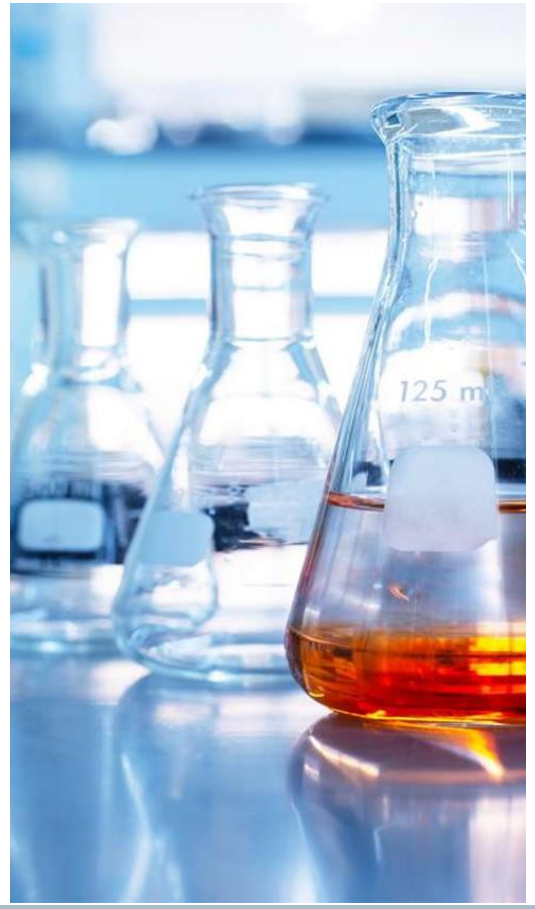
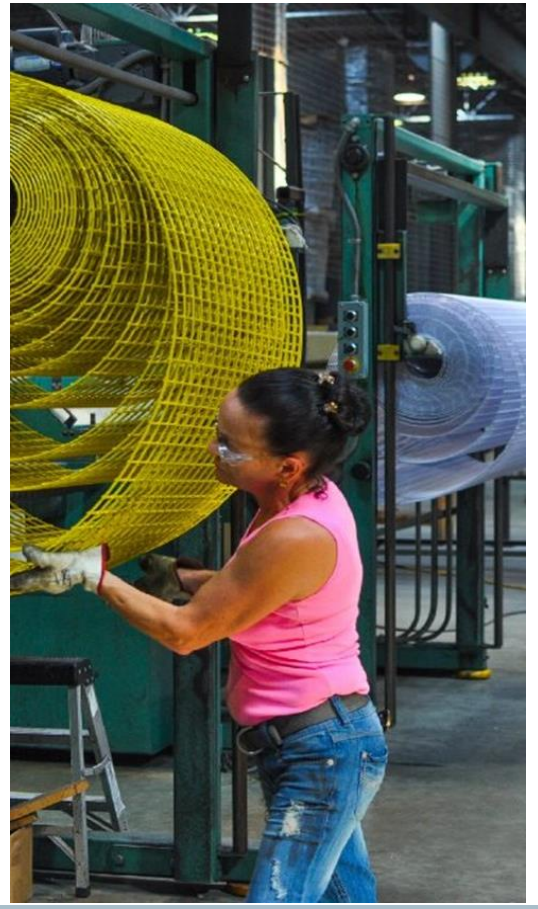
Evaluating and Prioritizing Chemicals of Concern



October 8, 2025

Webinar produced by TURI



Agenda for this webinar

- Overview of the Massachusetts process for evaluating and prioritizing chemicals of concern
  - Aryl phosphate esters
  - Nanomaterials
  - Quaternary ammonium compounds
- Evolution of ChemSec's SIN list
- ZDHC's Manufacturing Restricted Substances List (MRSL)

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Current activities of the TURA Science Advisory Board

Heather Tenney
Karen Thomas
Colin Hannahan

Role of the SAB

The Toxics Use Reduction Act of 1989 created a Science Advisory Board (SAB) to work with the Institute as described in Chapter 21I, Section 6(J).

The Board's primary role is to consider petitions to add or delete substances from the TURA list of toxic or hazardous substances and make recommendations to the Institute accordingly. The SAB also makes recommendations for Higher and Lower Hazard Substances.

The Institute may call on the SAB for scientific or technical advice concerning other TURA-related issues.

Science Advisory Board Nominations and Composition

The Board consists of 11 members appointed by the Governor

- 3 by the Institute
- 3 by the Secretary of Economic Affairs
- 3 by the Secretary of Environmental Affairs
- 1 by the Secretary of Labor
- 1 by the Secretary of Human Services

Members serve three-year terms

The Governor makes the final appointments to the Board

To be nominated to the SAB, an individual must have extensive professional experience and/or academic expertise

Toxicology, epidemiology, occupational medicine, environmental science or chemistry.

Look for expertise that balances the Board

SAB Considerations

Makes recommendations based solely on science of the substance

Makes recommendations based on the inherent hazard of the substance, not risk

Uses an expert judgment approach

Discussions and recommendations are in open public meetings

SAB Criteria for Listing Chemicals under TURA

1. Human Health Hazards

- Cancer
- Reproductive effects
- Neurological disorders
- Genetic mutations
- Chronic conditions
- Acute toxicity

2. Environmental Hazards

- Toxicity
- Persistence in the environment
- Bioaccumulation
- Other impacts like Ozone depletion, Climate change, Toxic breakdown products

3. Other

Adverse health effects from **likely use, handling, or disposal conditions**

Relevant Information

Health hazards	Environmental and ecosystem hazards	Safety and physical hazards
Health-based exposure limits and values	Environmental exposure values	Chemical information and physical characteristics
	Global environmental impacts	

Human Health Hazards

Information	Lists
PubChem Safety and Hazards – start here	Pharos – has GreenScreen (ISCL)
CompTox Hazard Data	California Prop 65 List
ChemInformatics – Hazard (it's a beta version!)	IARC
CompTox Literature – PubMed Abstract Sifter	ChemSec SIN List
CompTox Literature – Google Scholar	ECHA Endocrine Disruptor Assessment List
SciFinder – GHS statements (expert curated)	TEDx List of Potential Endocrine Disruptors
ECHA	European Commission – Endocrine Disruptors
UML LIbrary	EPA's Endocrine Disruptor Screening Program Universe of Chemicals (on CompTox)
	Chemical Neurotoxic Agents
If needed: NTP Report on Carcinogens	Grandjean & Landrigan 2006 and 2014 – Developmental neurotoxicants
	AOEC

Environmental Hazards

Information	Lists
ECOTOX	Pharos
EPA PBT Website	Ozone-Depleting Substance List
CompTox Literature – PubMed Abstract Sifter	Global Warming Potentials List
CompTox Literature – Google Scholar	Greenhouse Gas list
ECHA	EPA List of Hazardous Air Pollutants
	ECHA PBT Assessment List
	UN Environment Program Stockholm Convention
	List of Persistent Organic Pollutants
	Persistence – Biomonitoring California

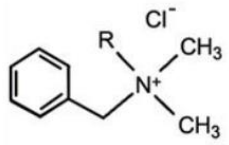
EHS Information – where to begin?

Notes:

- All links for resources can be found on the TURI EHS LIbGuide except for SciFinder and Pharos
- LibGuide: **https://guides.turi.org/beyond_sds**
- Course on how to use these resources: https://www.turi.org/tool%20posts/beyond-the-sds-2/
- These resources do not necessarily cover safety adequately (see NIOSH, OSHA)
- Additional considerations when researching categories, e.g., biomonitoring data sources

SAB EHS Summaries

Updated EHS Summary of Alkyl Dimethyl Benzyl Ammonium Chloride (ADBAC) for the MA TURA Science Advisory Board Meeting – May 20, 2021

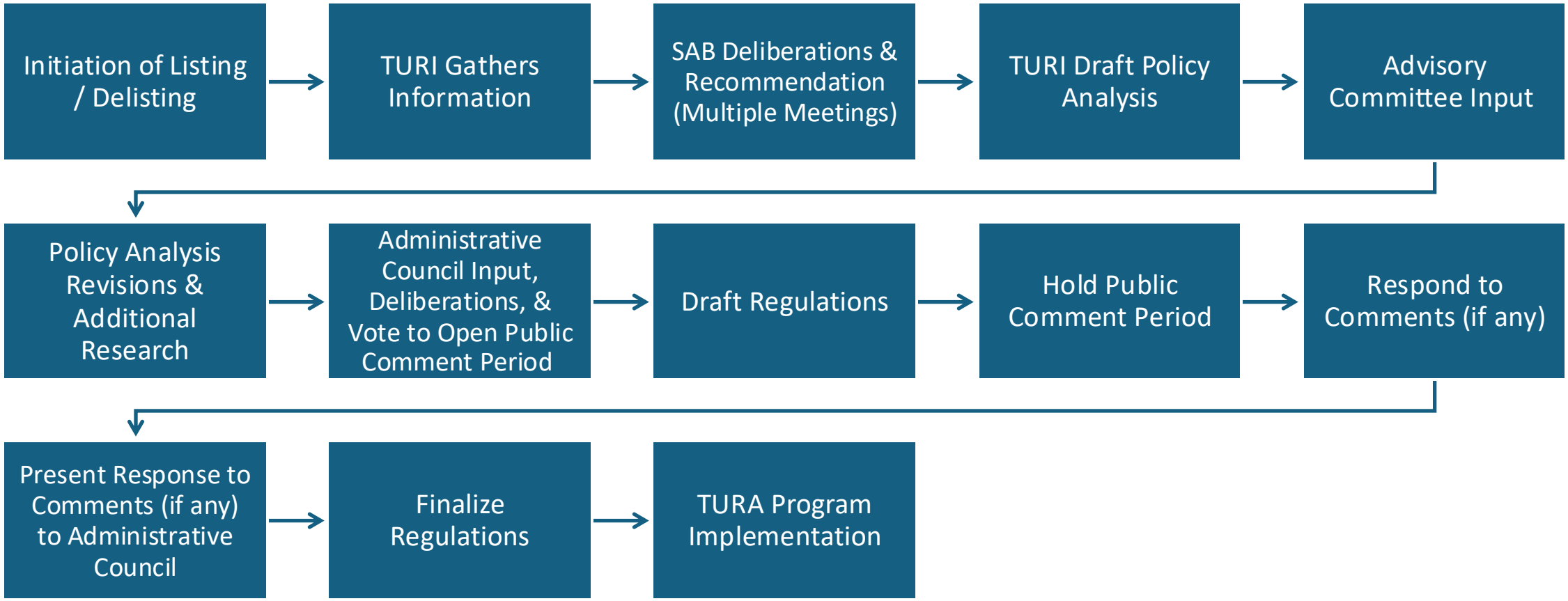
CAS #: 68424-85-1 Representative CAS # for ADBAC 	**NAME: Alkyl Dimethyl Benzyl Ammonium Chloride (ADBAC)** **Synonym[1]s:** n-alkyl (C14 50%; C12 40%; C16 10%) dimethyl benzyl ammonium chloride; Alkyl(C12-16)dimethylbenzylammonium chloride; Ammonium, alkyl(C12-C16)dimethylbenzyl-, chlorides; Barquat MB 80; Benzyl-C12-C16-alkyldimethyl ammonium chlorides; Bioquat 501; Bioquat 80; Black alg aetrine; BTC 835; Catigene T80; Cyncal 80; EINECS 270-325-2; Gardiquat 1250AF; Hyamin cdm/BC; Tret-O-lite WF 82 Alkyldimethylbenzylammo **RTECS #[1]:** UZ2995000 **EINECS #[2]:** 270-325-2 **Molecular Weight[3]:** 377 **Molecular Formula[4]:** RC R= n-alkyl (C_{12} 40%, C_{14} 5 **EPA PC Code[4]:** 069105 **Related CAS #'s: (See lis**
PHYSICAL CHARACTERISTICS	
Primary Use	ADBAC is an antimicrobi commercial/ institutiona medical settings[4]. There are 667 EPA-regist ingredient, 664 of which that are conventional pr 2011 through 2014 indic ADBAC are sold per year "Due to their amphiphili active agents against mi membranes through ele charged head group and adsorption, and then pe intramembrane region. them sensitive to the hy
Physical state, odor at room temperature & pressure	Crystalline sold in pure f Clear yellow to straw co
Melting point; Boiling point	**MP:** 241.02˚C

Specific Gravity	
SAFETY/PHYSICAL HAZARDS	
Vapor Pressure	3.53x 10^{-12} mm Hg[4]
Flammability	
Flashpoint	
Flammability Rating	
Auto Ignition Point	
Combustion products	
Explosivity (UEL, LEL, shock sensitive)	
Oxidizer	
Corrosivity	**Industrial** Acute Tox, Skin Corros Serious eye Hazardous **Ready-to-u** Skin corros Serious eye e.g., MD St **Institution** e.g., Alpha corrosion C
pH	7.59[4]
Reactivity	
Viscosity	
Odor Threshold	
Particle size, shape, respirable fraction	
Other physical hazards associated with process: Heat, gases under	

ergonomic hazard	
HEALTH HAZARDS	
Acute Toxicity	
Oral LD_{50}	LD_{50} Rat = 304.5 mg/kg (combined) LD_{50} Rat = 510.9 mg/kg (males) 280.8 mg/kg (females)[4] EPA Toxicity Category II[4]
Dermal LD_{50}	LD_{50} Rat = 930 mg/kg (combined) LD_{50} Rat = 1100 mg/kg (males) 704 mg/kg (females)[4] EPA Toxicity Category III[4]
Inhalation LC_{50}	0.054 < LC_{50} (Rat) < 0.51 mg/L[4] EPA Toxicity Category II[4]
Intraperitoneal LD_{50}	
Chronic or Sub-chronic Toxicity	
IARC rating	Not classified by IARC Monographs, Volumes 1-123
Carcinogenicity	The carcinogenic effects of DDAC and C12–C16 ADBAC have been investigated in multiple chronic mice and rats. All available stud ADBAC are carcinogenic via the with the conclusions of both EP Furthermore, EPA's Cancer Asse C12–C16 ADBAC and DDAC as "

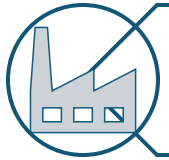
	Benchmark score."
ENVIRONMENTAL & ECO-SYSTEM HAZARDS	
PBT	
Persistence	"We have determined the occurrence of 19 QACs in residential dust collected before and during the COVID-19 pandemic. QACs were detected in >90% of the samples collected during the pandemic at concentrations ranging from 1.95 to 531 µg/g (n = 40; median of 58.9 µg/g). The total QAC concentrations in these samples were significantly higher than in samples collected before the COVID-19 pandemic ($p < 0.05$; n = 21; median of 36.3 µg/g). Higher QAC concentrations were found in households that generally disinfected more frequently ($p < 0.05$). Disinfecting products commonly used in these homes were analyzed, and the QAC profiles in dust and in products were similar, suggesting that these products can be a significant source of QACs. Our findings indicate that indoor exposure to QACs is widespread and has increased during the pandemic."[54]
Bioaccumulation	
BAF	
BCF	The whole body BCF in fish was estimated to be 79.[2] "There is potential for acute exposure to aquatic organisms in the water column because of the high solubility of ADBAC in water… However, bioconcentration in aquatic organisms is not expected despite the high log K_{ow} of 3.91 (>3) because ADBAC is highly soluble in water and, being a positively-charged compound, is tightly

TURA Program Decision Making Process

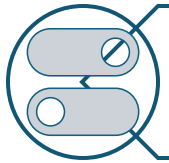


TURI Policy Analyses

Summary of Science



Uses in Massachusetts

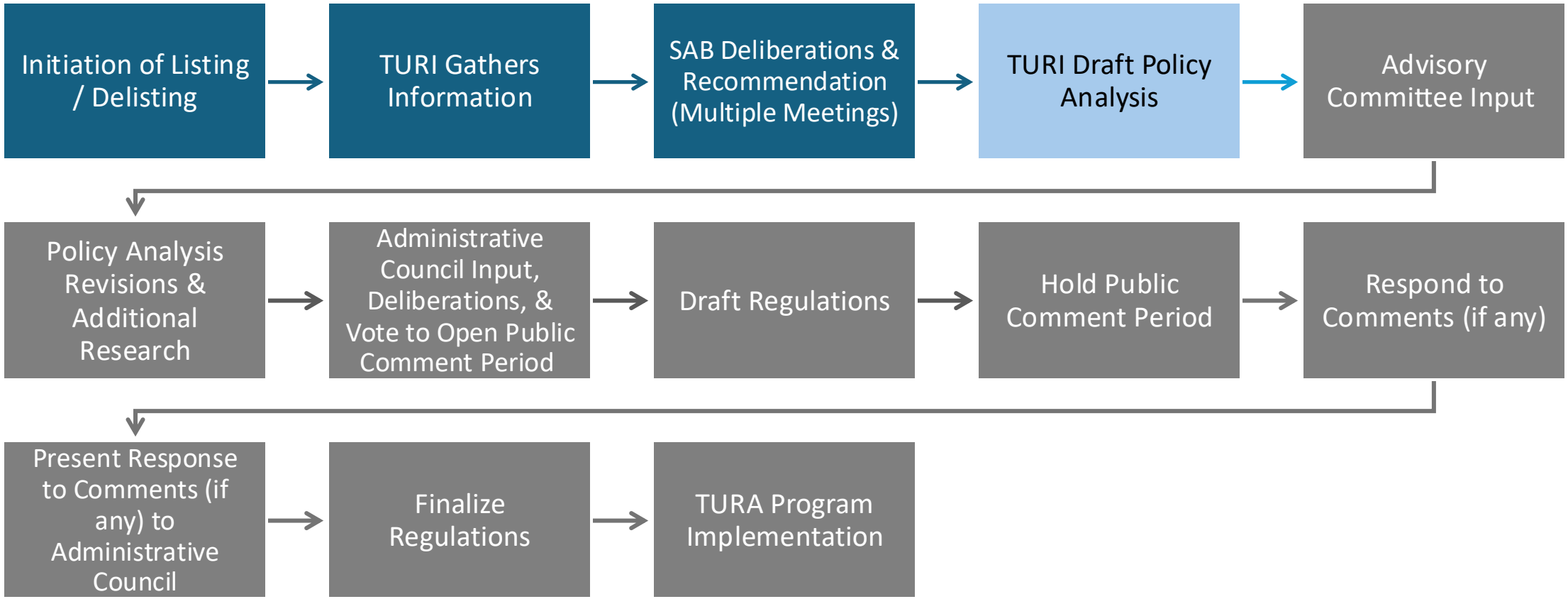


Potential alternatives

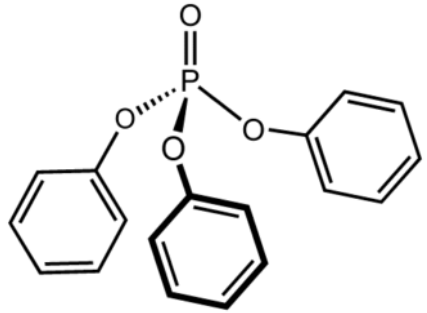
Regulations

Impact on TURA Program

TURA Program Consideration of **Aryl Phosphate Esters Category**



Aryl Phosphate Esters Category

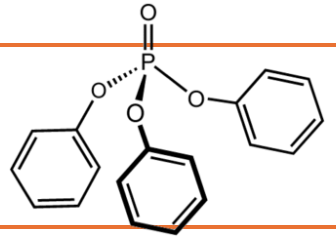


Why did the SAB consider APEs?

- FRs being considered state-wide per the 2020 Mass FR Law (ban)
  - "AN ACT TO PROTECT CHILDREN, FAMILIES, AND FIREFIGHTERS FROM HARMFUL FLAME RETARDANTS"
- APEs appeared as a potential substitute for the banned FRs
- Would they be a regrettable substitute?
- TURI decided to ask the SAB to investigate under TURA since APEs not currently listed

What are APEs?

APEs look like some variation of the most common APE – TPP

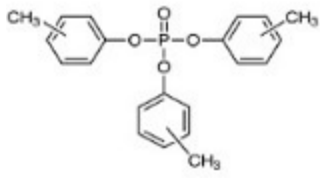


Used as flame retardants, plasticizers, lubricants (e.g., hydraulic fluids, textile coatings and plastic material/products)

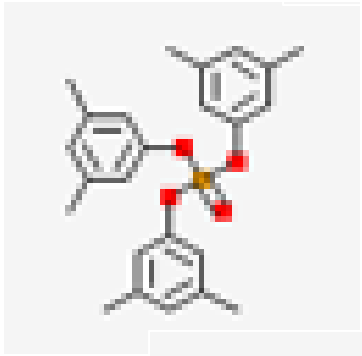
SAB considered this potential category during 4 meetings: December 2024, Feb/Apr/June 2025

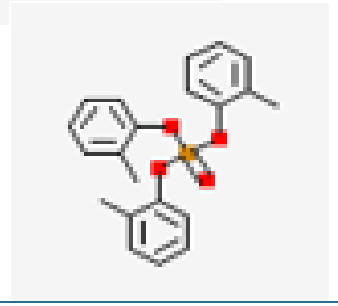
Hazard endpoints of consideration: aquatic toxicity, bioaccumulation, neurodevelopmental effects, endocrine disruption

The SAB made a recommendation - TURI now drafting the Policy Analysis for consideration at the TURA Advisory Council



Cresyl (methyl) and derivatives





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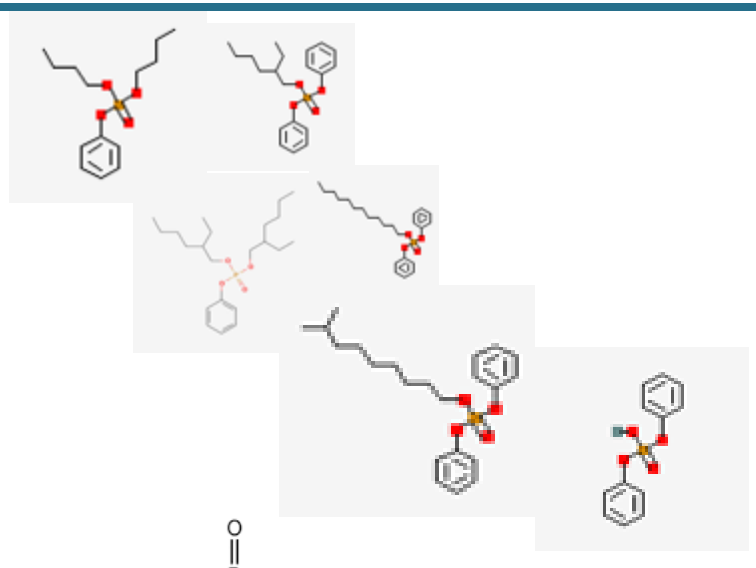
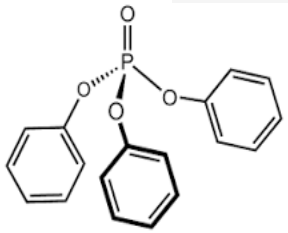
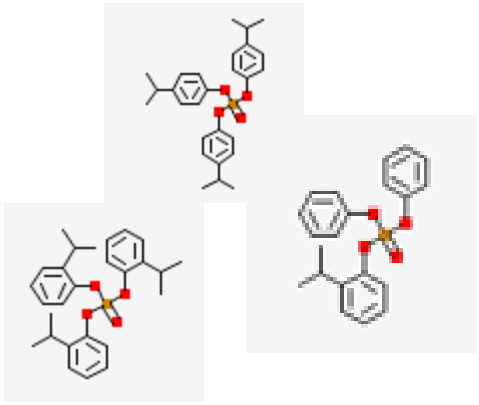




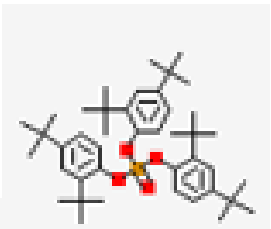
TPP and derivatives

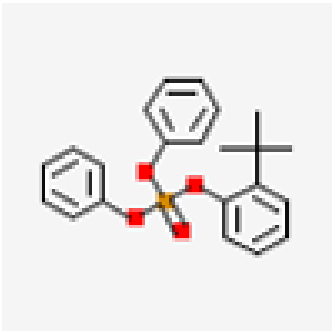
1

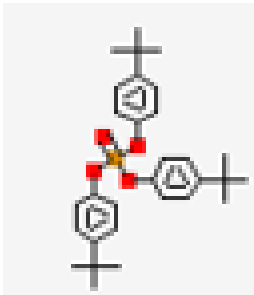


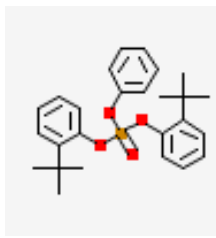
Isopropyl and derivatives

3





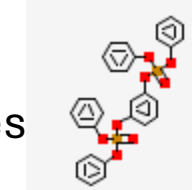


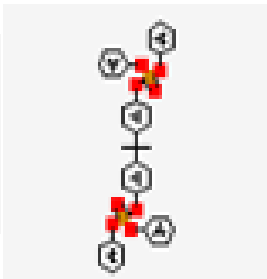


Butyl and derivatives

4

Poly and derivatives





5

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Process of Consideration for APEs

Start with SAB Criteria for listing and delisting

Special consideration for category vs single chemical

Are the potential members of the category similar enough **structurally** and would they be assumed to behave similarly with regard to **toxicity**?

Information Considered – Getting Started on APEs

Sources used:

- State, federal and international research and policy documents; academic and NGO research articles; and chemical databases (e.g., EPA CompTox)
- ~ 29 policy documents from EPA, US states, ECHA, EU member states, among others guided the initial research, providing valuable background information, toxicological concerns and policy options

Information gathered:

- Chemical structures (approx 30 CAS numbers), physical and chemical characteristics, possible neurological and developmental toxicity, possible endocrine disruption properties, and possible environmental hazards

Information Considered – Digging into the Science of APEs

Studies on the possible **neurological and developmental toxicity** of the category members

- Focused on studies from the last 5 years
- The Board looked at 67 research articles including 12 that studied possible **endocrine disruption**

The primary potential environmental hazard is **chronic aquatic toxicity** and some **bioaccumulation potential**

- One member considered 25 research papers (1980s vintage)
- Narrowed to 4 studies based on transparency and validity of study design and documented measurement of actual exposure concentration

The Recommendation

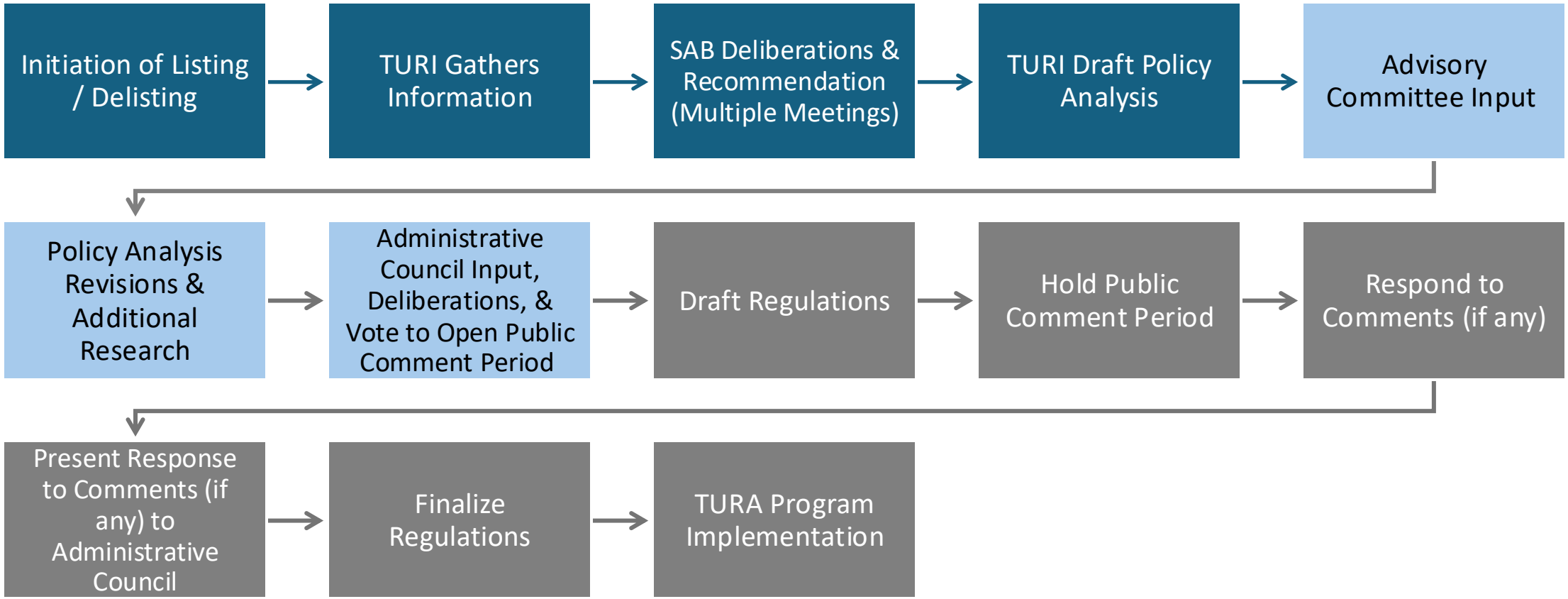
Recommendation to list aryl phosphate esters due to evidence of **aquatic toxicity** and **bioaccumulation**

- Aquatic toxicity consistent across the group.
- Holes in the data are scattered, giving more confidence that members of the group will act similarly.
- Bioaccumulation is moderate to high across the group and increases with molecular weight.

Additional concerns for **persistence, endocrine disruption, neurodevelopmental effects**

- Persistence likely increases with Log K_{ow} especially if Log K_{ow} is higher than 4.5 (most members of the group).
- There is concern for endocrine disruption, with varying levels of information and potency across the group. Evidence indicates that TPP and DPP interact with steroid hormone receptors.
- Altered behavior in rodents and human neurodevelopment effects have been shown in limited studies of some members.

TURA Program Consideration of **Carbon Nanotubes and Nanofibers**



Petition

June 2020

Petition filed by Clean Water Action (CWA) and Public Employees for Environmental Responsibility (PEER) to list Carbon Nanotubes (CNT) and Carbon Nanofibers (CNF) under TURA

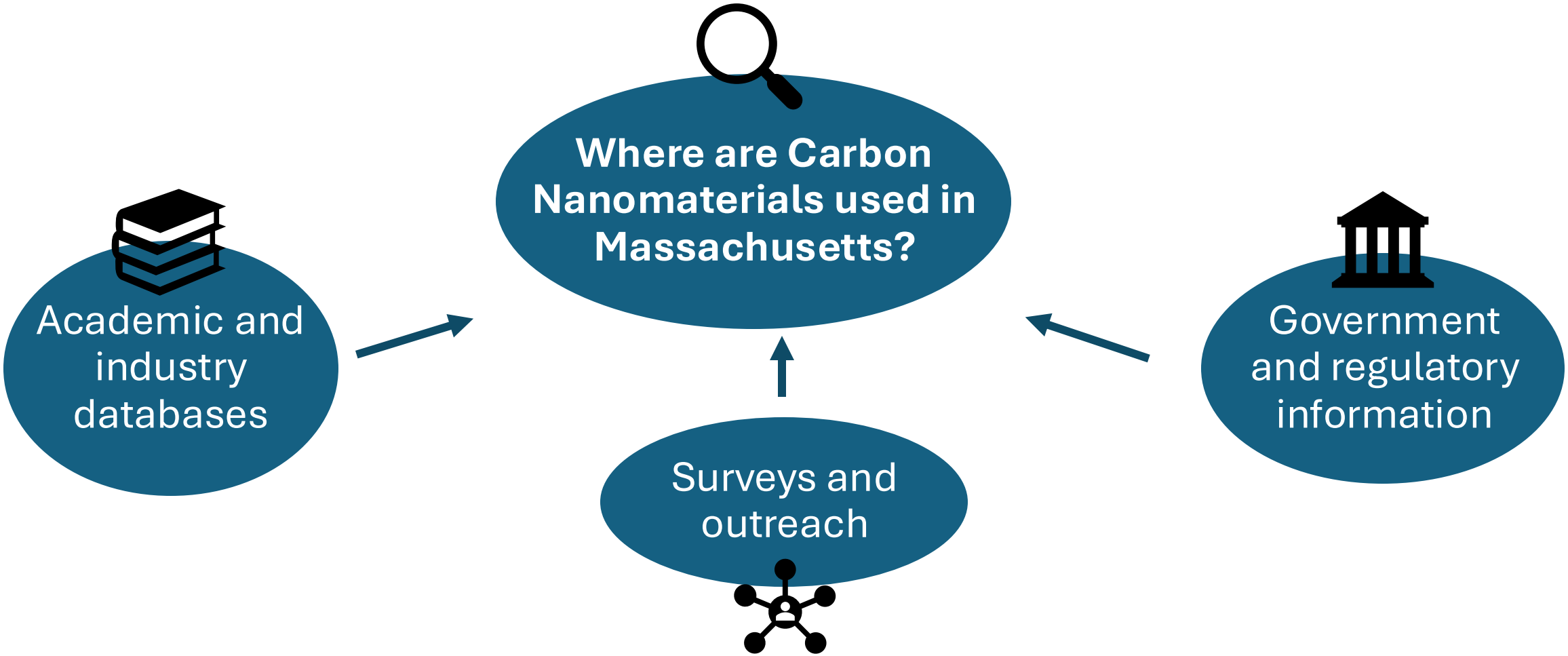
- Requested to list Carbon Nanotubes and Carbon Nanofibers as Higher Hazard Substances (HHS)
  - Would lower use reporting threshold to 1000 lb/year
- Proposed to include CNTs and CNFs on TURA list as a group
- Requested 100g use reporting threshold

Recommendation from the Science Advisory Board

TURA Science Advisory Board recommends Single Walled Carbon Nanotubes, Multi Walled Carbon Nanotubes, and Carbon Nanofibers be **added as three distinct categories** to the TURA List of Toxic Substances

- Recommended **MWCNT** category be listed as HHS
  - Evidence of pulmonary toxicity, lung cancer, mesothelioma and environmental persistence. And concerns for genotoxicity and toxic environmental degradation products.
- Recommended listing SWCNT and CNF as standard categories
  - **SWCNT** - evidence of pulmonary toxicity and environmental persistence. Concerns for reactive oxygen species (ROS) production and DNA damage.
  - **CNF** - evidence of pulmonary toxicity.

Policy Analysis: Potential Uses in Massachusetts



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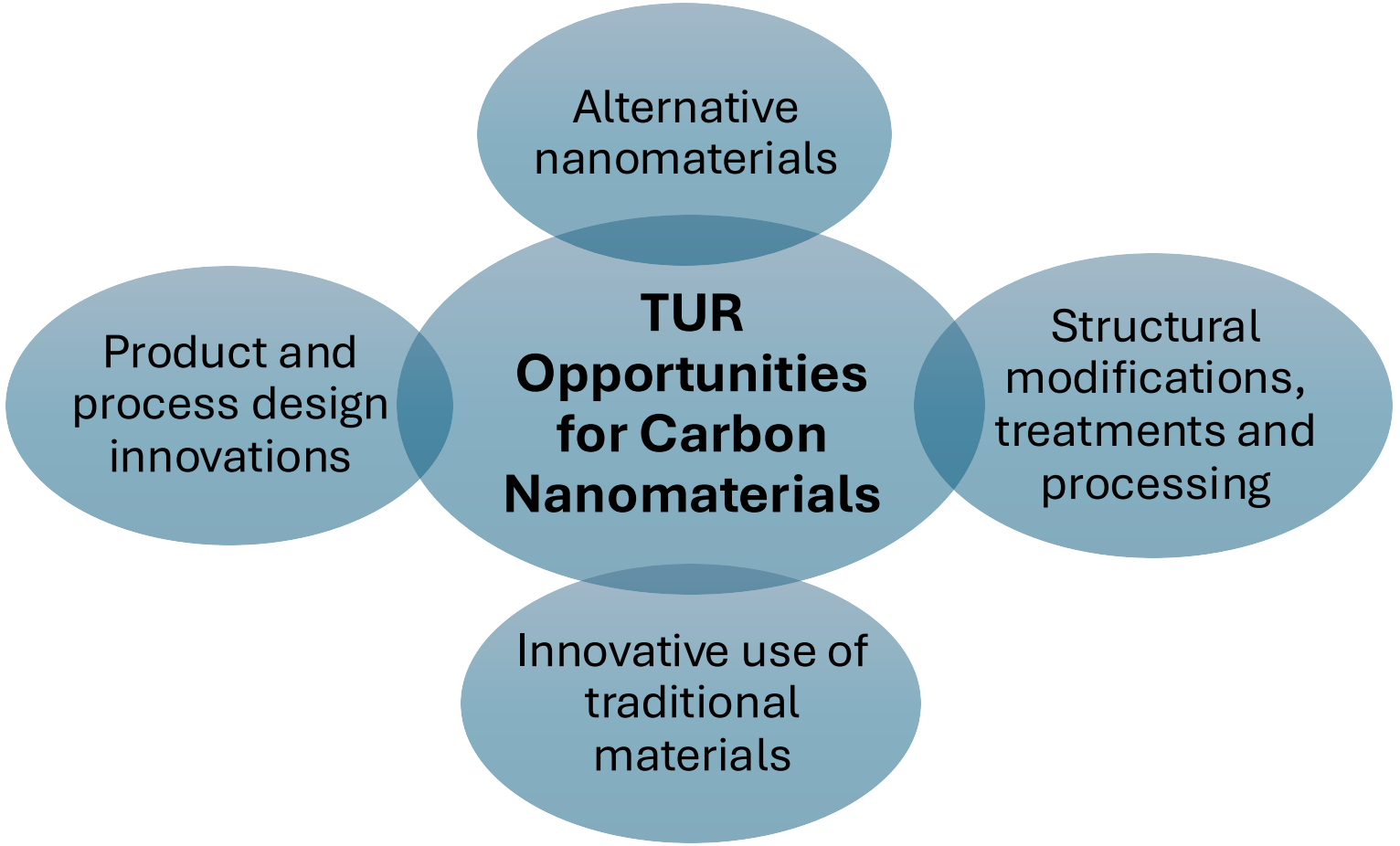
Regulatory Review

Overview of regulations, official guidance and initiatives that cover carbon nanomaterials

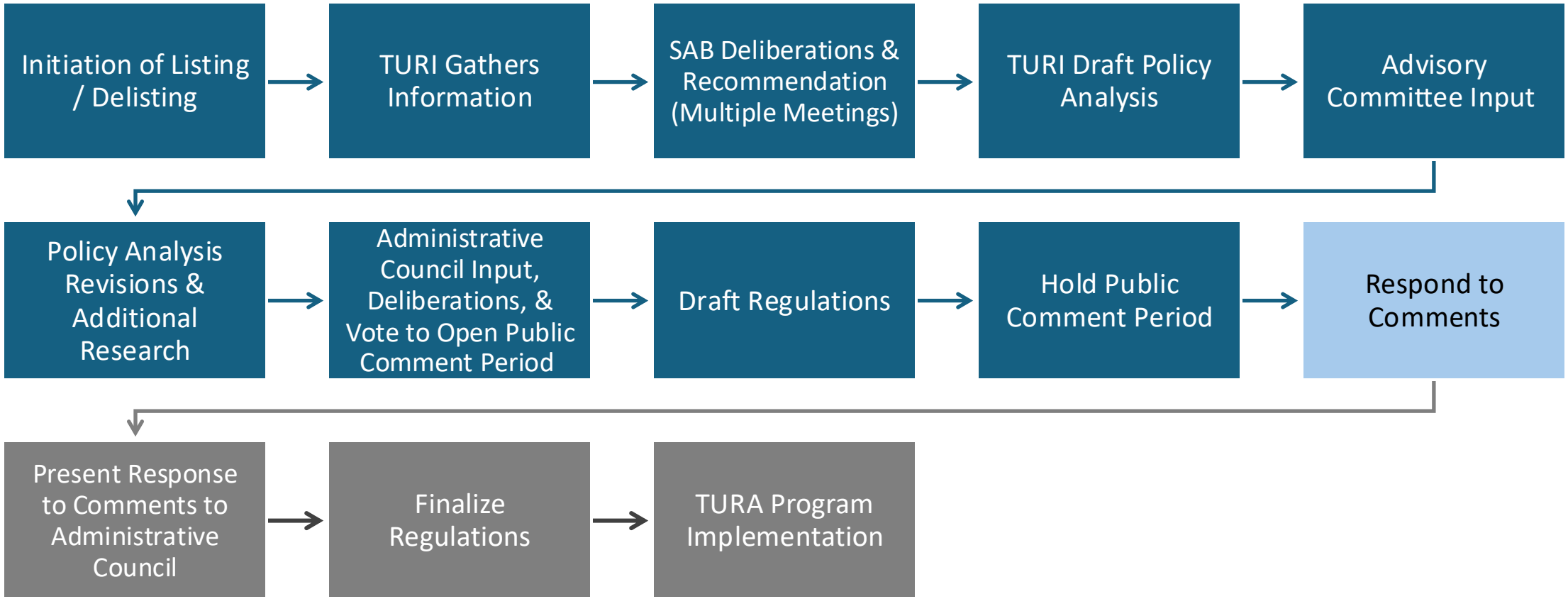
International	Federal	State and Local
• OECD Strategic Programme on Safety Evaluation and Risk Assessment • EU REACH Registration and Nanoform Guidance	• TSCA Section 5 (Premanufacturing Notices and Significant New Use Rules) • Recordkeeping Rule • NIOSH Recommended Exposure Limit	• California DSTC Formal Request Letters • Cambridge nanotechnology committee and Berkeley, CA disclosure requirements

TUR Opportunities

Do opportunities exist to reduce the use of carbon nanomaterials and the associated hazards along the lifecycle without compromising their unique characteristics and potential benefits to society?



TURA Program Consideration of **Quaternary Ammonium Compounds**



Considerations of Quats (QACs)

Quats are a group of substances used primarily for disinfection, wood preservation and some applications in personal care products

TURI initiated the quat review during the pandemic when quat use became more widespread

The SAB recommended listing 24 specific ADBAC and DDAC quats due to **respiratory irritation** and **inflammation**, **corrosivity**, **hazard to aquatic life**, **environmental fate** and **persistence**.

Safer Alternatives to Quats (QACs)

Chemical alternatives

- Caprylic acid, citric acid*, L-lactic acid*, Hypochlorous acid
- Hydrogen peroxide*
- Alcohols such as isopropyl alcohol and ethanol*

Non-chemical alternatives

- Steam
- UV light

***Substances have been evaluated by the U.S. EPA Safer Choice Program and are considered safer active ingredients**

Thank you!

Heather Tenney (Heather_Tenney@uml.edu)
Karen Thomas (Karen_Thomas1@uml.edu)
Colin Hannahan (Colin_Hannahan@uml.edu)

www.turi.org

Toxics Use Reduction Institute
University of Massachusetts Lowell

Upcoming Webinars

19 Nov., 12:00 PM – 1:30 PM

Implementing TUR: Company examples

Using machine learning to support TUR

9 Dec., 10:00 AM – 11:30 AM

Reminder

- To receive CEUs for attending today's webinar you must:
  - Attend the full webinar
  - Complete the survey, which will be distributed in the next few days

- Please never hesitate to reach out to TURI's training team if you have questions:
  - training@turi.org
  - Pam Eliason, Training Director: Pamela_Eliason@uml.edu
  - Agnes Cheng, Training Associate: Agnes_Cheng@uml.edu