Pushing the limits to minimize bias in DBP calculated toxicity due to left censored data and elucidating the true exposure risk

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BACKGROUND

- Formation of disinfection byproducts (DBPs) is a major concern during disinfection of drinking water (Fig.1)
- More than 700 DBPs identified
- Only 11 are regulated in U.S
- Adverse health effects i.e., bladder and colorectal cancer, birth defects
- DBP toxicity; a function of conc. and intrinsic toxic potency
- Cytotoxicity and genotoxicity assays on Chinese based on hamster ovary (CHO) cells

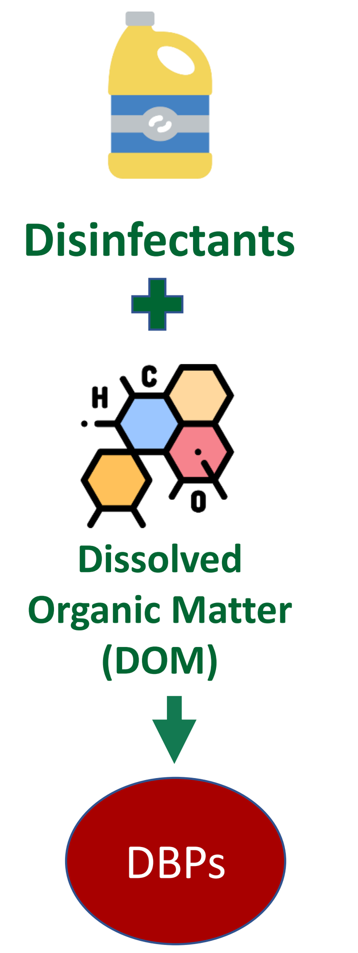
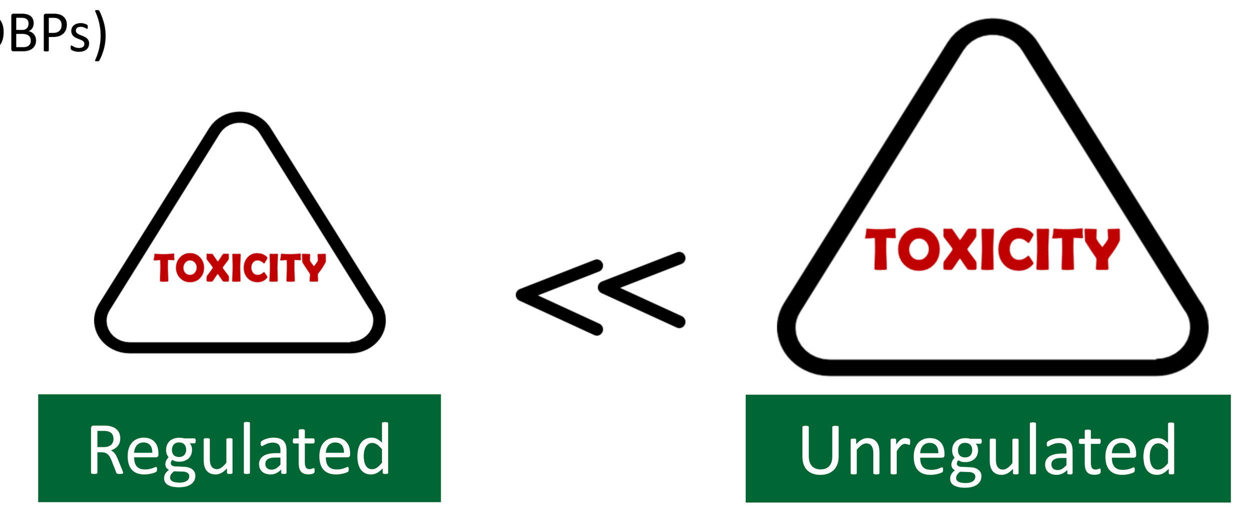


Fig 1.DBP Formation

UNREGULATED DBPS & LEFT CENSORING

- Toxicity of regulated VS unregulated DBPs (concept of priority DBPs)



- Left censoring of data due to method detection limits (MDLs), Fig.2
- Bias in toxicity calculations due to MDLs
- Left Censored Data: datapoints below a certain value but the value is currently unknown
- Pushing the MDLs to minimize the bias for true exposure risk

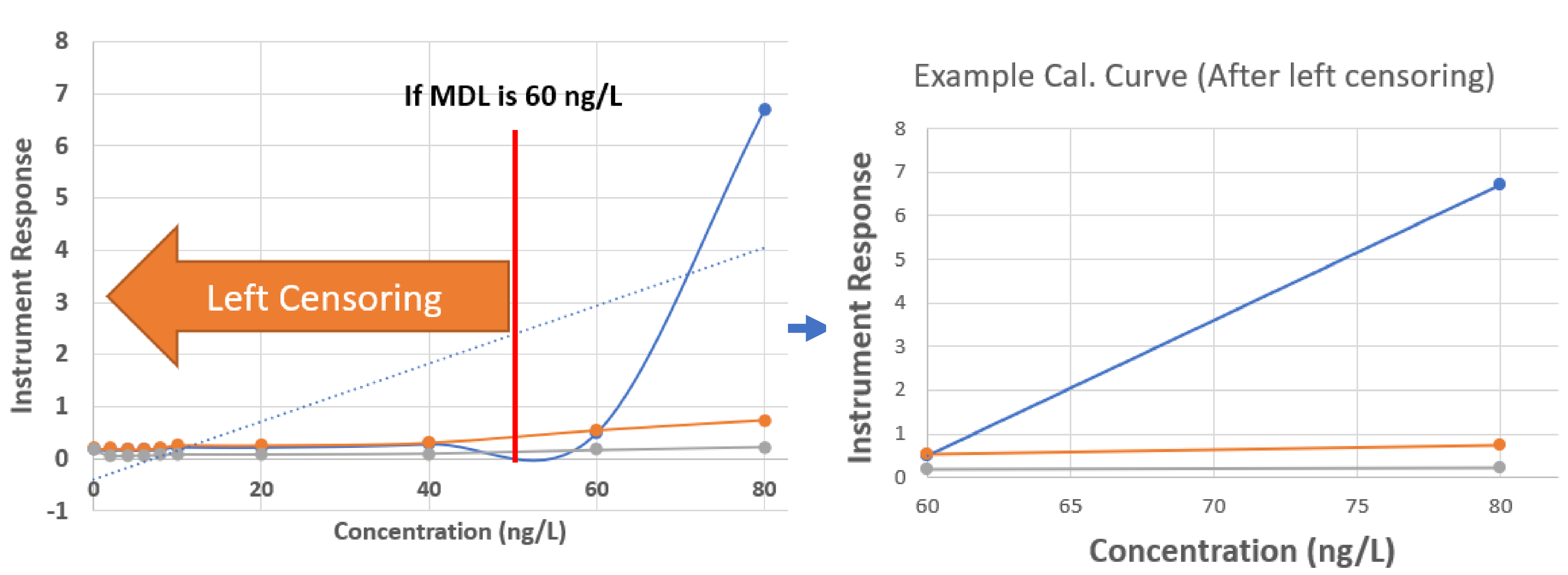


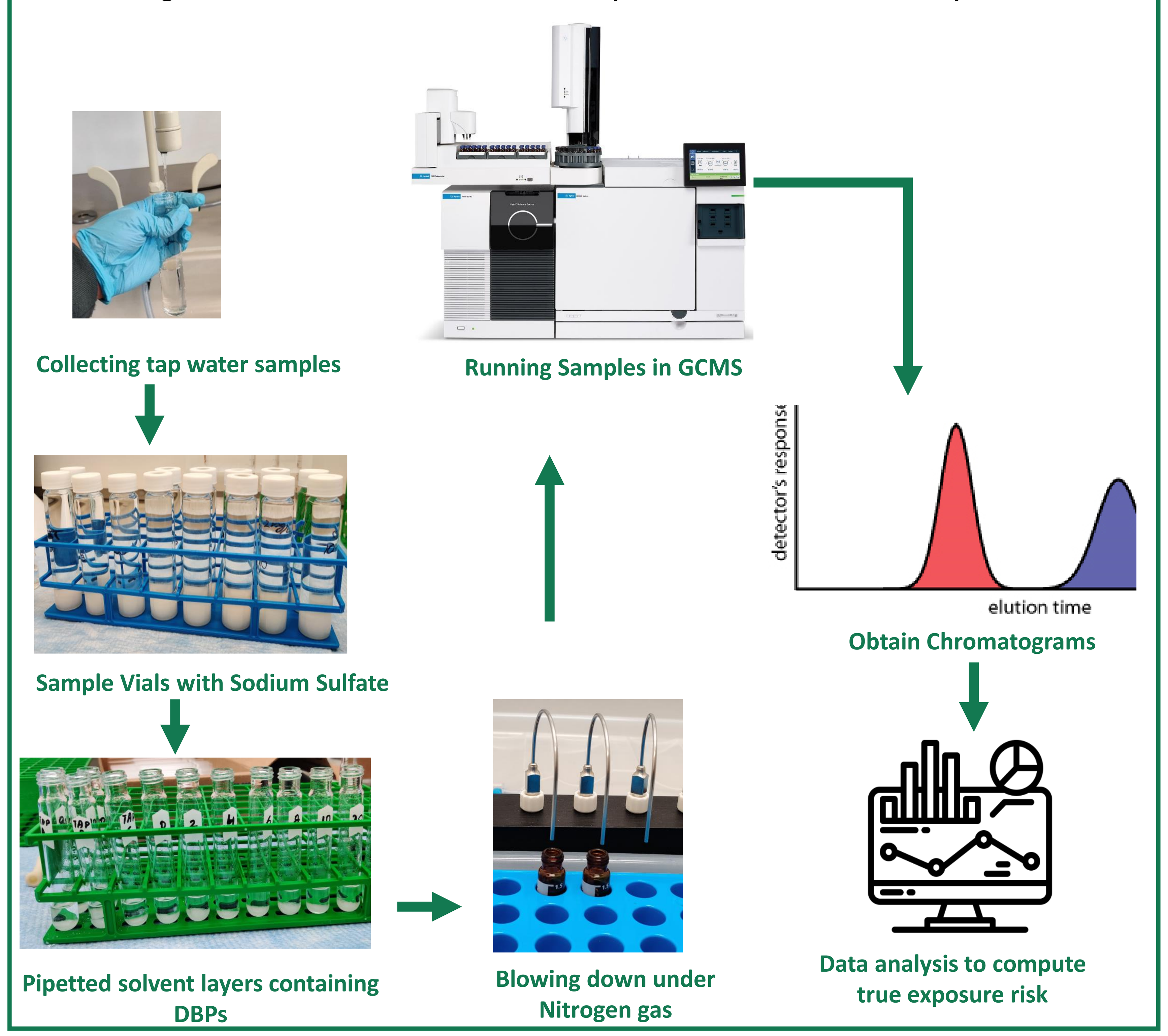
Fig.2 – Example of Cal. Curve affected by MDL

OBJECTIVES

- Utilizing the latest GCMS (TQ-Triple Quad) with high efficiency ion source (Agilent 7010b) for analysis
- Develop a highly sensitive GCMS analytical method
- Quantitation of ~45 volatile and semi-volatile DBPs with substantially lower reporting limits (~ 0.001 µg/L or 1ng/L)
- Based on the new MDLs calculate new concentrations
- Minimize the bias introduced by left-censoring of data
- Evaluate impact of bias by comparing previously reported censored data and the new data on cumulative toxicity

METHODS

A. Collect real raw drinking water samples from taps
B. Extraction of DBPs using Liquid-Liquid and Solid-Phase Extraction (LLE & SPE) techniques
C. Run samples with GCTQ and obtain chromatograms
D. Data analysis to quantify trace concentrations
E. Using statistical methods to compute bias and true exposure risk



RESULTS & NEXT STEPS

Results

- Method development completed for some of the priority DBPs
- MRM (multiple reaction monitoring) vs SIM (selected ion monitoring) allowing trace analysis through ultra high selectivity
- Newly established MRLs are approximately a hundred times lower than the previously established MRLs (Table-1)
- Drinking water samples from Corbalis and Griffith drinking water treatment plants were analyzed with the new method to quantify DBP concentrations
- Method development phase nearing completion for haloacetic acids (HAAs) and haloacetamides (HAMs)

Next Steps

- Test variety of real tap water samples from mid Atlantic region
- Statistical analysis for computing bias in cumulative toxicity calculations leading to publication

Table-1. Comparison of previously and newly established MRLs for some priority DBPs

DBP Compound	Previously Reported MRLs (ug/L)	Newly Established MRLs (ug/L)
Dichloroacetonitrile (DCAN)	0.10	0.001
Bromochloroacetonitrile (BCAN)	0.10	0.001
Dibromoacetonitrile (DBAN)	0.10	0.005
Bromodichloroacetaldehyde (BDCAL)	0.10	0.005
Tribromoacetaldehyde (TBAL)	0.10	0.005
Trichloroacetonitrile (TCAN)	0.10	0.001

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REFERENCES

- Clasen, T., & Edmondson, P. (2006). International Journal of Hygiene and Environmental Health, 209(2), 173–181.
- McKenna, Elizabeth, David Hanigan. 2020” Environmental Science: Processes & Impacts 22 (3): 708–18.
- Li et al. Environ. Sci. Technol. 2018.
- Han et al. Environ. Sci. Technol. 2021.
- Zeng, T., Plewa, M. J., & Mitch, W. A. (2016). Water Research, 101, 176–186.
- Mark et al. Environ. Sci. Technol. 2007.