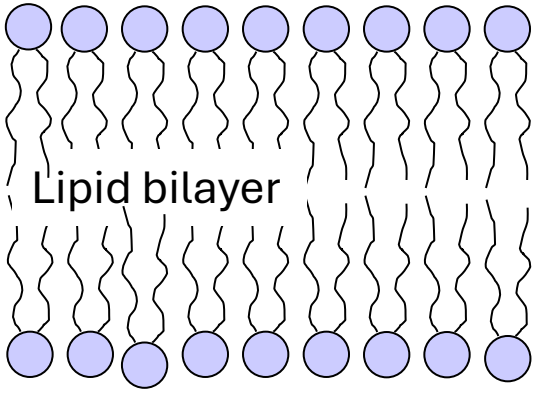
Cationic Polymer
Too Large

Short Chainlengths 6-8
Water soluble,
low cell interaction

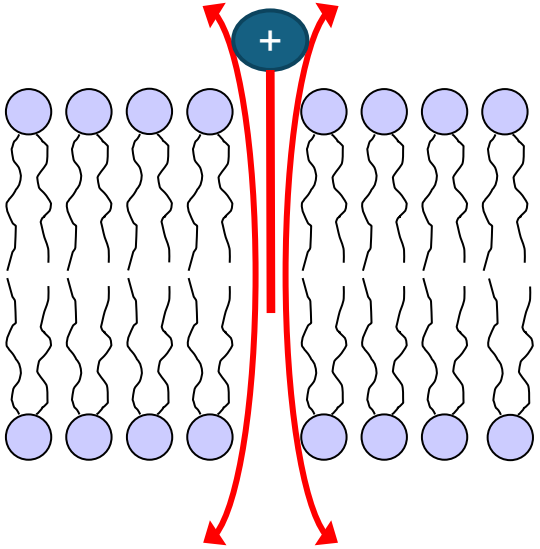
Specific Chainlengths 8-14
Antibacterial Properties

Long Chainlengths 18-22
Not water soluble,
Low cell interaction

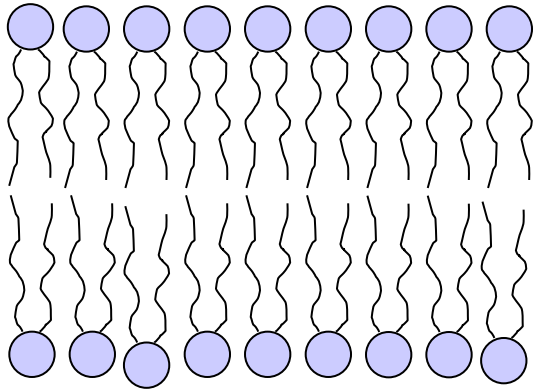
Cationic Polymers
Not water soluble,
Low cell interaction

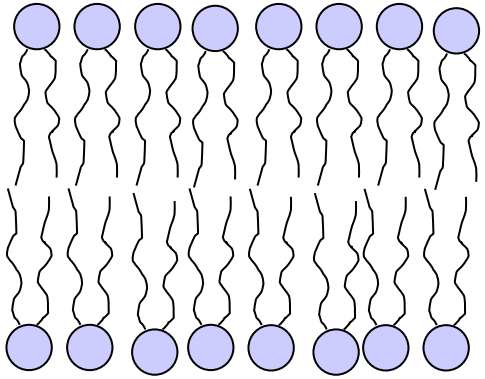


Inner Cell: phospholipids, etc.



Disrupts the membrane
Cells become vulnerable

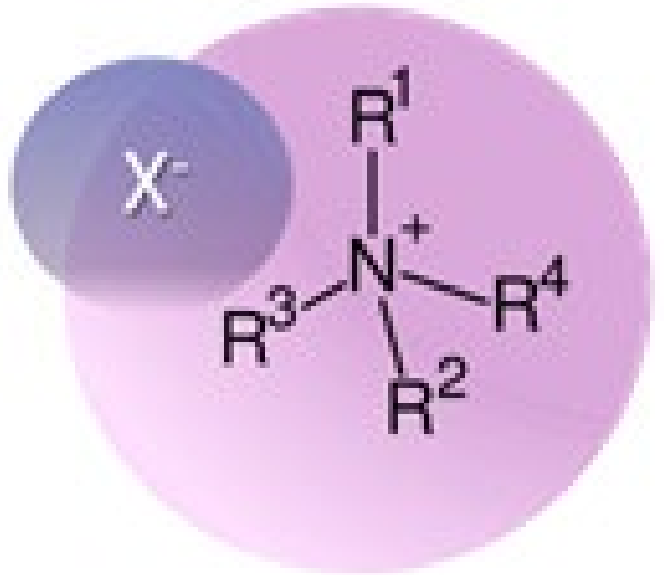




***Amphoterics/Zwitterionic**
No Charge – Water phase

Quats Definition and Benefits

- Nitrogen center with four "R groups"
- R groups can vary from Hydrogen, benzyl, amides, esters or various alkyl chains and polymers
- The Alkyl groups can vary from C_8-C_{22} and this will dictate the solubility and function of the molecule
- Molecular weight and charge density of polymers dictate functional benefits
- The ingredient has many different functions:
  - Hair and Skin Conditioners
  - Hydrotropes
  - Wetting agents
  - Emulsifiers
  - Clay treatments

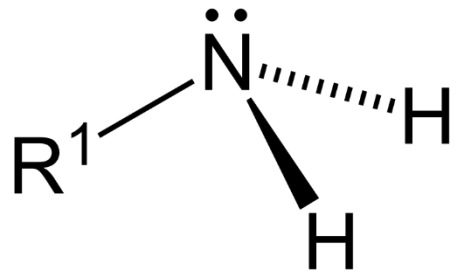


What are different amines and quats?

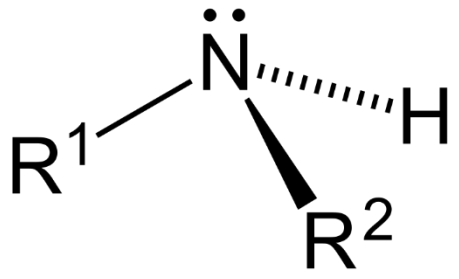
Organic compound derived from ammonia

- One or more hydrogen atoms have been replaced
- **One R group** is attached then it is a primary **1º amine**
- **Two R groups** are attached then it is a secondary **2º amine**
- **Three R groups** are attached then it is a tertiary **3º amine**
- **Four R groups** are attached then it is a quaternary **4º amine**

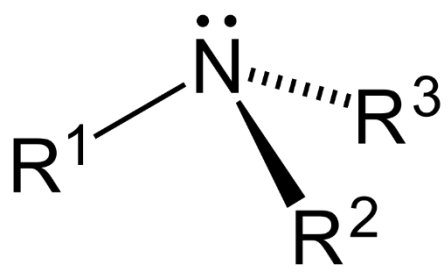
1°



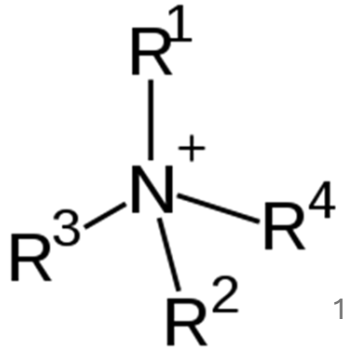
2°



3°



Quats

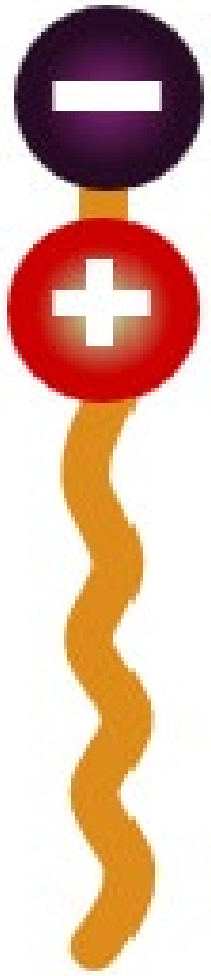


Type of Quats Used

Application	Quaternary
Fabric softeners	Esterquats (EQ)
Hair & skin conditioners	Alkyltrimethyl ammonium chloride Esterquats, Amidoquats, Polyquats
Hard Surface cleaners	Alkyltrimethyl ammonium chloride Alkyldimethyl ethoxylated ammonium chloride
Organoclays	Alkylbenzyldimethyl ammonium chloride Dialkyldimethyl ammonium chloride
Asphalt emulsifiers	Quaternized polyamines Alkyltrimethyl ammonium chloride
Corrosion inhibitors	Alkyltrimethyl ammonium chloride Esterquats
Flocculating agents	Esterquats, Polyquats
Biocides	Alkylbenzyldimethyl ammonium chloride Dialkyldimethyl ammonium chloride Polyquats

Functional Uses for Quats in Personal Care Products

- Amphoteric/Zwitterionic Surfactants
  - Primary use in Shampoos and Bodywashes.
- Cationic Surfactants
  - Primary use in Hair Conditioners and Lotions.
- Cationic Polymers
  - Primary use in Shampoos in combination with anionic surfactants for deposition of health actives.
- Organo-Clays
  - Primary use in nail products for suspension.

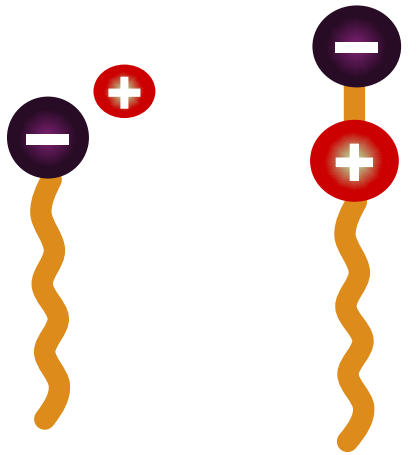


Amphoteric/Zwitterionic Surfactants (Betaines)

- Chemical Structure
  - Amphoteric/Zwitterionic compounds: they have both a + and a - charge, but the molecule overall is neutral.
  - Typically consist of a Quat group (+) and a Carboxylate group (-).
- Charge and Solubility
  - Highly water-soluble and mild on skin.
  - Good compatibility with both anionic and cationic surfactants.
- Applications
  - Used in shampoos, body washes, and other personal care products.
  - Known for their **mildness**, foam-boosting, and conditioning properties.
- Toxicity and Environmental Impact (to be discussed in later meetings)
  - Generally considered **biodegradable** and **low toxicity**.
  - Preferred in formulations aiming for gentleness and environmental fate and effects.

Why Amphoterics? Surfactants are Paired to Enhance Efficiency

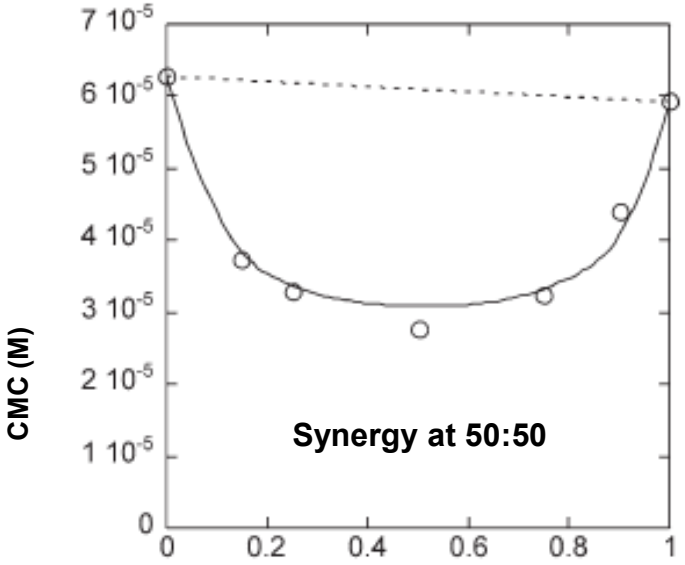
-Anionic surfactants (negative charge) interact with Amphoteric/Zwitterionic surfactants (both positive and negative charges)



Anionic **Amphoteric/ Zwitterionic**

-These synergistic interactions result in enhanced surfactancy as seen in the graph below

Lower Surface Tension
Better Cleaning
More Lather



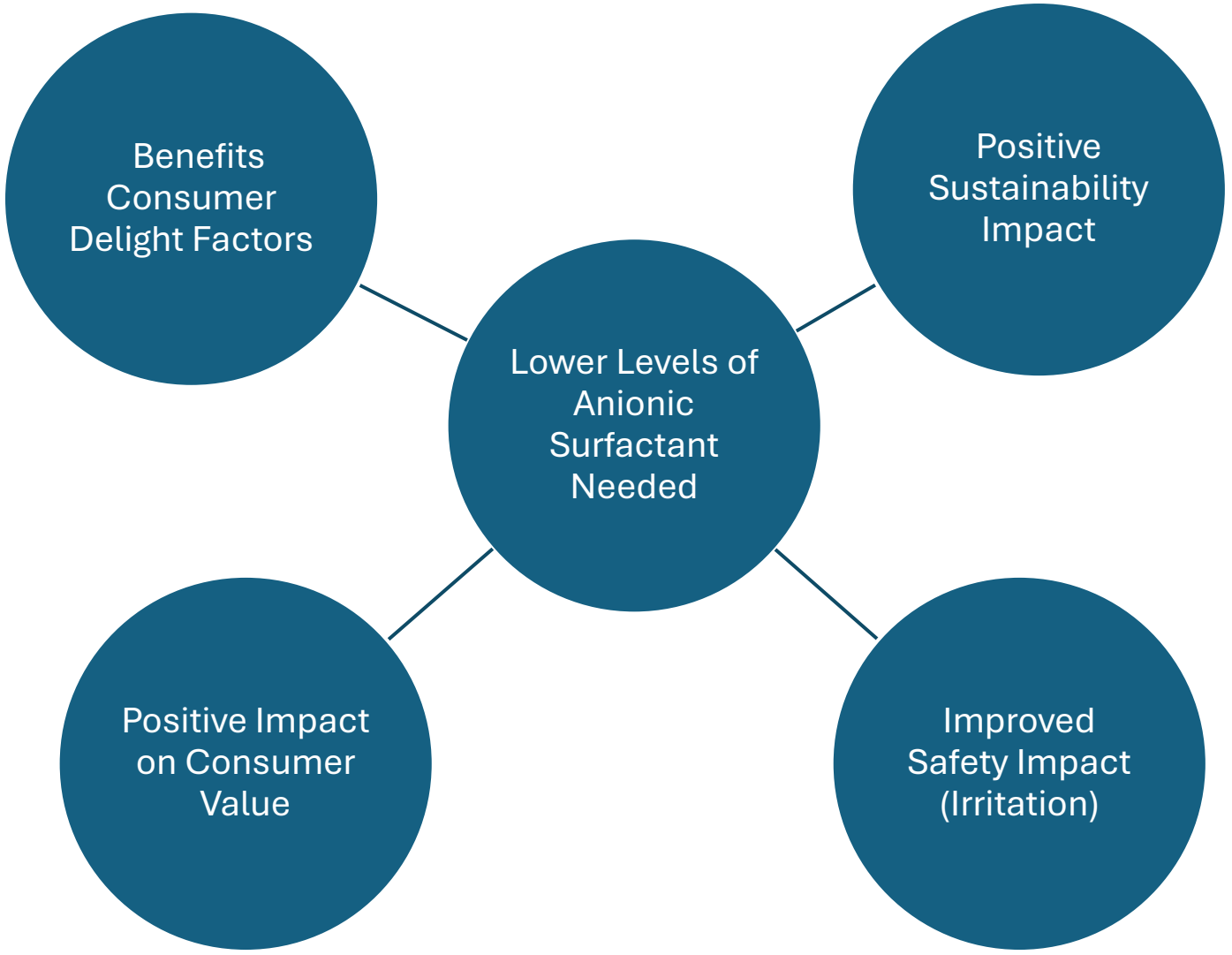
100% Anionic (SLS)

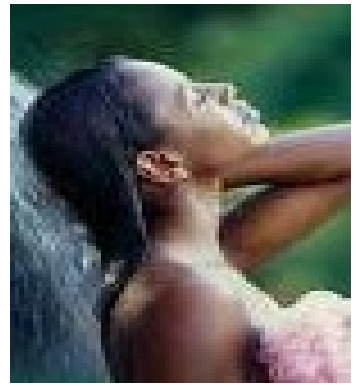
100% Amphoteric/Zwitterionic (Betaine)

Surfactant System: Less surfactants needed for efficacy

Impact of Amphoteric/Zwitterionic Surfactants (Betaines):

Synergy from Combinations of Anionic and Amphoteric/Zwitterionic Surfactants, lower surfactant levels required

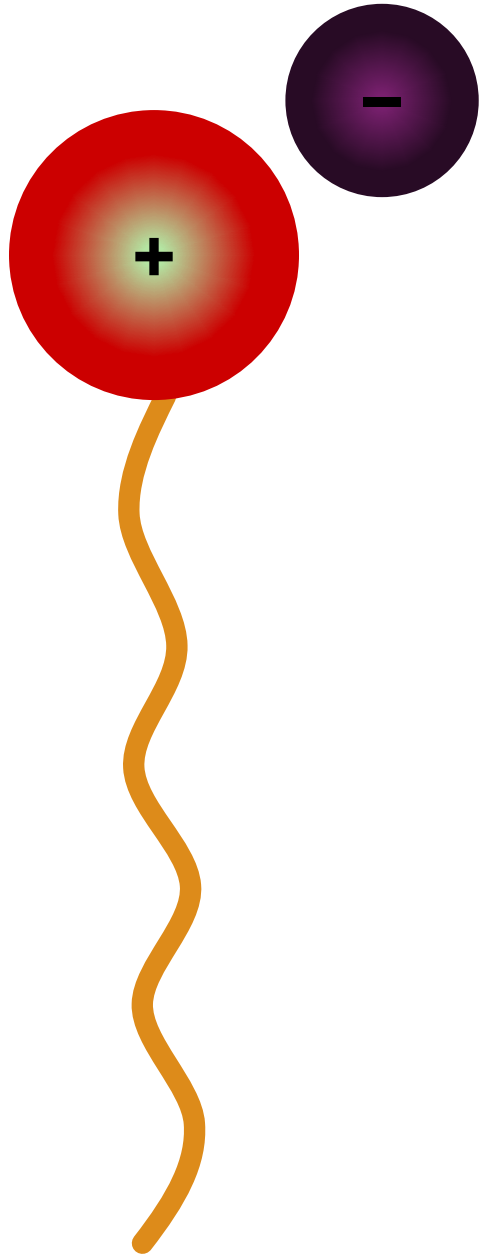




Cationic Ingredients

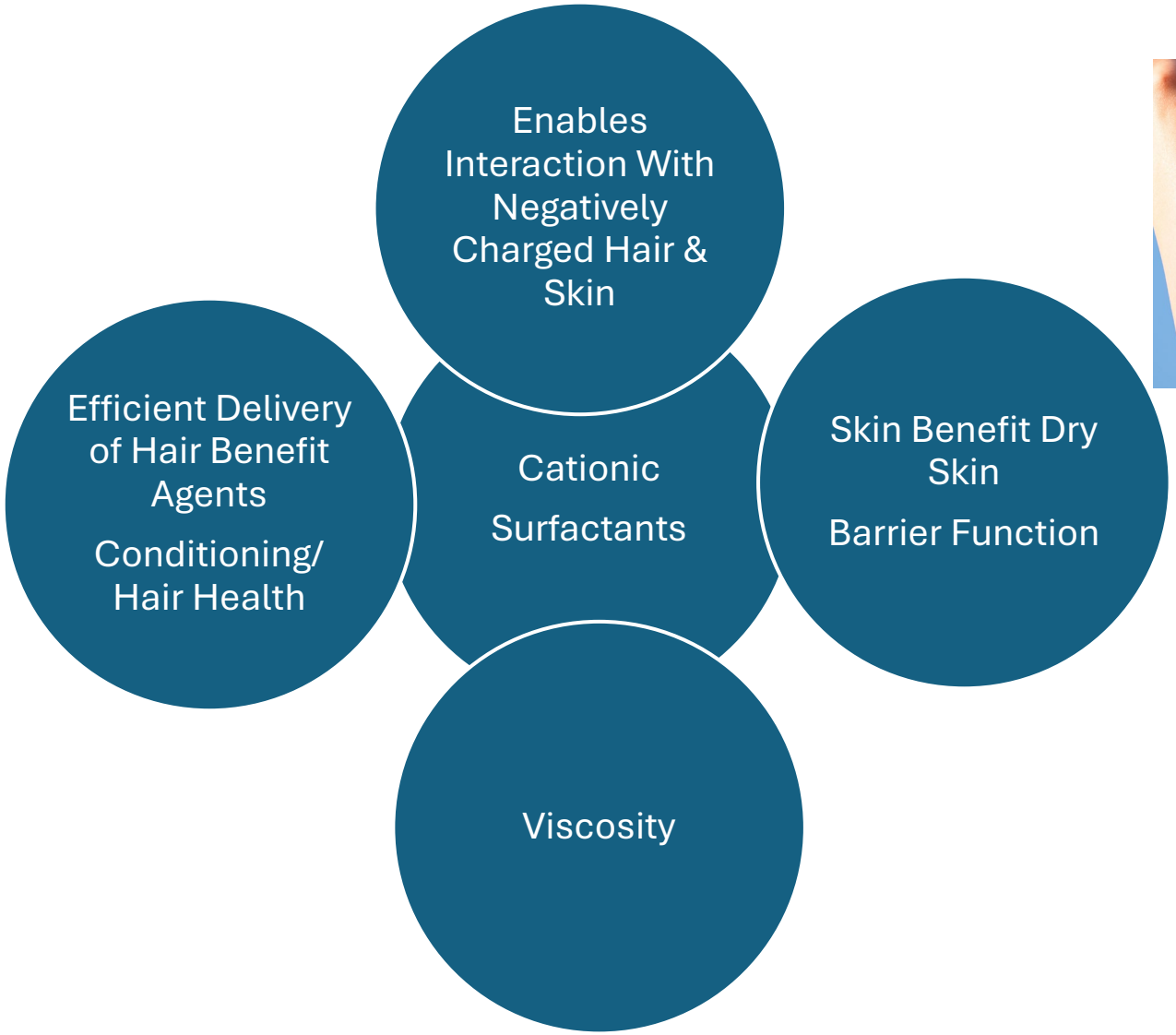
Alkyl Surfactants

Polymers



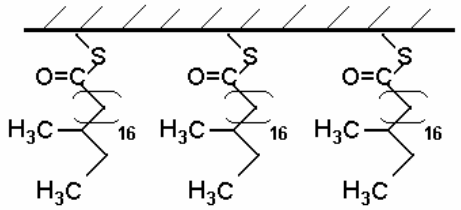
Cationic Surfactants

Structures that utilize linked cationic charges for ingredient synergy



Unhealthy Hair is Negatively Charged, So the Cationic Surfactant Charge is Key to Repair Cuticle

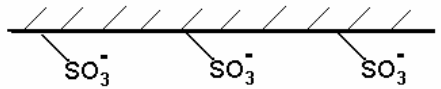
Healthy Hair



Hydrophobic Protective Layer

Everyday Damage

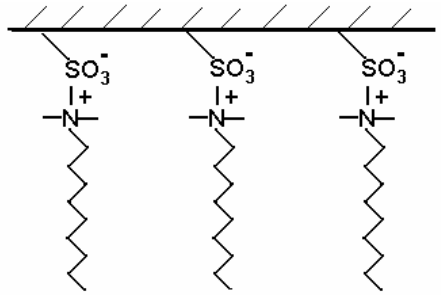
Unhealthy Hair



Hydrophobic Protective Layer Missing Negatively Charged Hair

Conditioner With Cationic Surfactant

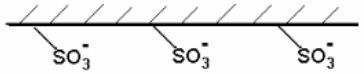
Unhealthy Hair Protected



Hydrophobic Protective Layer Restored

Primary Cationic Surfactants/Polymers Drive Hair Health

Unhealthy Hair

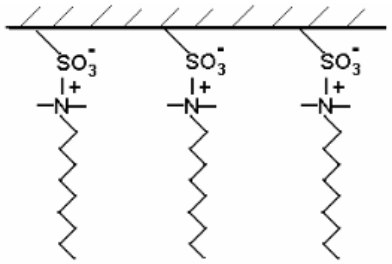


Hydrophobic Protective Layer Missing Negatively Charged Hair

Unhealthy Hair

Healthy Hair

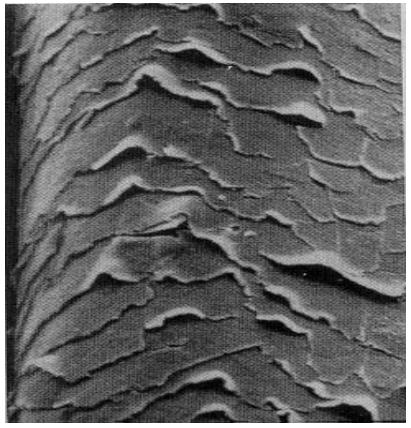
Unhealthy Hair Protected



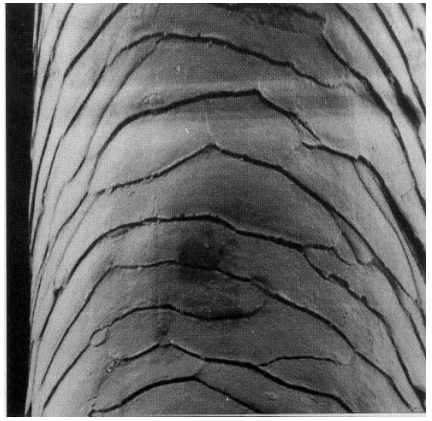
Hydrophobic Protective Layer Restored

By Protecting the Hair Cuticle from Damage

Cuticle Damage Due to Washing, Combing, Brushing, Drying, etc.



Cuticle Repair

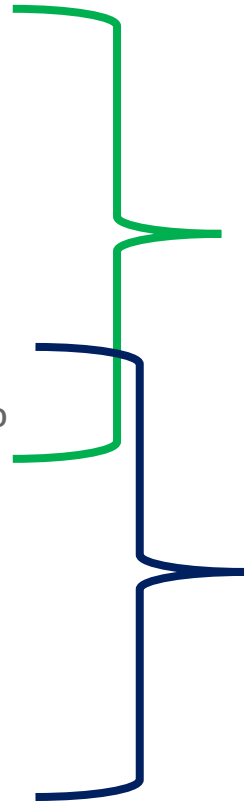


Expected Consumer Benefit from Hair Products

Cationic Surfactants are Core to Multiple Conditioner Hair Health Benefits

Ingredients

- Water, >80%
- Fatty alcohols, 1.5-7%
- **Cationic Surfactants/Polymers** 0.5-3.5%
- Silicones, 0.5-5%

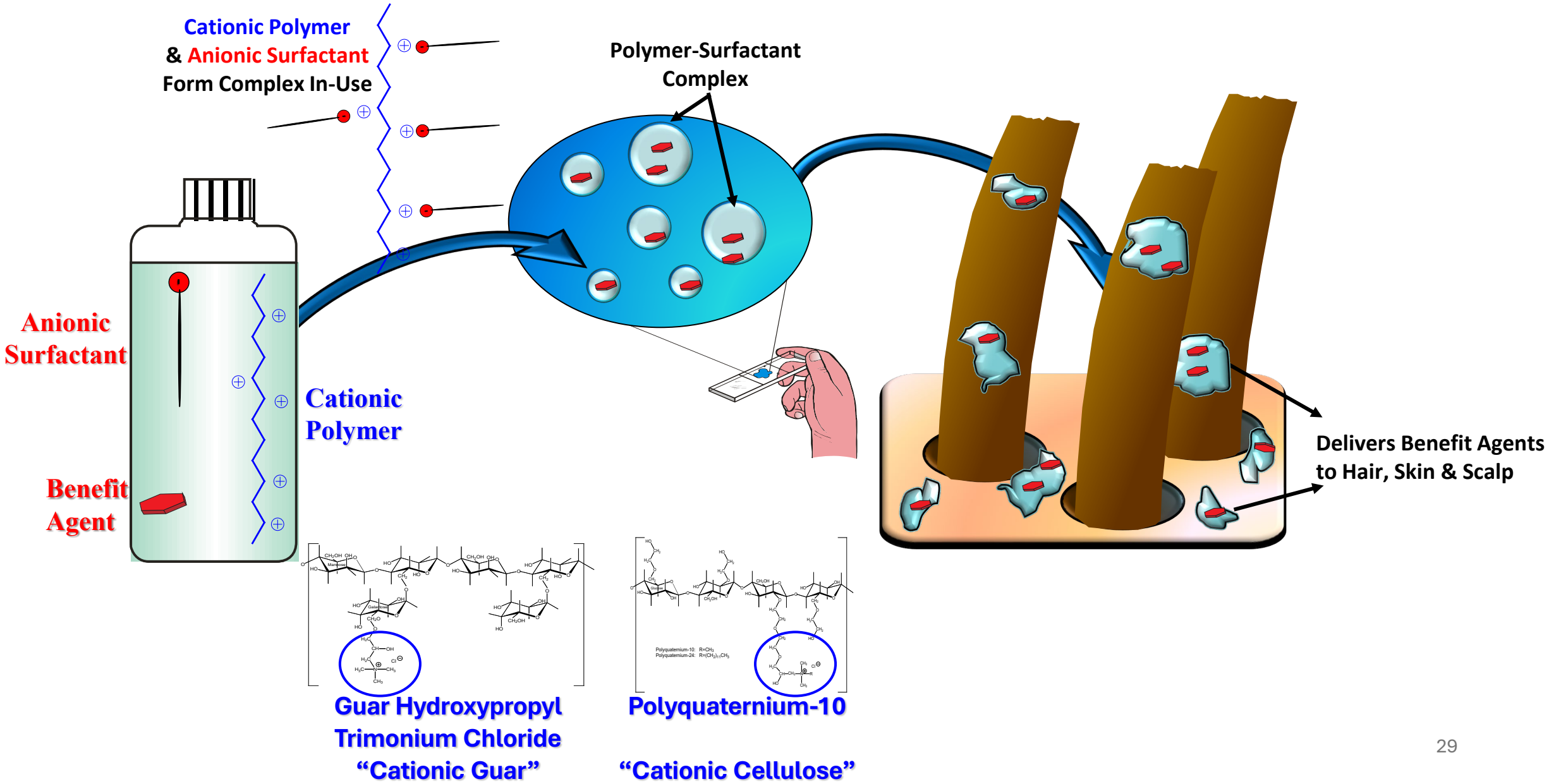


Benefits

Ingredients Form Gels to provide Smooth texture and Minimize Damage During Use

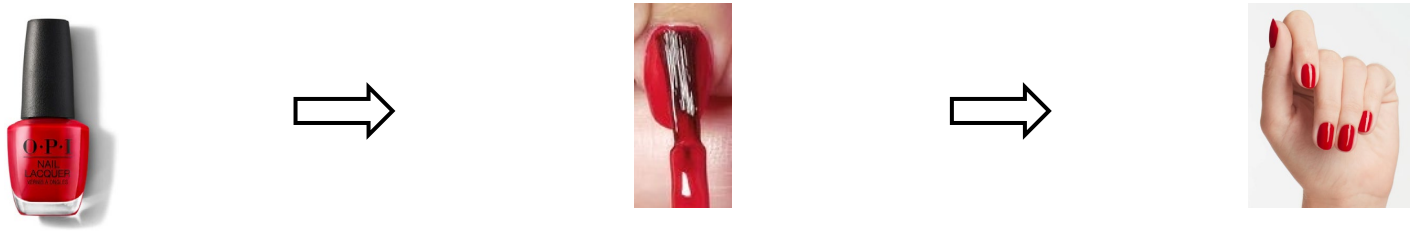
Ingredients Deposit on Hair for Dry Conditioning Benefits
(surface modification & damage protection)

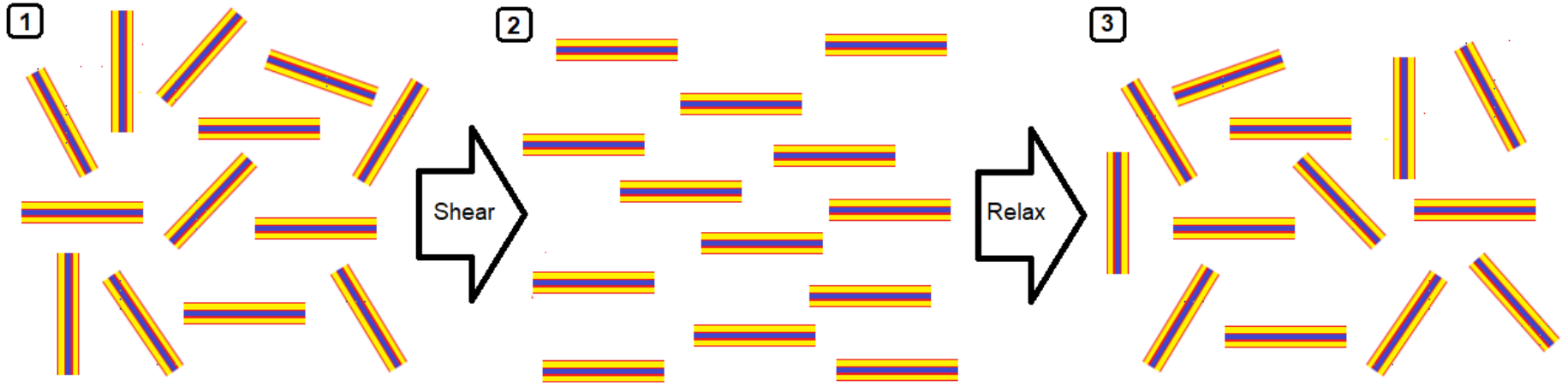
Cationic Polymers Interact with Anionic Surfactant to Enable Benefits from Cleaning Formulas



Organo-Clay

Organo-Clay Functional Behavior





Platelet structure enables gel networks (thixotropic) that respond to movement:

1. Disorganized, randomly oriented platelets create a thickening effect.
2. Under shear (flow), platelet structures align reducing viscosity and allowing smooth application
3. Removal of the shear, allows the platelets to randomly re-orient again, restoring viscosity so the lacquer can stiffen and remain in place to dry on the nail

Performance in low-polarity solvents requires a hydrophobic quaternary stearate (C18)

Organo-Clay Material and Structure

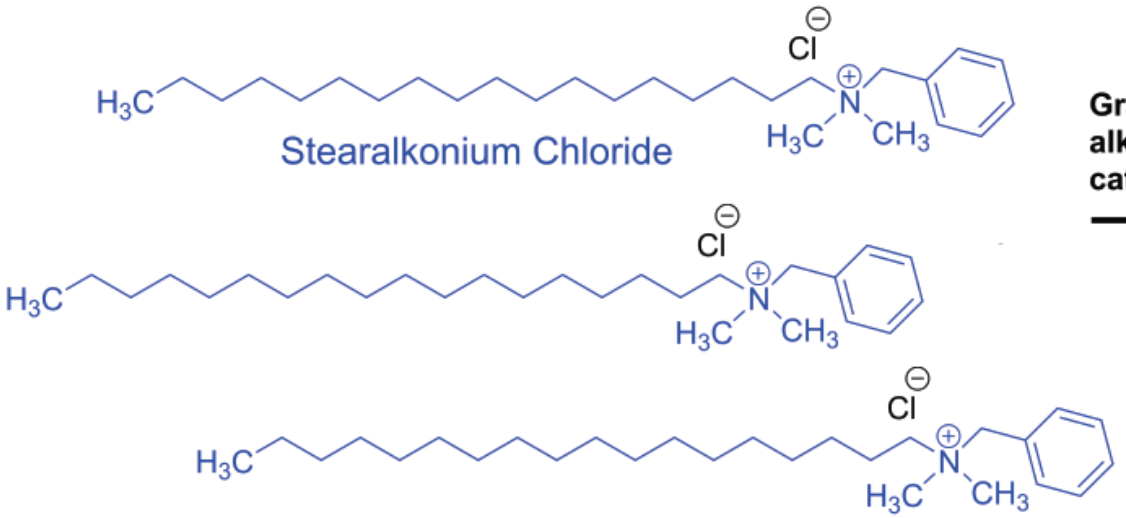
Materials - Stearalkonium Bentonite & Stearalkonium Hectorite (C18)

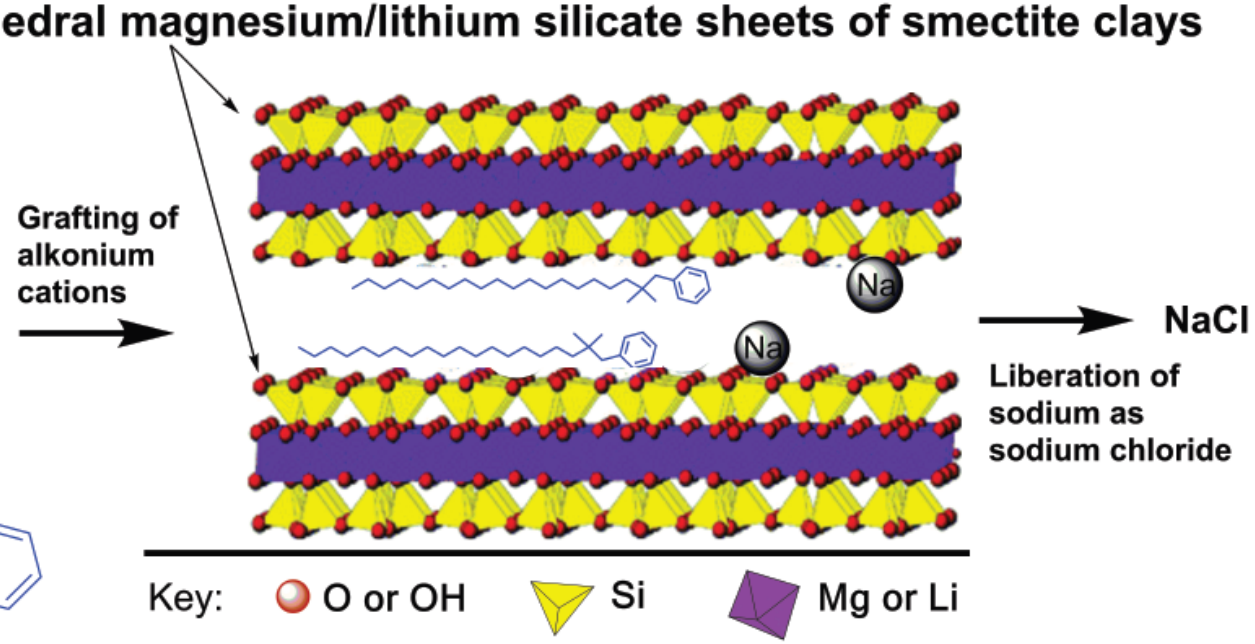
- Stearalkonium (C18) clays are used as **suspension agents** in nail polish**,** and they are **not soluble**
- They stay on nail surface and will not penetrate into cells.

Structures

- Modified smectite clays with layered plate structure and stearalkonium ions inserted between the layers
- Stearalkonium ions are bound to the clay via strong ionic bonding and remain strongly associated in the material, limiting their bioavailability and biological activity under typical cosmetic use conditions.

Figure 1. Synthesis of alkonium clays.





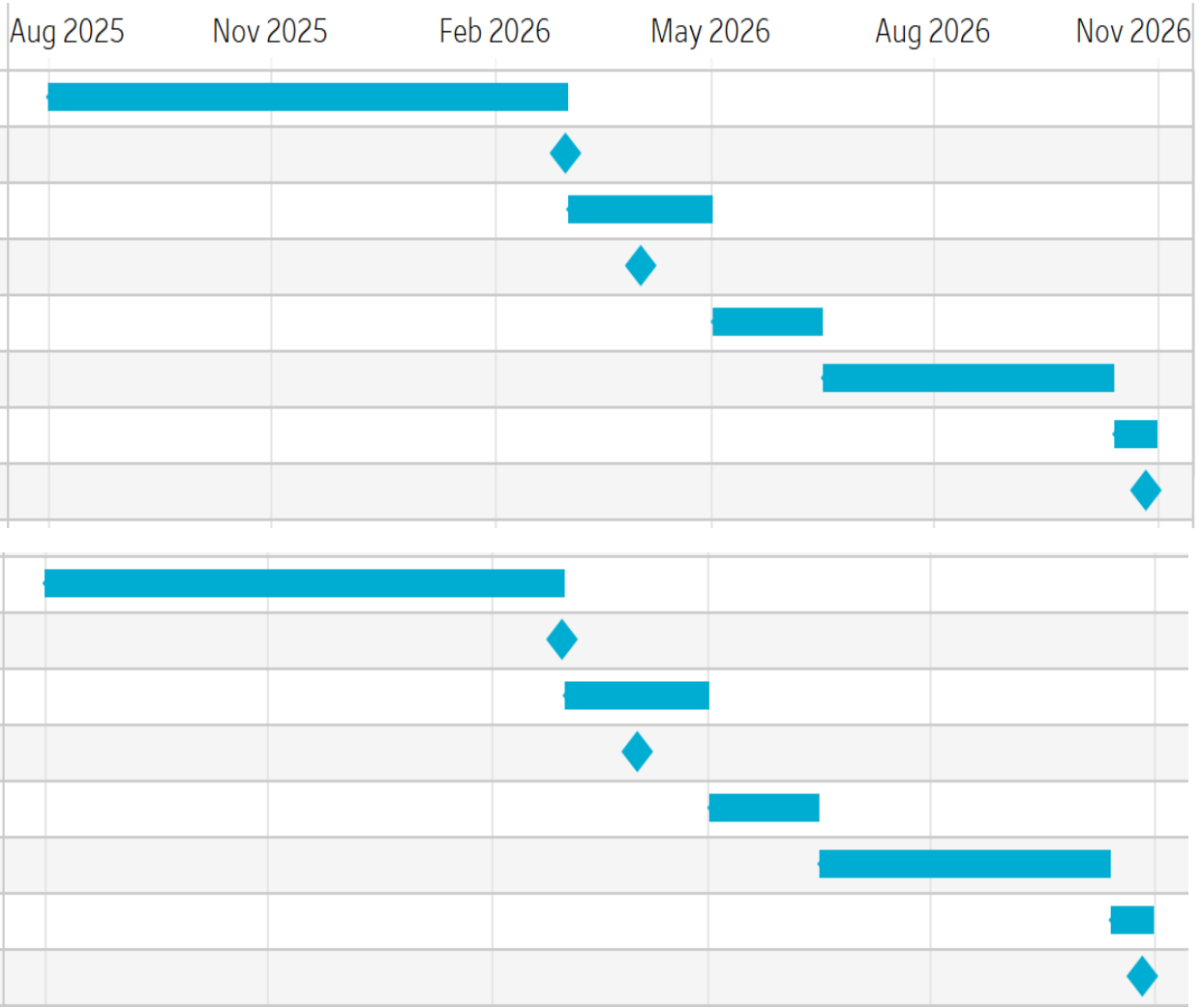
ADAPTED FROM: "Safety Assessment of Alkonium Clays as Used in Cosmetics", *Cosmetic Ingredient Review*, Final Report, April 26, 2016.

No Alternatives for Reformulation

- The benefits of the positively charged ingredients in these products cannot be unappreciated or understated
- The vast majority of hair conditioners and shampoos are formulated using QAC surfactants and polymers to interact with more typical anionic materials to provide conditioning and efficacy
- Only technology that delivers the thixotropic structure and stability in nail lacquer
- There are no positively charged alternatives to quats

Current Success!

Project Name	Activity or Milestone
Antibacterial hand soaps and body washes containing benzyl alkyl dimethyl ammonium compounds (BACs) and benzethonium compounds (BZT)	DTSC prepares Product-Chemical Profile
	DTSC releases draft Product-Chemical Profile
	Pre-regulatory public comment period
	Pre-regulatory workshop
	DTSC considers public comments
	External Scientific Peer Review
	DTSC finalizes Product-Chemical Profile
	DTSC releases final Product-Chemical Profile
Hand sanitizers and antiseptic skin wipes containing benzyl alkyl dimethyl ammonium compounds (BACs)	DTSC prepares Product-Chemical Profile
	DTSC releases draft Product-Chemical Profile
	Pre-regulatory public comment period
	Pre-regulatory workshop
	DTSC considers public comments
	External Scientific Peer Review
	DTSC finalizes Product-Chemical Profile
	DTSC releases final Product-Chemical Profile



Next Steps

- The pause in DTSC's pursuit of quats in PCPs products is most likely temporary
- Does not impede other states from their own activities
- Update on Environmental Literature Scan
  - Based on Sept 2025 SACX recommendation, ESC is conducting a literal review of available studies
  - Conducted initial ERAs for the priority cosmetic QACs and these will be refined with data identified in the literature review (Emily Burns)
  - Work is being done in the ESC's ERA subgroup and is a 2026 priority (welcoming member participation!)


Questions?