The New Pharos

Compound Groups

Teresa McGrath

HBN HEALTHY BUILDING NETWORK
KNOW BETTER

HBN HEALTHY BUILDING NETWORK

MISSION

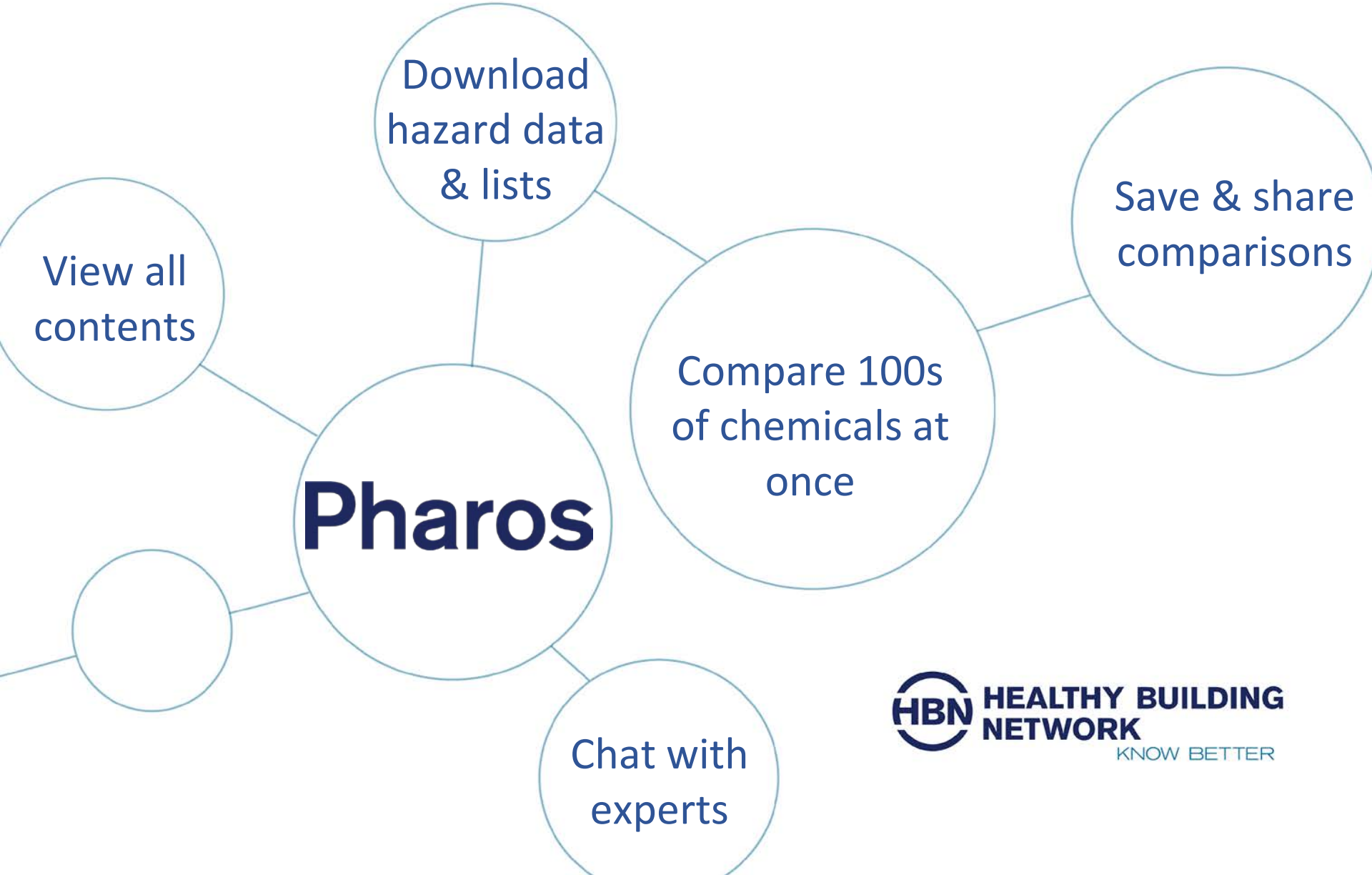
To advance human and environmental health by improving hazardous chemical transparency and inspiring product innovation

About Pharos

Comprehensive independent database of chemicals, polymers, metals and materials.

- Save hours of time by searching hazard information on >160,000 chemicals across 85 hazard lists
- Avoid regrettable substitutions with >600 compound groups
- Understand upstream concerns with process chemistry data

New Features



HBN HEALTHY BUILDING NETWORK
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Compound Groups Population Project

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Compound Group Population Project

A project to systematically identify the individual members of chemical groups identified with specific health hazards by scientific bodies (such as lead compounds or organic mercury compounds) in order to improve list based chemical hazard screening, harmonize tools, and avoid regrettable substitutions.

https://pharosproject.net/compound-group-population-project

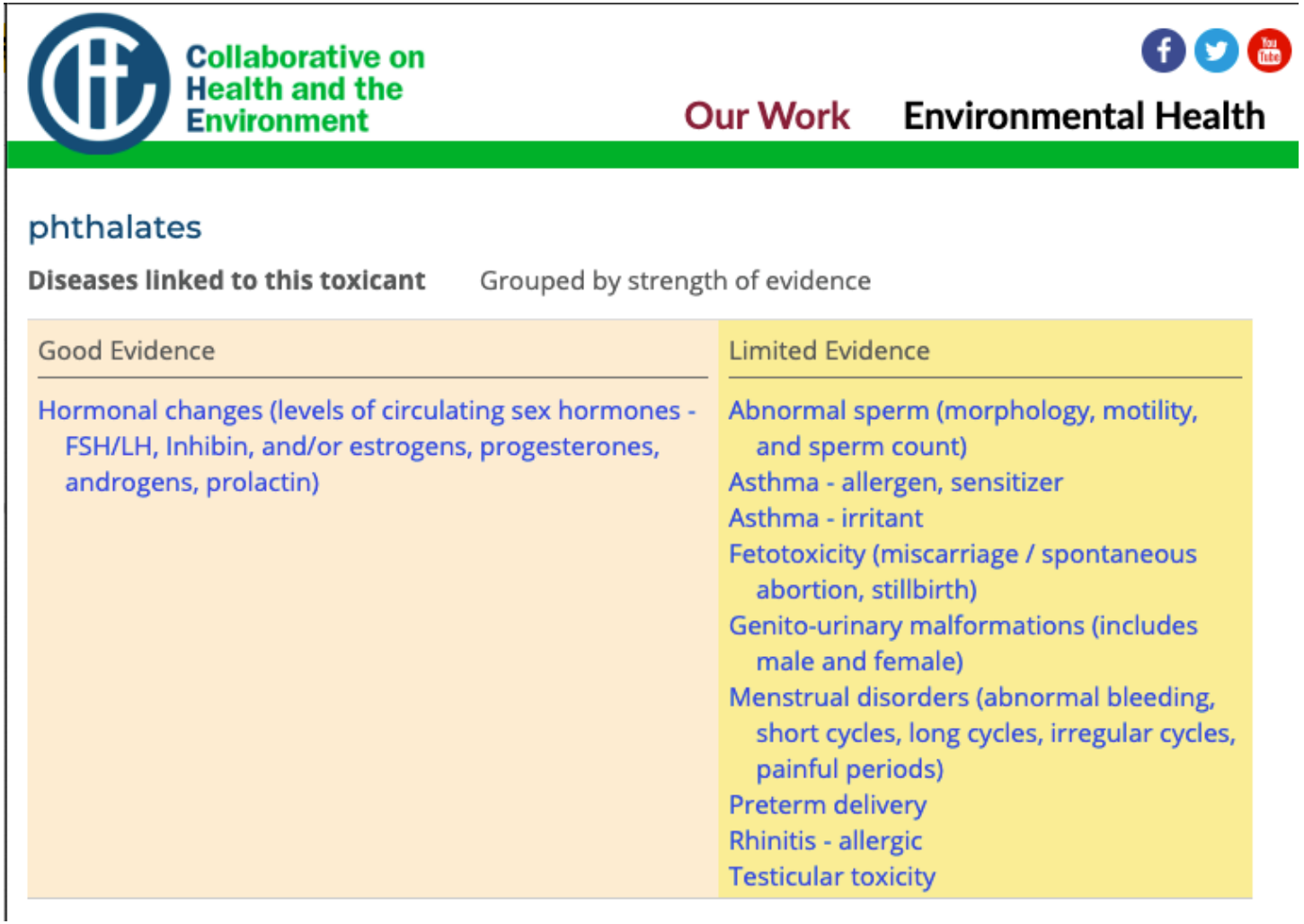
Methodolgy

1. Propose definitions of groups.
2. Develop algorithms to search chemical structure databases to identify members of the groups.
3. Use an open collaborative peer review process to improve definitions of groups, establish credibility and build buy in.
4. Establish a public registry / open standard of the group definitions and members.
5. Encourage use of these standardized group definitions and chemical lists by tool developers and list publishers to increase consistency.

Peer Review of Compound Groups

- Jointly managed by Clean Production Action and Healthy Building Network
- Volunteer scientists discuss group definitions and members and provide recommendations
- Priority groups are those with GreenScreen List Translator LT-1 hazards (~80 Compound Groups)

Orthophthalates (aka phthalates) are listed as toxic by CHE



Collaborative on Health and the Environment

Our Work Environmental Health

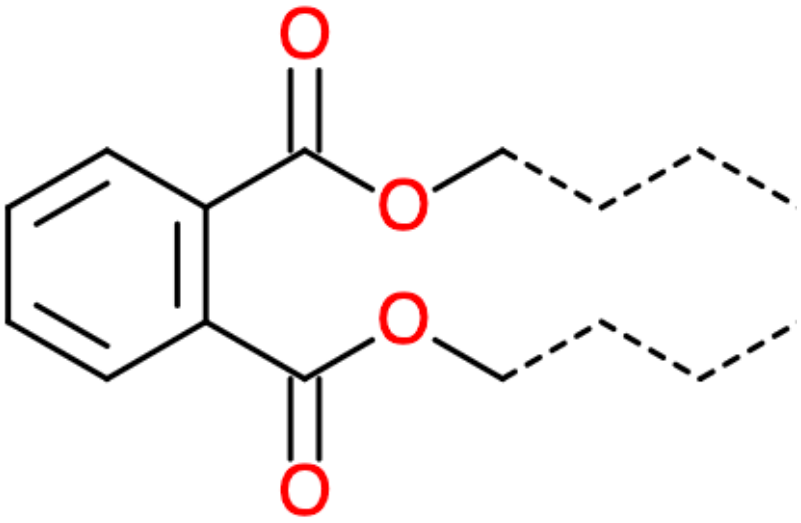
phthalates

Diseases linked to this toxicant Grouped by strength of evidence

Good Evidence	Limited Evidence
Hormonal changes (levels of circulating sex hormones - FSH/LH, Inhibin, and/or estrogens, progesterones, androgens, prolactin)	Abnormal sperm (morphology, motility, and sperm count) Asthma - allergen, sensitizer Asthma - irritant Fetotoxicity (miscarriage / spontaneous abortion, stillbirth) Genito-urinary malformations (includes male and female) Menstrual disorders (abnormal bleeding, short cycles, long cycles, irregular cycles, painful periods) Preterm delivery Rhinitis - allergic Testicular toxicity

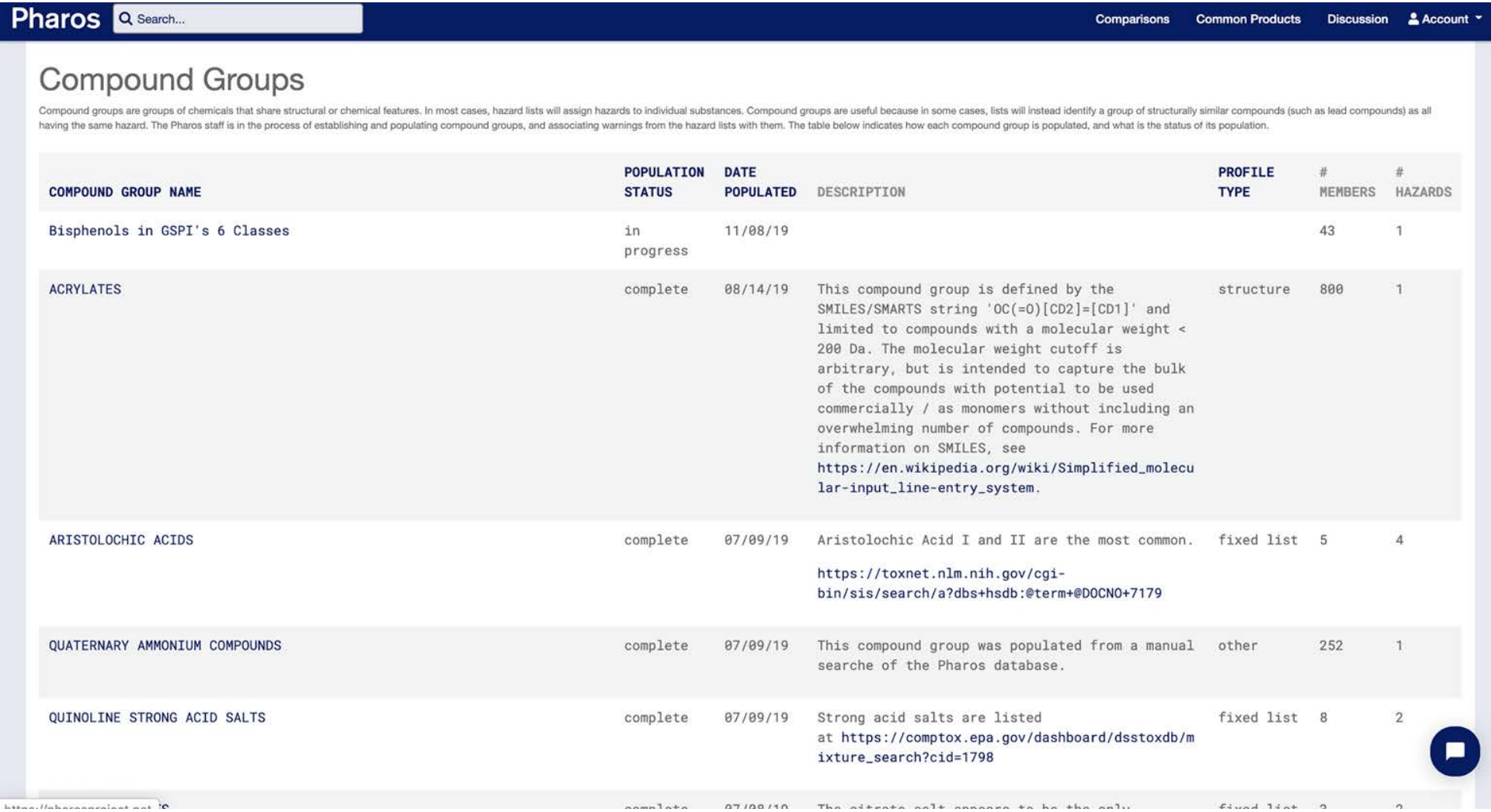
Search for Orthophthalates using a common structure

There are hundreds or orthophthalates, and they all share the same structure (denoted with solid lines).



Using the common structure to search databases like PubChem and ChemIDplus provides a list of all orthophthalates they contain.

>600 Compound Groups in Pharos

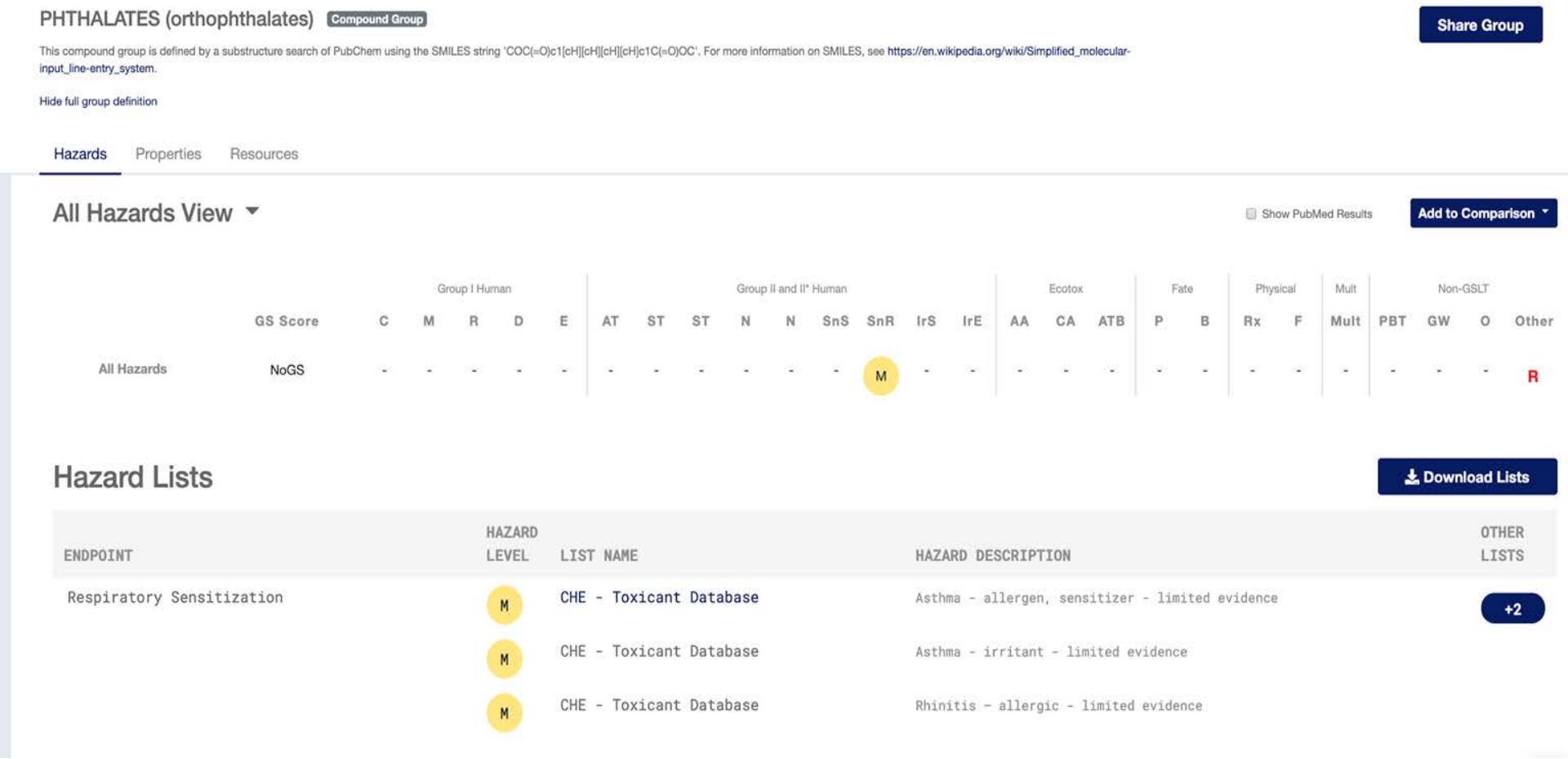


Compound Groups

Compound groups are groups of chemicals that share structural or chemical features. In most cases, hazard lists will assign hazards to individual substances. Compound groups are useful because in some cases, lists will instead identify a group of structurally similar compounds (such as lead compounds) as all having the same hazard. The Pharos staff is in the process of establishing and populating compound groups, and associating warnings from the hazard lists with them. The table below indicates how each compound group is populated, and what is the status of its population.

COMPOUND GROUP NAME	POPULATION STATUS	DATE POPULATED	DESCRIPTION	PROFILE TYPE	# MEMBERS	# HAZARDS
Bisphenols in GSPI's 6 Classes	in progress	11/08/19			43	1
ACRYLATES	complete	08/14/19	This compound group is defined by the SMILES/SMARTS string 'OC(=O)[CD2]=[CD1]' and limited to compounds with a molecular weight < 200 Da. The molecular weight cutoff is arbitrary, but is intended to capture the bulk of the compounds with potential to be used commercially / as monomers without including an overwhelming number of compounds. For more information on SMILES, see https://en.wikipedia.org/wiki/Simplified_molecular-input_line-entry_system.	structure	800	1
ARISTOLOCHIC ACIDS	complete	07/09/19	Aristolochic Acid I and II are the most common. https://toxnet.nlm.nih.gov/cgi-bin/sis/search/a?dbs+hsdb:@term+@DOCNO+7179	fixed list	5	4
QUATERNARY AMMONIUM COMPOUNDS	complete	07/09/19	This compound group was populated from a manual searche of the Pharos database.	other	252	1
QUINOLINE STRONG ACID SALTS	complete	07/09/19	Strong acid salts are listed at https://comptox.epa.gov/dashboard/dsstoxdb/mixture_search?cid=1798	fixed list	8	2

Compound group: Orthophthalates



PHTHALATES (orthophthalates) Compound Group

Share Group

This compound group is defined by a substructure search of PubChem using the SMILES string 'COC(=O)c1[cH][cH][cH][cH]c1C(=O)OC'. For more information on SMILES, see https://en.wikipedia.org/wiki/Simplified_molecular-input_line-entry_system.

Hide full group definition

Hazards | Properties | Resources

All Hazards View

Show PubMed Results | Add to Comparison

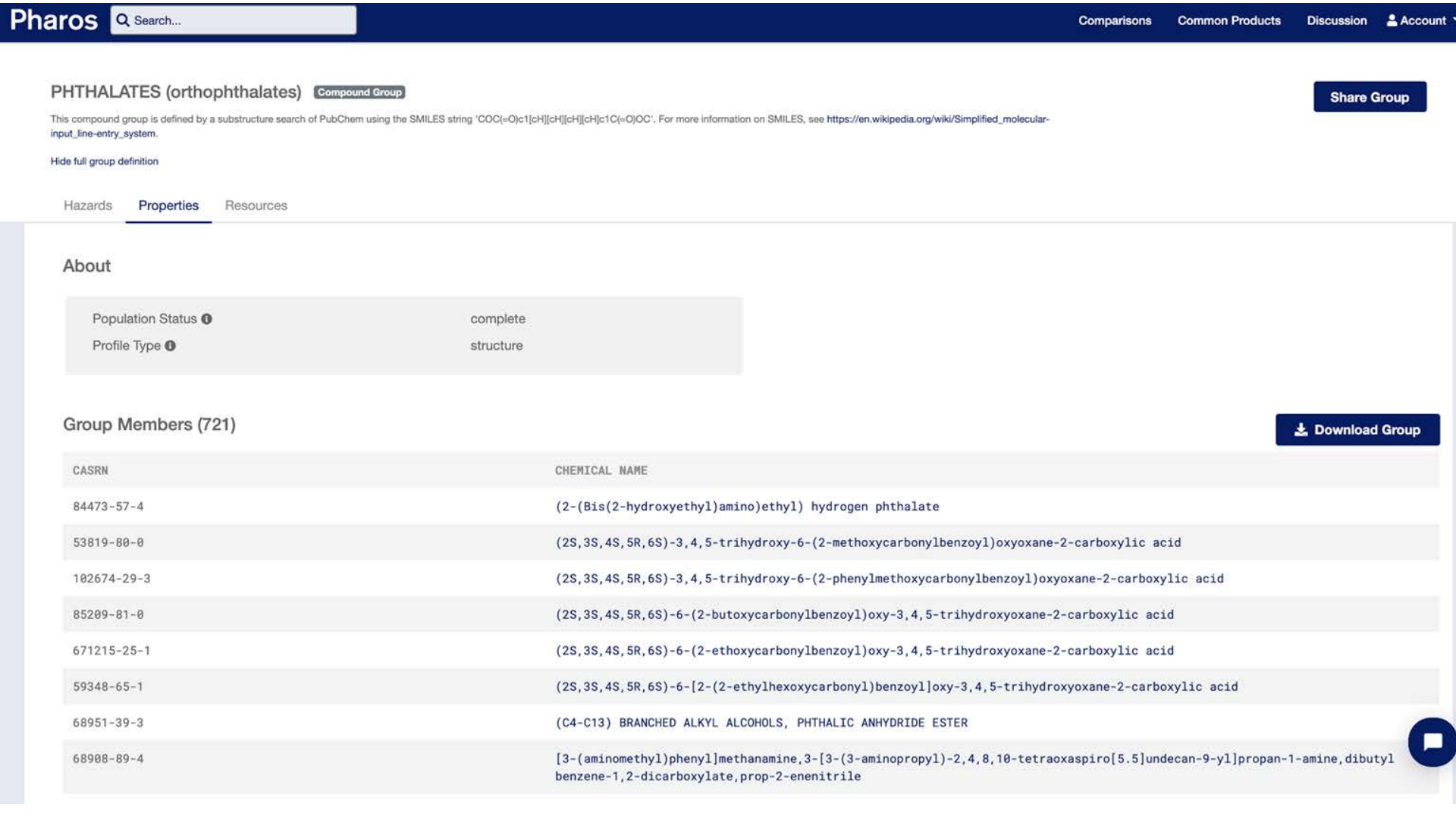
		Group I Human					Group II and II* Human									Ecotox			Fate		Physical		Mult	Non-GSLT			
	GS Score	C	M	R	D	E	AT	ST	ST	N	N	SnS	SnR	IrS	IrE	AA	CA	ATB	P	B	Rx	F	Mult	PBT	GW	O	Other
All Hazards	NoGS	-	-	-	-	-	-	-	-	-	-	-	M	-	-	-	-	-	-	-	-	-	-	-	-	-	R

Hazard Lists

Download Lists

ENDPOINT	HAZARD LEVEL	LIST NAME	HAZARD DESCRIPTION	OTHER LISTS
Respiratory Sensitization	M	CHE - Toxicant Database	Asthma - allergen, sensitizer - limited evidence	+2
	M	CHE - Toxicant Database	Asthma - irritant - limited evidence	
	M	CHE - Toxicant Database	Rhinitis – allergic - limited evidence	

Compound group: Orthophthalates



Pros/Cons of Compound Group Population Project

- Pros
  - Harmonized between systems
  - Better defined compound groups
  - Higher confidence in hazard assignments
- Cons
  - Lists change more rapidly than process to update groups
  - Not as nimble to add chemicals known to be part of the group
- Lessons learned
  - Choose smaller sets of chemicals to QC
  - Need a mechanism for adding chemicals in short tat

Next Steps

- Phase 1 & 2 : 80 compound groups
  - Nearing completion.
  - Select groups in second round of review.
- Publish findings Feb
- Harmonize tools

Thank You!

For more information contact:
Teresa McGrath
tmcgrath@healthybuilding.net

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Small Group Discussion

1) Are chemical classes part of your work (or your organization's work)?

If yes:

- How are chemical classes part of your work?
- Which chemical classes are you working with?

If no:

- How might a class approach be helpful in your work?
- How could you better avoid regrettable substitutes by using chemical classes?

2) What is it that you want to do with classes (what actions do you want to take)?