OVERVIEW OF AQUATIC RISK ASSESSMENT OF POLYMERS – EVIDENCE FROM CATIONIC POLYMERS

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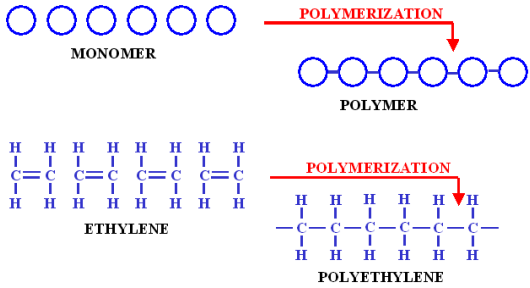
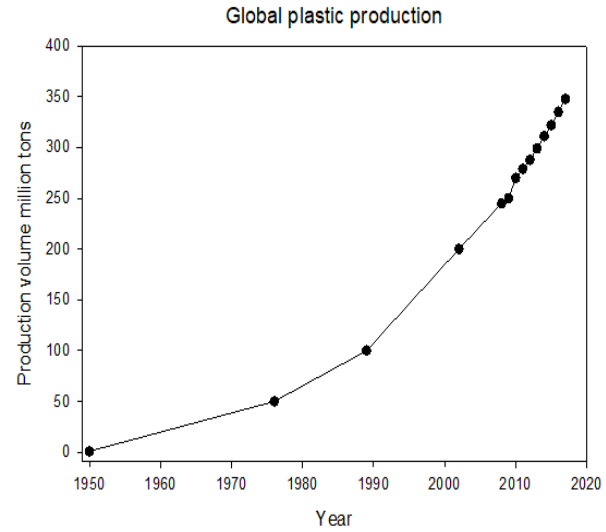
WHAT ARE POLYMERS?



- Large macromolecule, mostly >1000s Da., with at least 3 covalently bound monomers
- Many different uses depending upon their designed properties:
  - Pharmaceutical; nano; cleaning; biocides; lubricants; plastics; flocculants etc.
- Different types of polymers:
  - Natural (DNA; starch; sugar etc.) and industrial biopolymers
  - Synthetic e.g. in chemical industries, plastics and rubbers
  - Different functionalities and properties
- Different compositions:
  - A mixture of monomers, smaller polymers and large polymers, impurities
  - Additives – e.g. stabilizers
- *So, what are they?:*
  - UVCB's; drugs; nanomaterials; microplastics?
    - Answer: *Depends on the specific polymer*

WHY POLYMERS?



- Large global volume and increasing uses – today they are a multi-million dollar industry
- First real regulatory interest in the 1990s by OECD - USEPA assessment and prioritization in TSCA in 1996 Boethling and Nabholz (1996) summarized hundreds of regulatory submissions from1980s to 1995 and developed USEPA position
- Polymer exemption from registration in certain regulatory programs (e.g., REACH) due to assumed low concern - these assumptions are now being reconsidered
- Toxicity and exposure is unknown for the most part – high persistence is however known

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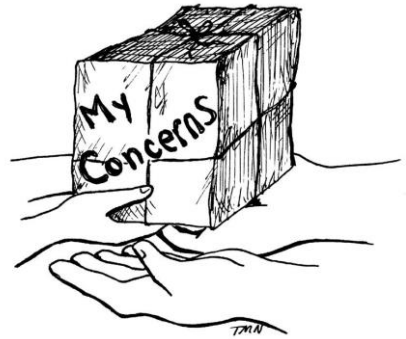
POLYMERS OF TOXICOLOGICAL CONCERN

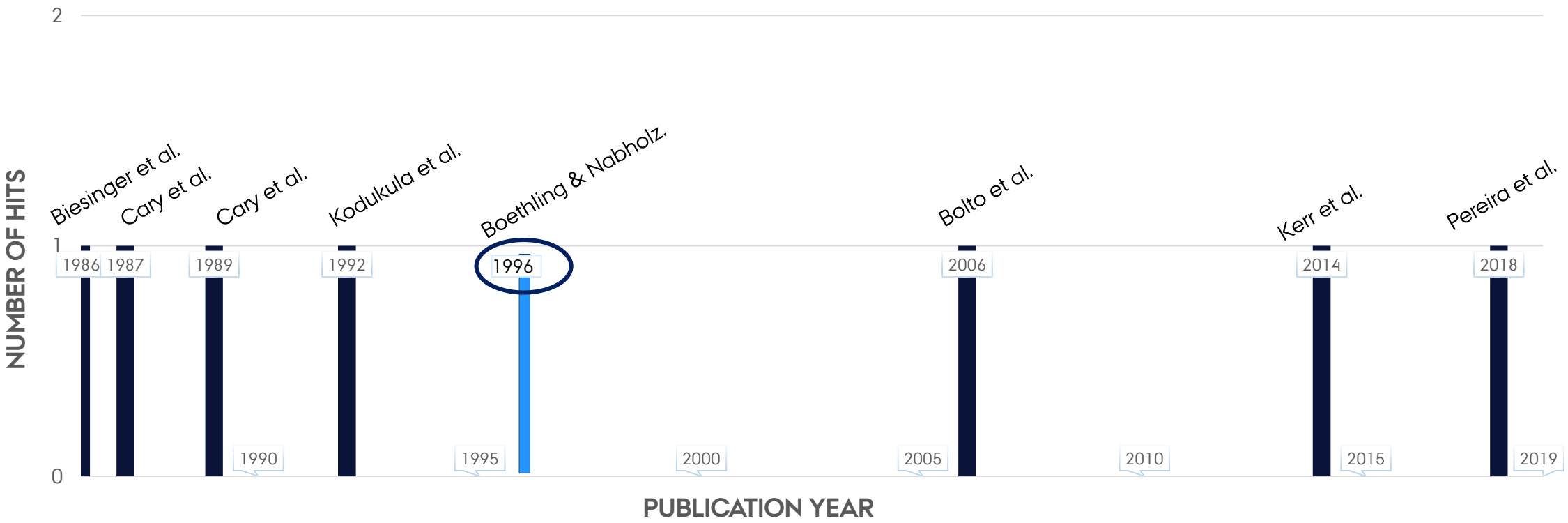


Characteristics:

- Backbone and composition (natural, carbon, silicon)
  - *No clear differences in toxicity*
- Molecular weight (MW) and distribution (Lipinski's rule on bioavailability)
  - *MW > 1000 Dalton → low concern (cannot pass cell membranes)*
  - *MW < 1000 Dalton and >1% oligomers → potential concern*
- Charge and ionic properties
  - *Cationic polymers are of potential concern due to aquatic toxicity (e.g. PQ6)*
- Size
  - *If they can degrade to smaller molecules → potential concern*
- Functions and functionalizations
  - *Biocidal or other functions, additions and substitutions → potential concern*
- Solubility (water and lipids)
  - *If they can overcome Lipinski's rule → potential concern*

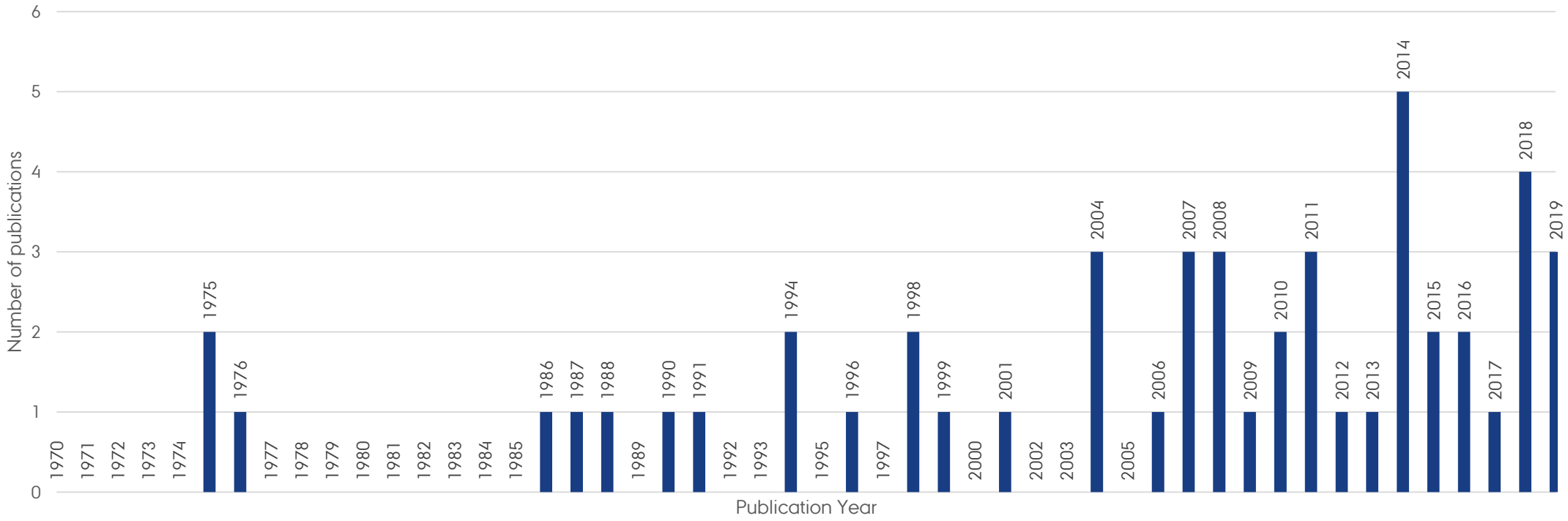
CATIONIC POLYMERS LIT REVIEW

SciFinder review: “Cationic + polymer + aquatic + toxicity” = 7 hits → not much data!



CATIONIC POLYMERS CURATED REVIEW

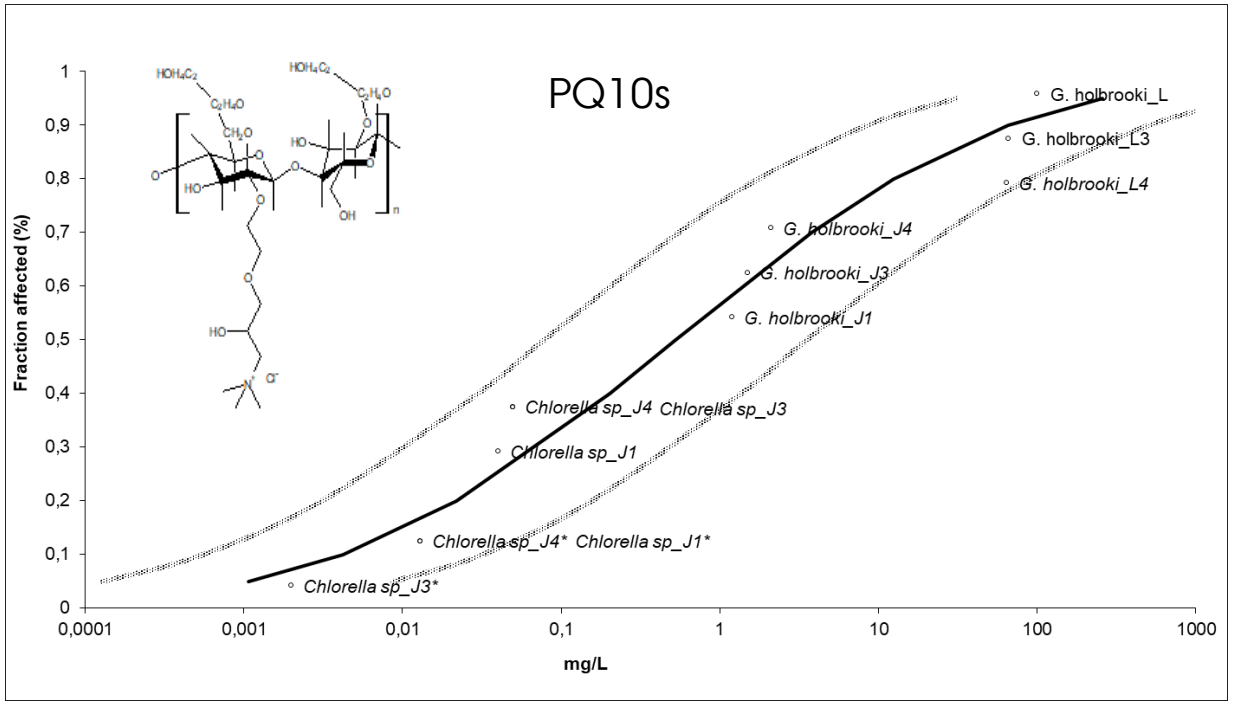
Curated review returned 50 relevant aquatic tox. publications (1970-2019) – not much data

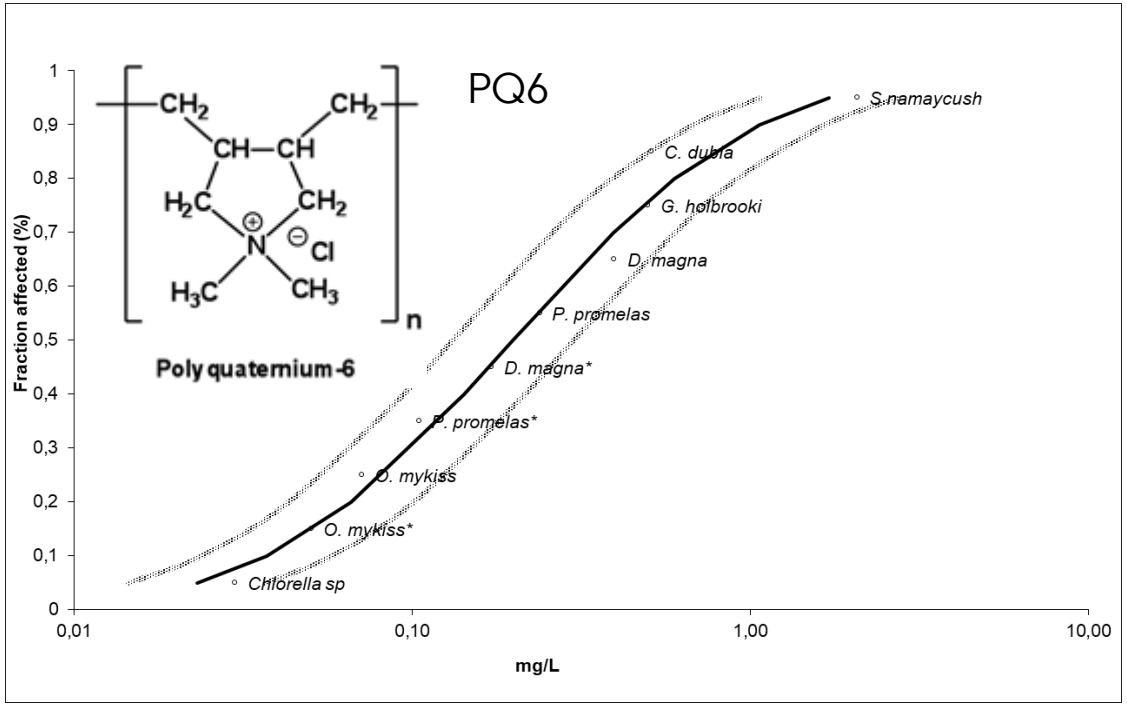


TOXICITY REVIEW OF POLYQUATERNIUMS

Distribution of published acute toxicity data for the PQ10 (mixed polymer) and mainly acute toxicity PQ6 (homo-polymer (PolyDADMAC)) (Pecquet et al. 2019):

→ Quite large variations in toxicities (nom. concentrations)

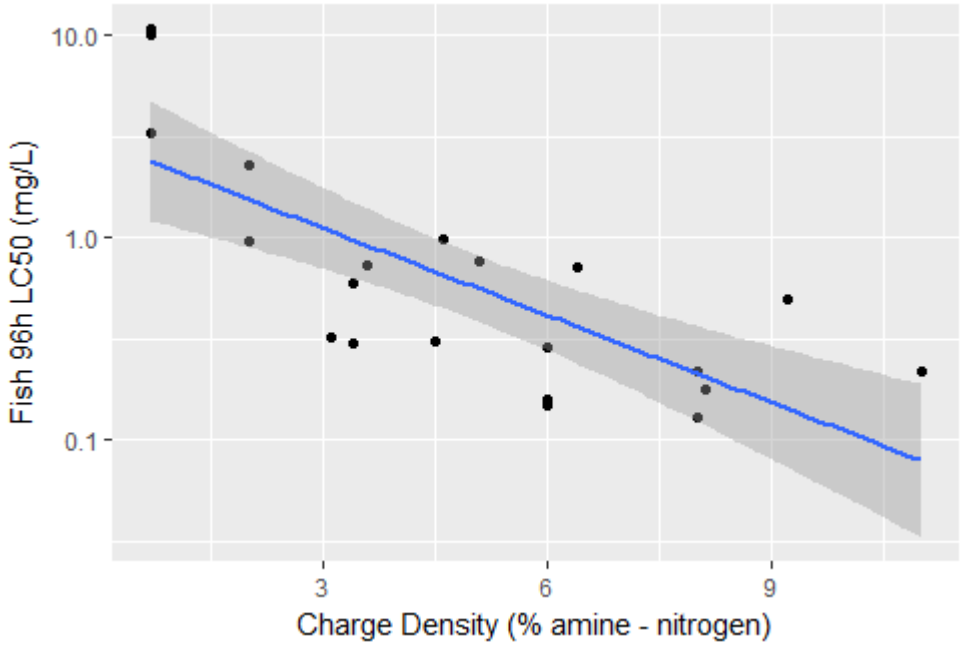


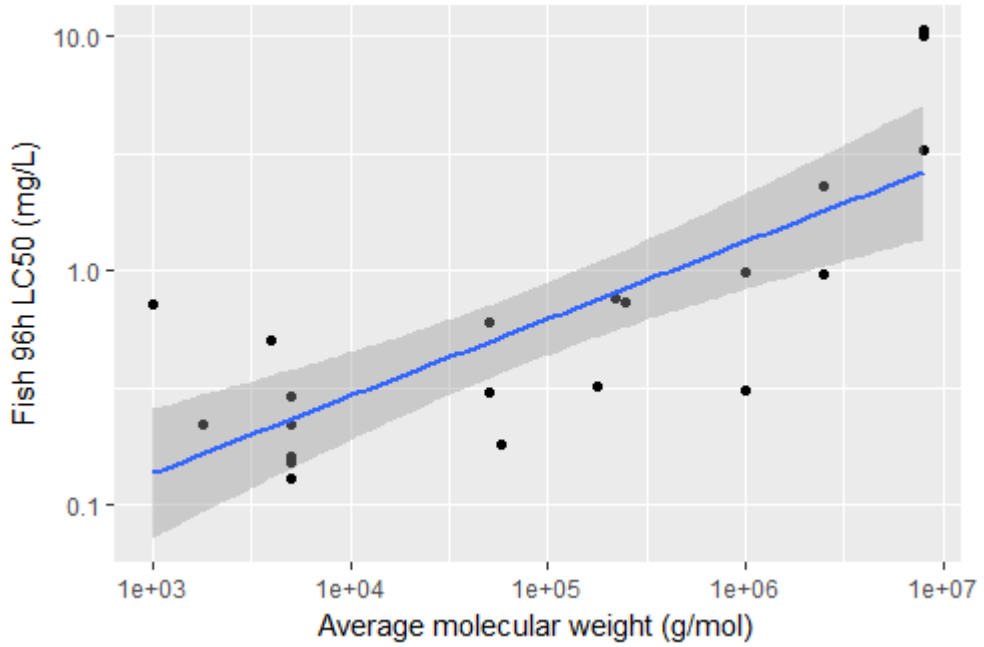


TOXICITY DESCRIPTOR REVIEW

Boethling and Nabholz (1996) reported 21 blinded cationic polymer datasets with associated important toxicity descriptor information:

- For acute fish there is a clear positive relationship between charge density and toxicity and negative relation ship between MW and toxicity - not so clear for *Daphnia* and algae - algae toxicity ranges from 0.006 to 1000 mg/L!
- Log Kow is not a good descriptor
- Acute to Chronic Ratios = 14-18 → not specific MoA





TOXICOLOGICAL CHALLENGES

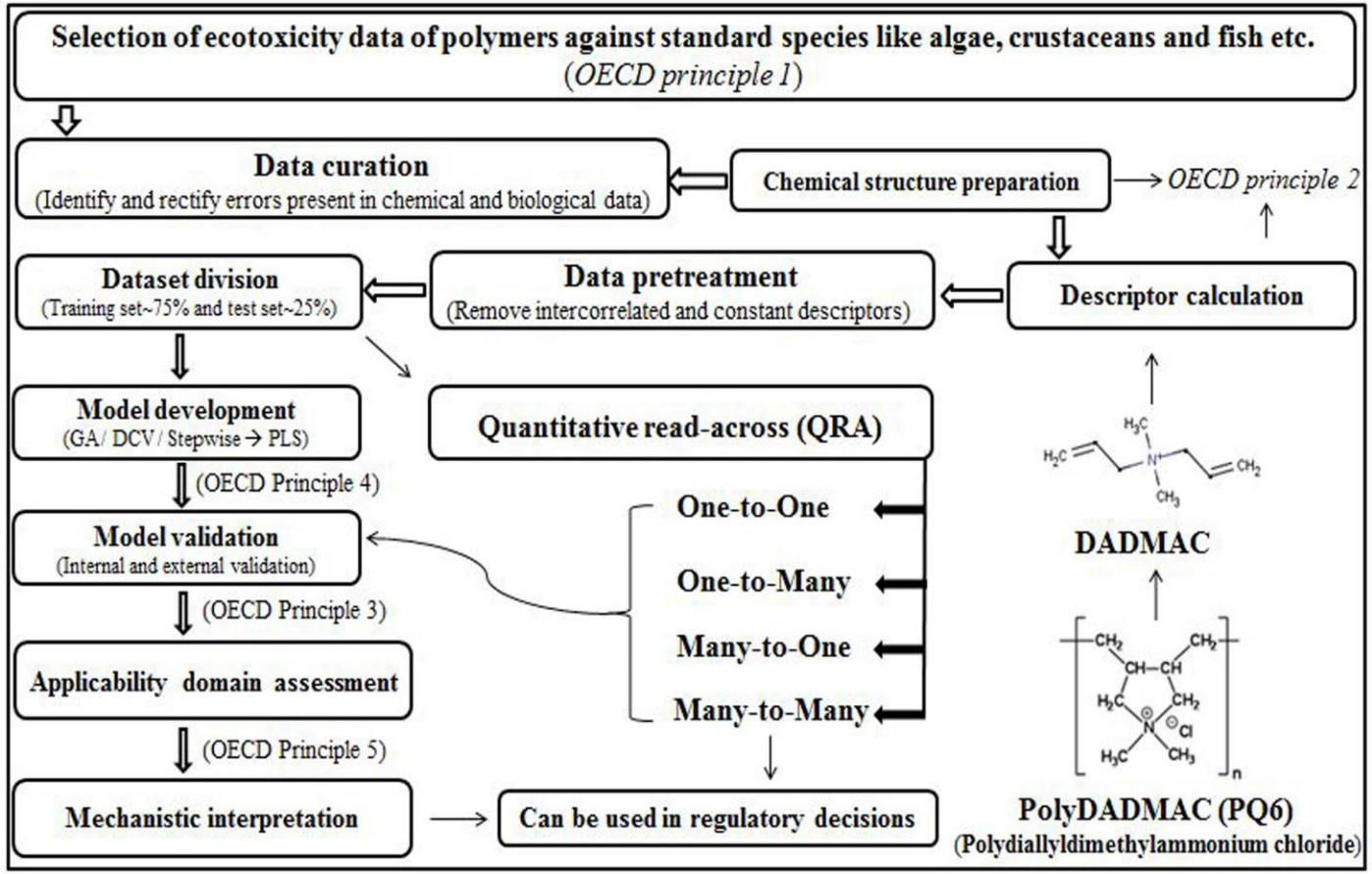
- Lack of publicly available data!
- Uncertainty about MoA – physical effects and modelling dose-response?
- Uncertainty about toxicological bioavailability?
- What are the relevant toxicological descriptors?
- Are these UVCBs – and how to test mixtures?
- Test methods – do they need update/amendments?
- Mitigating factors – humic acid, solids, in the tests – guidance?
- Need analytical methods to verify exposures!
- Need to develop computational models when the above is resolved?

→ Need consensus and guidelines for these issues

QSAR MODELLING?

TOXICITY = f(CHEMICAL STRUCTURE)

- Follow OECD principles?
- Lack of ecotox data → 2d fragment based QSAR modelling – ongoing work
- Other models can other descriptors be transferred – ongoing work



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RISK ASSESSMENT CHALLENGES

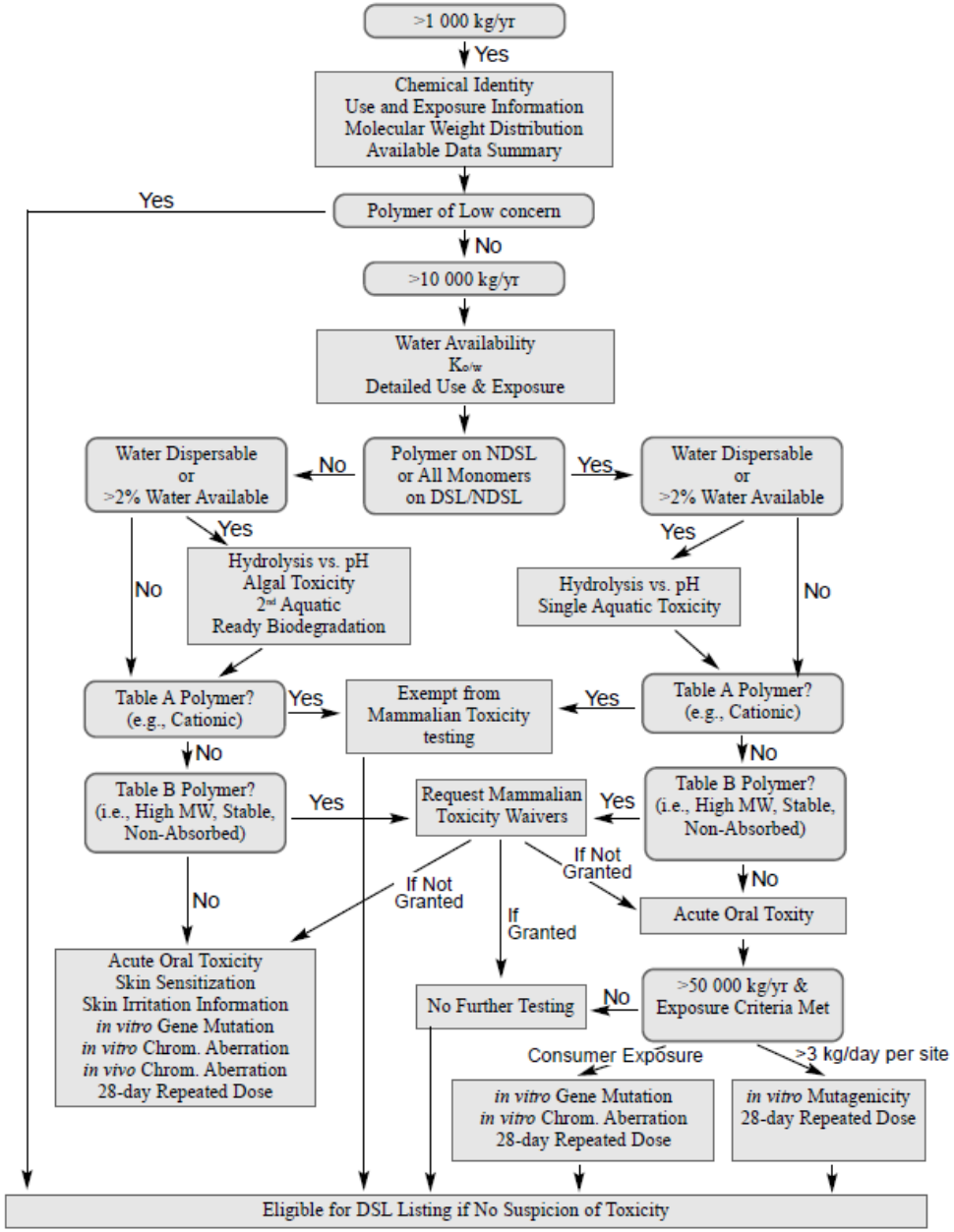
Canada: Polymers in CEPA (2001) – determine if the polymer is of low concern – mainly volume; WS (Log Kow); algal toxicity. See poster by ECCC (MP074) for updates.

USA: Three categories for soluble polymers:

1. Low MW → can assess toxicity
2. Large polymers with low MW → can maybe assess toxicity
3. Large polymer with high MW → consider physical effects

Europe: ECHA is reviewing how to prioritize the polymers of concern – need data which is not currently publicly available. Knowing that toxicity assessments are less suited and that sound ecotox models does not exist – issues needs solving?

Environmental relevance and mitigating factors of the tests needs clarification and optimization (?) – guidance...



CONCLUSIONS

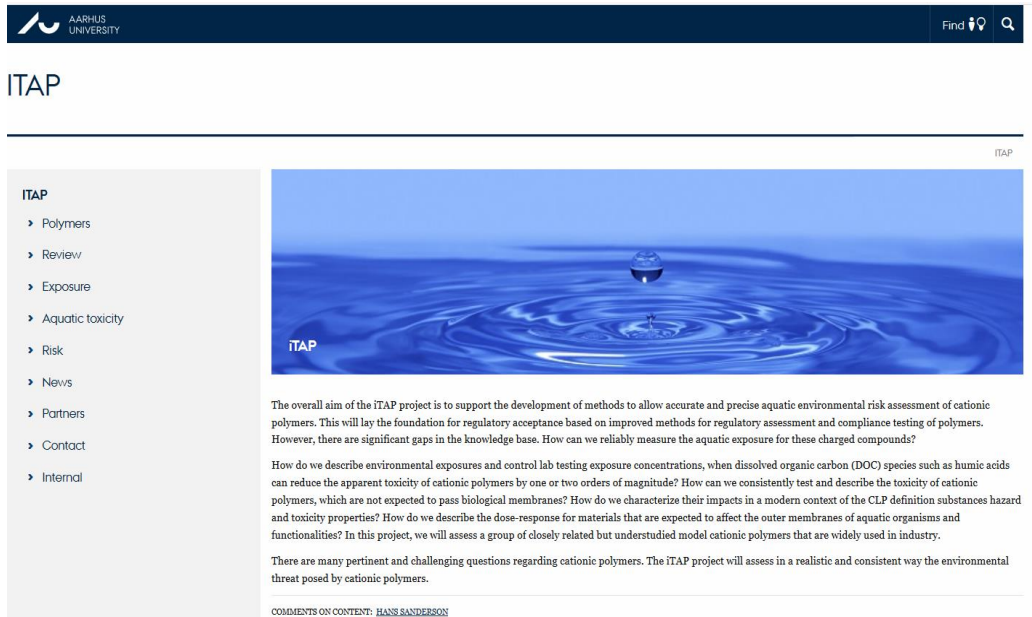
Ongoing work see the next presentations and follow the iTAP project:

http://cefic-lri.org/projects/eco-46-improved-aquatic-testing-and-assessment-of-cationic-polymers-itap/ or https://projects.au.dk/itap/

SETAC-Europe session: *Environmental Risk assessment of Polymers*

Under track 4: Ecological risk assessment and human health risk assessment of chemicals, mixtures and stressors and risk mitigation strategies

Abstract deadline: **Nov 27th!**



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