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Update on Screening Chemicals in Commerce to Identify New Persistent and Bioaccumulative Chemicals in the Great Lakes

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Goals of Our Study

- Develop a “North American” list of potentially PB&T chemicals
  - Greater relevance to the Great Lakes and trans-boundary long range transport than Canadian CMP priorities
- Using Quantitative Structure-Property relationships, and scientific judgment, identify chemicals in commerce that may be P and B and have not been previously measured in environmental media
- Include degradation products where possible e.g. perfluoroalkyl acids
- Assess whether selected chemicals can be analyzed by existing methods in use for POPs and new PB&T chemicals in the Great Lakes
- Screen for various toxicity endpoints

Development of a Combined Canadian and US database of chemicals in commerce (Howard and Meylan 2007)

Source	No. Substances	Reporting Threshold	Reporting Date
US EPA High production volume (HPV) program*	3549	1,000,000 lbs/yr (454 t/yr)	Post-1990
US EPA TSCA Inventory update rule (IUR) web site**	14,458 organics (combined HPV and EHPVs)	>10,000 lbs/yr (4540 kg/yr)	IUR reporting years; 1986 to 2002
Canadian DSL categorization***	11,317 organics	>100 kg	Mid-1980s
UVCBs****** (1400 on the DSL)	3059 organics	>100 kg	Mid-1980s
Total (after duplicates removed)	**22,043**		

*available from http://www.epa.gov/HPV/hpvchmlt.htm
** available from http://www.epa.gov/oppt/iur
*** available from Environment Canada - http://www.ec.gc.ca/substances/
**** UVCB = Unknown, of Variable Composition, or of Biological Origin – organic chemicals

Further Prioritization Based on Lessons Learned from POPs in the Great Lakes

1. High bioaccumulation/biomagnification potential, i.e., in top predators
2. Persistence – sequestered in bottom sediments in the open lakes implying a low rate of biodegradation
3. Long range transport potential i.e., found in mid-lake, in Lake Superior and remote lakes such as Siskiwit Lake
4. Quantity in use and potential for emissions i.e., open use or as an additive vs. as a chemical intermediate

Selection Characteristics	#	Notes
Predicted BCF >1000, Atmospheric Oxidation >1 day, and Log Kaw >-5 and <-1	105	Using EPIsuite. Mainly chemicals with LRT potential
By chemical class (Br, Cl, F, I, Si, cyclic hydrocarbons) and considering biodegradability	495	By expert judgment – includes chemicals and their degradation products with low LRT but potential for persisting in sediments and in the water column
Total	600	**62% halogenated; 10% siloxanes**

Information on measurement and analyzability of the 600 substances

Analyzable	Well monitored in the GL region and Arctic (ie. programs such as IADN, NCP)	Chemicals that may have been analysed in any GL, Arctic or other environmental measurement studies	Analyzable using existing methods for neutral POPs or other neutrals such as pesticides and PAHs*	Analysable by LC-MS/MS ESI mode (anionic) or positive CI mode
Yes	**48**	**98**	**396**	**43**
% Yes	**8%**	**16%**	**66%**	**7%**
No	**552**	**502**	**125**	
Maybe			**39**	**24**

*Numbers analyzable was determined by expert judgment

Comparison with Environment Canada's Chemicals Management Plan list of priority chemicals

CMP category	Total in each CMP category	Overlap with the 600 P&B chemicals in this study
HC priorities	917	23
P&B priorities	657	29
PBiT challenge	148	37
Eco-hi- medium-low	2989	124
TOTAL	4711	213

Conclusion – 387 chemicals are unique to this study

Toxicity Estimates of Priority Chemicals

- 429 chemicals have been further evaluated to identify and estimate whether these compounds are toxic to aquatic organisms and to mammals utilizing:
  - Analog Identification Methodology (AIM)
  - ECOSAR
  - OncoLogic

Results of toxicity screening of 429 chemicals using QSARs

	Number of chemicals tested or within model domain	Results	Number	%
AIM tool	429	Included in 45 classes	277	65
ECOSAR	349	Predicted EC50 <1 ug/L = >1 – 10 ug/L = >10-100 ug/L =	 115 42 61	 27 9.8 14
OncoLogic	146	High High-moderate Moderate Low-Moderate Marginal Low	0 10 24 34 29 49	0 6.8 16 23 20 34

Future Work

- Further prioritization of the 600 chemicals
  - Further work on analyzability (Muir)
    - •Identifying chemicals for which analytical standards are available
  - QSAR screening of remaining chemicals (171) using AIM, ECOSAR and OncoLogic
- Addition of chemicals from the TSCSA 2006 IUR
- Fate, Transport and Exposure Potential assessment (Howard)
  - Select High release
  - Degraded during use (intermediates)
  - Known degradation products e.g. perfluoroalkyl acids

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