

Preliminary Screening of Quaternary Ammonium Compounds

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Presentation to the Scientific Guidance Panel

July 25, 2019



Purpose of agenda item

- Respond to Panel's request for preliminary screening of quaternary ammonium compounds (QACs)
- Obtain Panel and public input on selecting a chemical class for future consideration as potential designated chemicals:
 - QACs
 - Classes previously screened by the SGP (e.g., some classes of pesticides)

Background: Criteria for recommending designated chemicals

- ***Exposure or potential exposure*** to the public or specific subgroups
- The ***known or suspected health effects*** resulting from some level of exposure based on peer reviewed scientific studies
- The ***need to assess the efficacy of public health actions*** to reduce exposure to a chemical
- The ***availability of a biomonitoring analytical method*** with adequate accuracy, precision, sensitivity, specificity, and speed
- The ***availability of adequate biospecimen samples***
- The ***incremental analytical cost*** to perform the biomonitoring analysis for the chemical

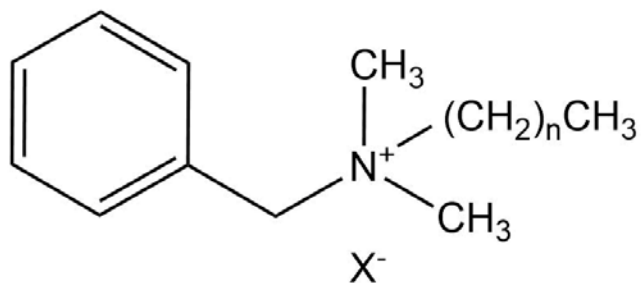
Overview of presentation

- Description of class
- Potential for exposure
 - Example uses and products
 - Volume of use
 - Environmental detections
- Possible health concerns associated with members of the class
- Biomonitoring information

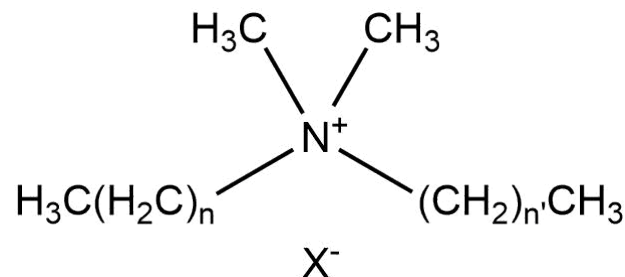
Description of class

- General chemical structure includes NR_4^+ , R often being an alkyl or benzyl group
- Chemical functions include:
 - Antimicrobial
 - Preservative
 - Antistatic
 - Softening
 - Surfactant

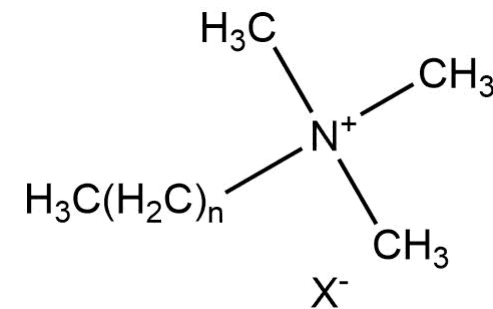
Chemical structures of selected QACs



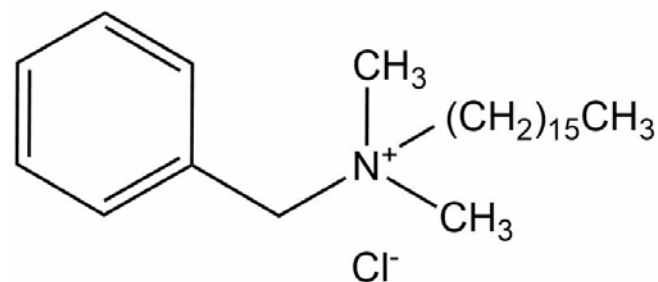
Benzylalkyldimethyl ammonium compounds (BACs)



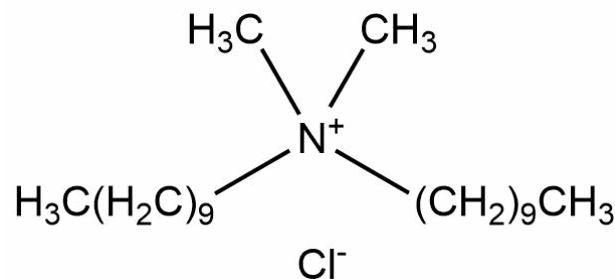
Dialkyldimethyl ammonium compounds (DADMACs)



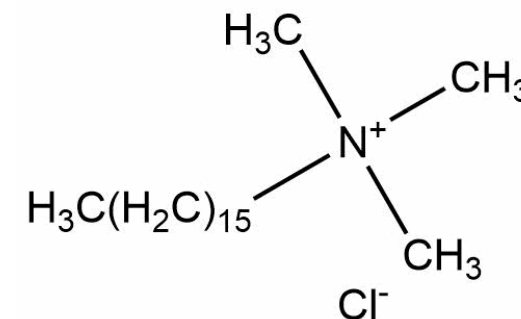
Alkyltrimethyl ammonium compounds (ATMACs)



Benzylhexadecyldimethyl ammonium chloride

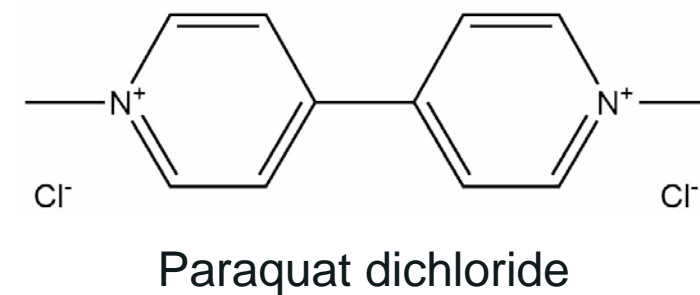
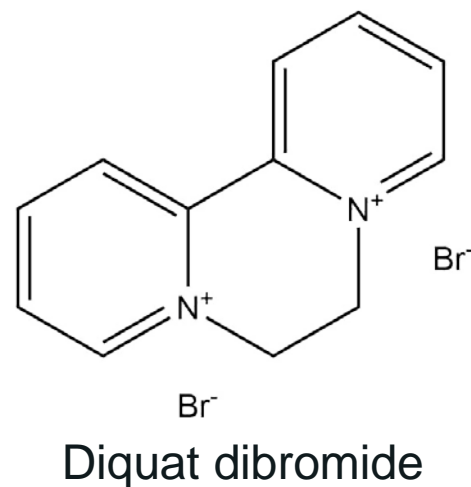
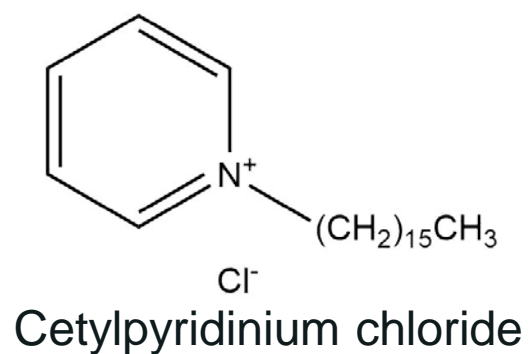
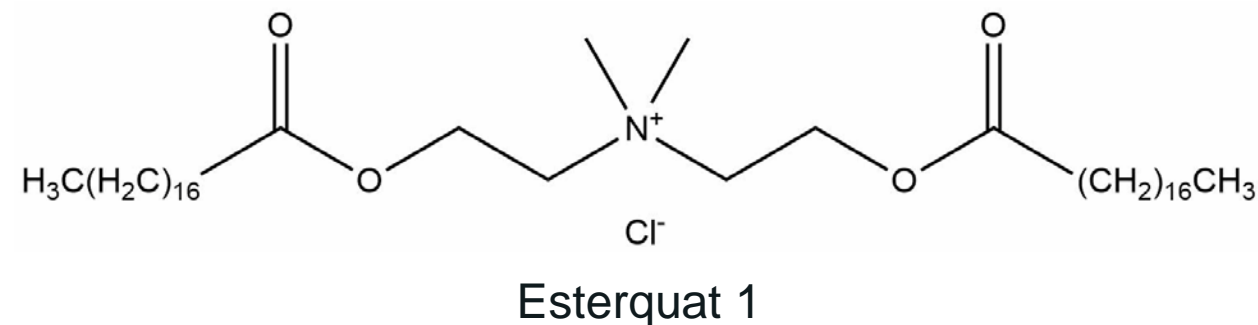
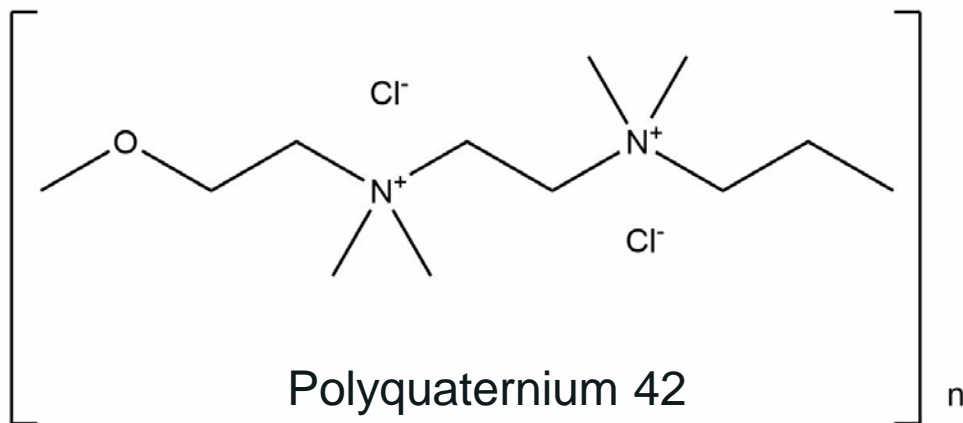


Didecyldimethyl ammonium chloride



Hexadecyltrimethyl ammonium chloride

Chemical structures of selected QACs (cont.)



Volume of use for QACs reviewed

- California pesticide sales
 - About half had sales >100K pounds in 2018
 - Several had sales >1M pounds in 2018
- California agricultural application
 - Paraquat dichloride applications >1M pounds (rank #23) in 2017
- National aggregate production volume
 - Located 20 QACs with >100K pounds produced in 2015
 - Of these, 11 were high production chemicals (>1M pounds)

Example products and QAC ingredients



Cleaning products

■ Disinfecting surface wipes and sprays

- Alkyl(50%C14, 40%C12, 10%C16)dimethylbenzyl ammonium saccharinate
- Alkyl(60%C14, 30%C16, 5%C18, 5%C12)dimethylbenzyl ammonium chloride
- Alkyl(68%C12, 32%C14)dimethylethylbenzyl ammonium chloride
- Alkyl(50%C14, 40%C12, 10%C16)dimethylbenzyl ammonium chloride
- Dioctyldimethylammonium chloride
- Octyldecyldimethyl ammonium chloride

■ Surface cleaners

- Alkyl(67%C12, 25%C14, 7%C16, 1%C8-C10-C18)dimethylbenzyl ammonium chloride
- Alkyl(50%C14, 40%C12, 10%C16)dimethylbenzyl ammonium chloride
- Alkyl(60%C14, 30%C16, 5%C18, 5%C12)dimethylbenzyl ammonium chloride
- Alkyl(68%C12, 32%C14)dimethylethylbenzyl ammonium chloride
- Polyquaternium 95

Example products and QAC ingredients (cont.)



Antibacterial hand soaps

- Benzalkonium chloride
- Cetrymonium chloride

Example products and QAC ingredients (cont.)



Hair conditioners

- Behentrimonium chloride
- Behentrimonium methosulfate
- Polyquaternium 37
- Polyquaternium 47
- Cetrimonium chloride
- Dicetyldimonium chloride
- Distearyldimonium chloride

Example products and QAC ingredients (cont.)



Other personal care products

► Shampoo

- Polyquaternium 6
- Polyquaternium 10

► Hair dye

- Polyquaternium 22

► Facial cleanser and body wash

- Polyquaternium 7

► Lotion

- Distearyldimonium chloride

► Mouthwash

- Cetylpyridinium chloride

Example products and QAC ingredients (cont.)



Cosmetics

► Foundation

- Quaternium 15

► Lipstick

- Quaternium 18

► Mascara

- Polyquaternium 10

Example products and QAC ingredients (cont.)



- Eye drops
 - Benzalkonium chloride
- Contact lens solution
 - Polyquaternium 1
- Topical antiseptics
 - Benzalkonium chloride
 - Benzethonium chloride
- Oral antiseptic pain relievers
 - Benzalkonium chloride

Example products and QAC ingredients (cont.)



Fabric softeners

- Diethylesterdimethyl ammonium chloride

Example products and QAC ingredients (cont.)



Pesticides used at home

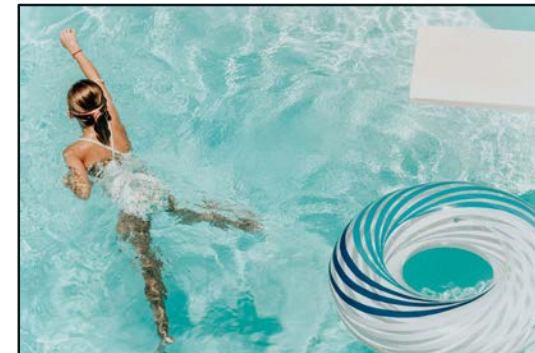
■ Weed and grass killers

- Diquat dibromide

■ Swimming pool algaecides

- Alkyl(50%C14, 40%C12, 10%C16)dimethylbenzyl ammonium chloride
- Polixetonium chloride (polyquaternium 42)

Example products



Widely used in oil and gas operations



- Oil field biocide
- Oil field foamer
- Oil emulsifier
- Mineral slurry dispersant
- Antistatic
- Surfactant
- Corrosion inhibitor
- Clay stabilizer

Environmental detections

➡ Widely detected in:

- Sediment
- Sludge
- Wastewater treatment plant (WWTP) influent and effluent

➡ Other detections:

- Indoor house dust samples collected in Germany
- Air samples from a US hospital
- Fish sampled from Nordic countries – mostly cod, some perch

Possible health concerns

- Skin irritation/sensitization
- Respiratory effects, including asthma
- Developmental and reproductive effects
- Altered cellular function and metabolism
- Antibiotic resistance

Biomonitoring information

- Very little biomonitoring data located
- Methods papers
 - Whitehead et al. (2010)- Spiked diquat dibromide and paraquat dichloride in human urine
 - Steuer et al. (2016)- Determination of phosphatidylcholine-derived QACs in human plasma, serum, and urine
- Preliminary biomonitoring research in progress

Previously screened chemical classes

➡ Pesticides

- Neonicotinoids*
 - Acetamiprid, clothianidin, imidacloprid, and thiacloprid newly added to designated chemical list
- Anilides

➡ Chemical classes used in UV applications

- Benzophenones
- Phenolic benzotriazoles

*Ospina M, Wong LY, Baker SE, Serafim AB, et al. (2019). Exposure to neonicotinoid insecticides in the U.S. general population: Data from the 2015-2016 national health and nutrition examination survey. Environ Res. Epub ahead of print.

Options for the Panel

■ The SGP could:

- Request that OEHHA prepare a potential designated chemical document on QACs
- Request that OEHHA prepare a potential designated chemical document on a previously screened chemical class
- Advise no further action on any of these classes
- Suggest other chemical classes for possible consideration