Critical Analysis of Benchmark-1 GreenScreen® Hazard Combinations

Samantha Vaccaro
Meg Whittaker
ToxServices LLC

18th BizNGO Annual Meeting
Oakland, CA
December 6, 2023

TOXSERVICES
TOXICOLOGY RISK ASSESSMENT CONSULTING

What is a Chemical of Concern?

- A chemical of concern displays one or more of the following traits:

  - Carcinogenicity, mutagenicity, reproductive or developmental toxicity
  - Potential concern for children's health
  - Used in children's products
  - Neurotoxic

  Human Health

  - Persistent, bioaccumulative, and toxic (PBT)
  - Very persistent or very bioaccumulative in the environment (vPvB)
  - Very persistent and Toxic (vPT)
  - Ozone depleting
  - Detected in biomonitoring programs

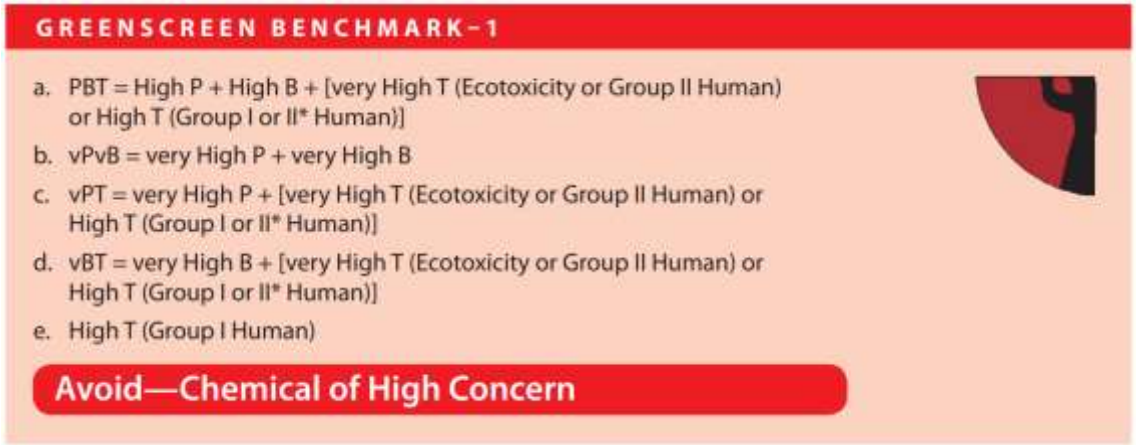
  Environmental Health

- Chemicals of concern are challenging to phase out:
  - Switching to a chemical with unknown hazards may result in a chemical that is more hazardous

What is a Benchmark-1 Chemical?

Benchmark-1 (BM-1) chemicals are defined as chemicals of high concern to human health and the environment based on high or very high endpoint-specific rankings

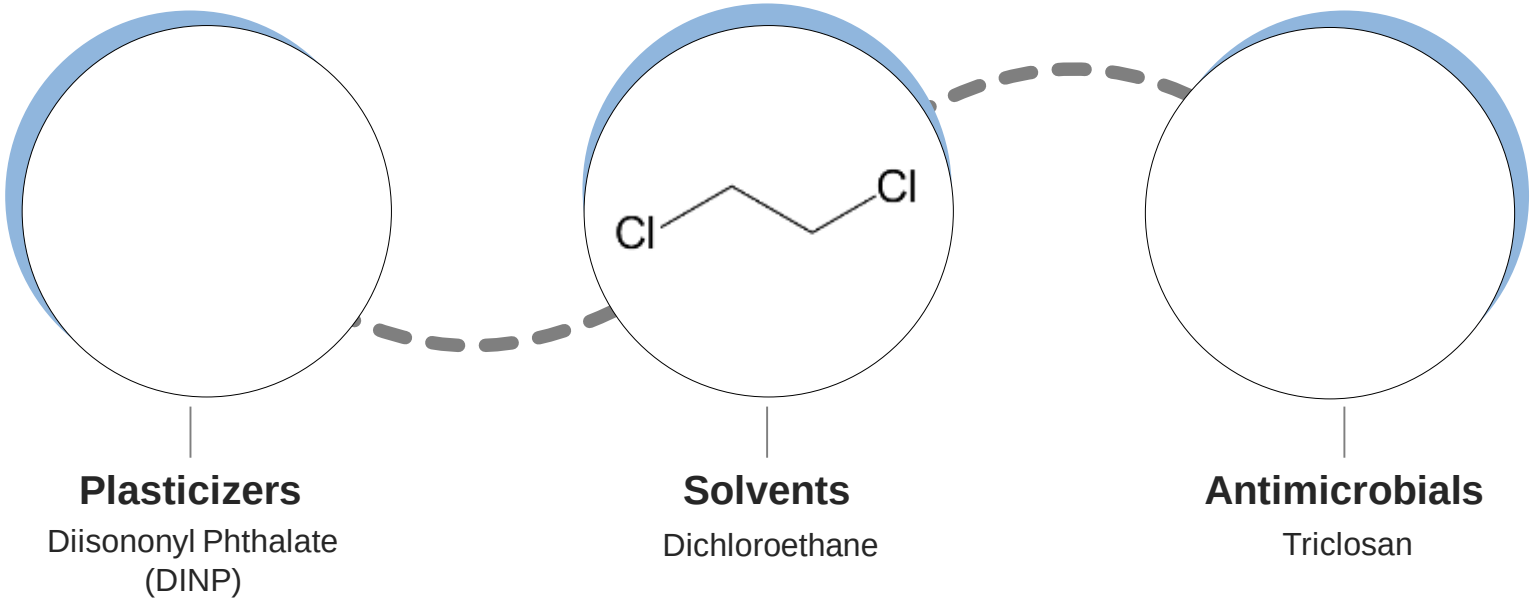
- Organic BM-1 chemicals are further classified into five subclasses BM-1A, BM-1B, BM-1C, BM-1D, and/or BM-1E, based on a chemical's hazard characteristics



- Inorganic BM-1 chemicals are classified into four subclasses BM-1A, BM-1B, BM-1C, BM-1D with no subclass for vPvB since inorganic compounds are recalcitrant (persist in nature and do not biodegrade)

What is a Benchmark-1 Chemical?

Example BM-1 chemicals include commonly used:



Industry Bans on Chemical Classes

sweetgreen

Sweetgreen and Chipotle will remove "forever chemicals" from their bowls by the end of 2020

by Joe Fassler
03.16.2020, 10:53am

Environment

CHIPOTLE

patagonia
VENTURA, CALIFORNIA

Made without PFCs / PFAS

We're converting all of our durable water-repellent membranes and finishes to non-fluorinated alternatives by 2025.

LOWE'S

LOWE'S SAFER CHEMICALS POLICY

As a responsible corporate citizen, Lowe's takes product safety and environmental sustainability very seriously. To manage chemicals more responsibly, Lowe's implements this safer chemicals policy through a number of strategic actions and commitments.

Flooring

- All vinyl flooring is free of ortho-phthalates
- All indoor wall-to-wall carpet is free of triclosan, organotins, ortho-phthalates, vinyl chloride, nonylphenol ethoxylates, coal fly ash, formaldehyde, added heavy metals
- All indoor residential carpet and rugs are free of PFAS chemicals

WHOLE FOODS MARKET

BLOG

Whole Foods, Trader Joe's Pledge Initial Action on Nonstick PFAS

December 12, 2018

Starbucks Innovates, Tests and Learns from Store Partners to Achieve Waste Goals

In further single use packaging optimization, we continue to replace traditional plastic straws with new compostable options around the globe. By the end of this year, will have eliminated PFAS from all packaging in the US and will eliminate PFAS globally in 2023.

Does Chick-fil-A's packaging contain PFAS?

Chick-fil-A is working to eliminate intentionally added PFAS from all newly produced packaging going forward in our supply chain. Products with oil and grease resistant coatings containing PFAS are expected to be phased out by the end of summer of 2022. We've spent the last four years working closely with our suppliers, an independent lab and 3rd party validator to provide our customers with innovative packaging products that meet all applicable regulatory standards. This is one important step in our ongoing journey to use more sustainable materials in our restaurants. Chick-fil-A is dedicated to offering the best food, packaging and overall experience to our guests.

Chick-fil-A

TRADER JOE'S

THE HOME DEPOT

PHASING OUT PRODUCTS CONTAINING PFAS

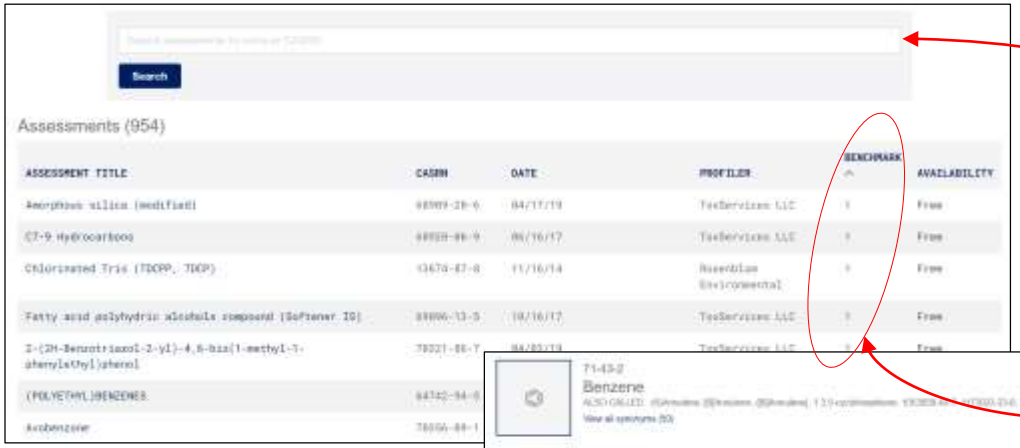
September 17, 2019

In partnership with suppliers, The Home Depot is working diligently to offer products that are innovative and safer for the environment. The Home Depot is committed to minimizing the environmental impact of the products on its store shelves and has led the industry in creating chemical standards to do just that.

To build upon the strategy, The Home Depot will be phasing out Perfluoroalkyl and Polyfluoroalkyl Substances (PFAS) December 31, 2019 in the U.S. and Canada in carpets and rugs.

Where to Find Benchmark-1 Chemicals?

The Pharos Chemical and Material Library



Search by CAS number or sort by BM score

https://pharosproject.net/

Where to Find Benchmark-1 Chemicals?

Toxnot / 3E Exchange Chemical Database

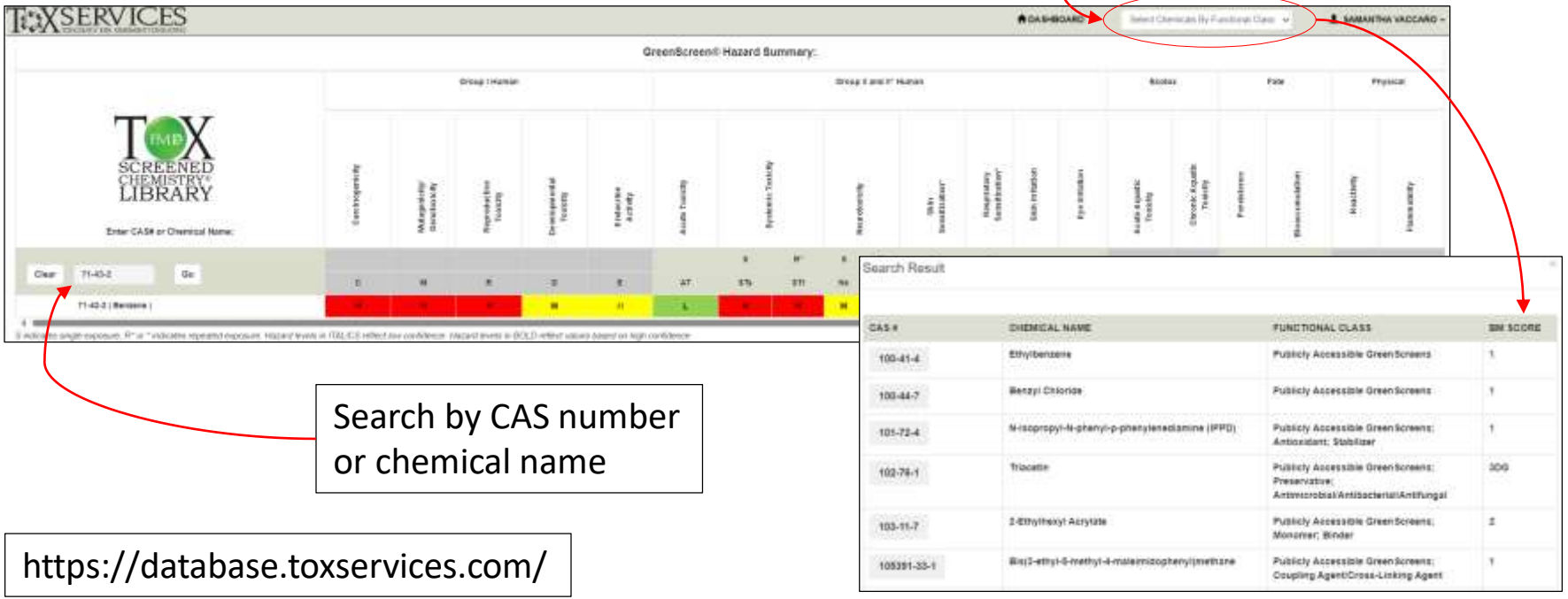
Search by CAS number or chemical name

https://exchange.3eco.com/

Where to Find Benchmark-1 Chemicals?

ToxServices' ToxFMD Screened Chemistry® Library

Search by functional class*



Search by CAS number or chemical name

https://database.toxservices.com/

*All BM-1 chemical GreenScreens are available via the "Publicly Accessible GreenScreens" functional class

Benchmark-1 Analysis

ToxServices' ToxFMD Screened Chemistry® Library

The ToxFMD Screened Chemistry® Library[1] contains GreenScreen® chemical hazard assessments for over 1,000 chemicals

Data Mining

Of the 1,000+ GreenScreen® chemical hazard assessments preformed by ToxServices, the library contains 204 BM-1 chemicals

Chemical Classification

The 204 BM-1 chemicals were assigned a chemical class using ClassyFire[2], a web-based application for structural classification

Subscore Hazard Combination Analysis

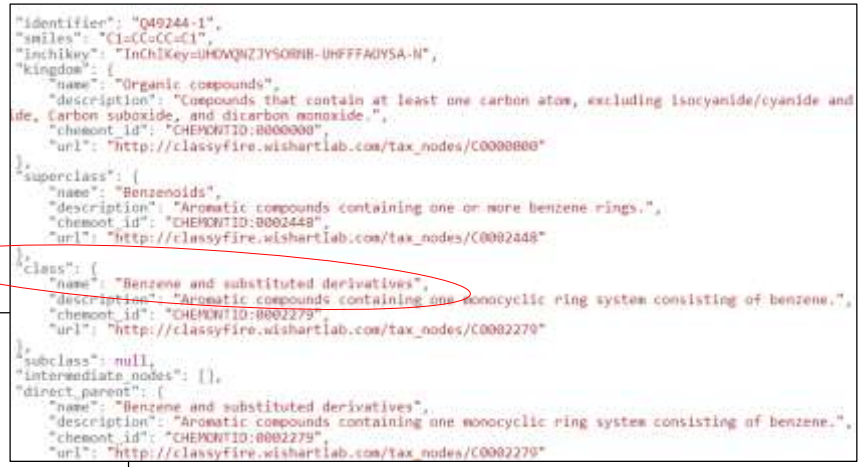
The 204 BM-1 chemicals were assigned a total of 278 subscores (1A, 1B, 1C, 1D, and/or 1E)

[1] https://database.toxservices.com/

[2] *Djoumbou Feunang Y, Eisner R, Knox C, Chepelev L, Hastings J, Owen G, Fahy E, Steinbeck C, Subramanian S, Bolton E, Greiner R, and Wishart DS. ClassyFire: Automated Chemical Classification With A Comprehensive, Computable Taxonomy. Journal of Cheminformatics, 2016, 8:61.* DOI: 10.1186/s13321-016-0174-y

ClassyFire

ClassyFire is a web-based application for automated structural classification of chemical entities. This application uses a rule-based approach that relies on a comprehensible, comprehensive, and computable chemical taxonomy.

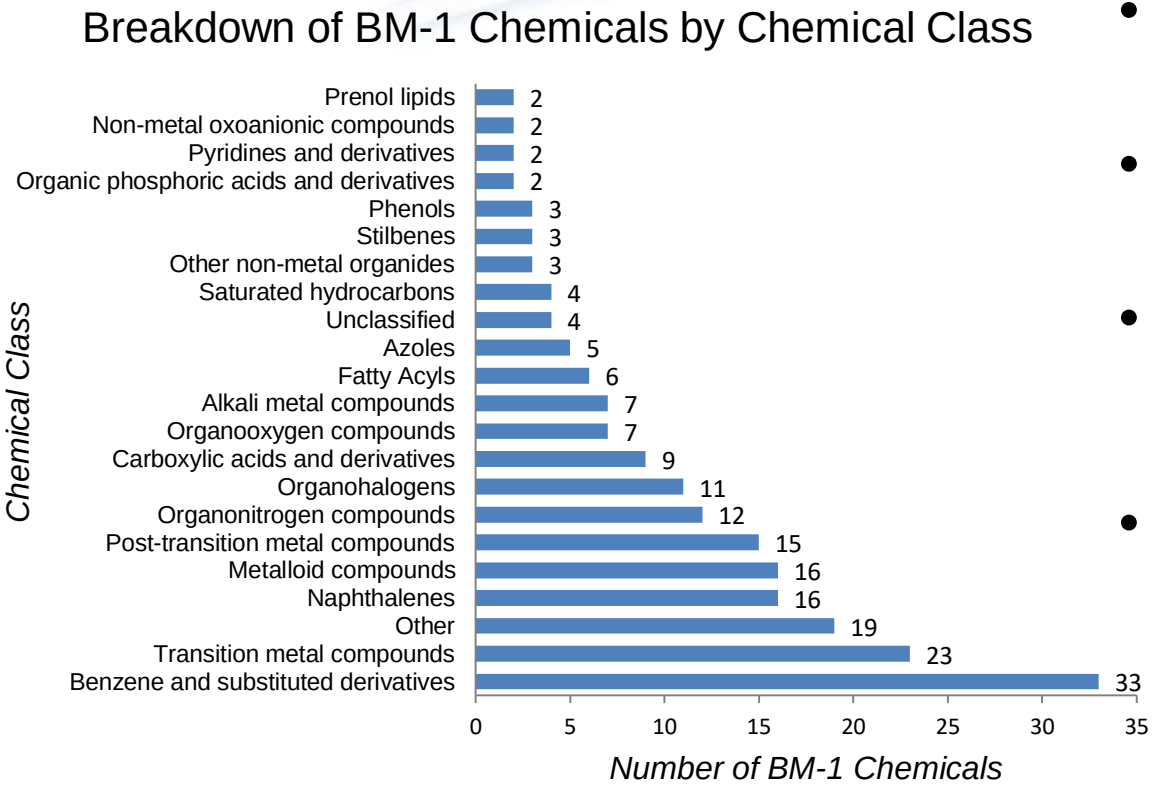


http://45.88.80.180/

ClassyFire's output is a hierarchical chemical classification of a chemical entity

Djoumbou Feunang Y, Eisner R, Knox C, Chepelev L, Hastings J, Owen G, Fahy E, Steinbeck C, Subramanian S, Bolton E, Greiner R, and Wishart DS. ClassyFire: Automated Chemical Classification With A Comprehensive, Computable Taxonomy. Journal of Cheminformatics, 2016, 8:61. DOI: 10.1186/s13321-016-0174-y

Benchmark-1 Analysis

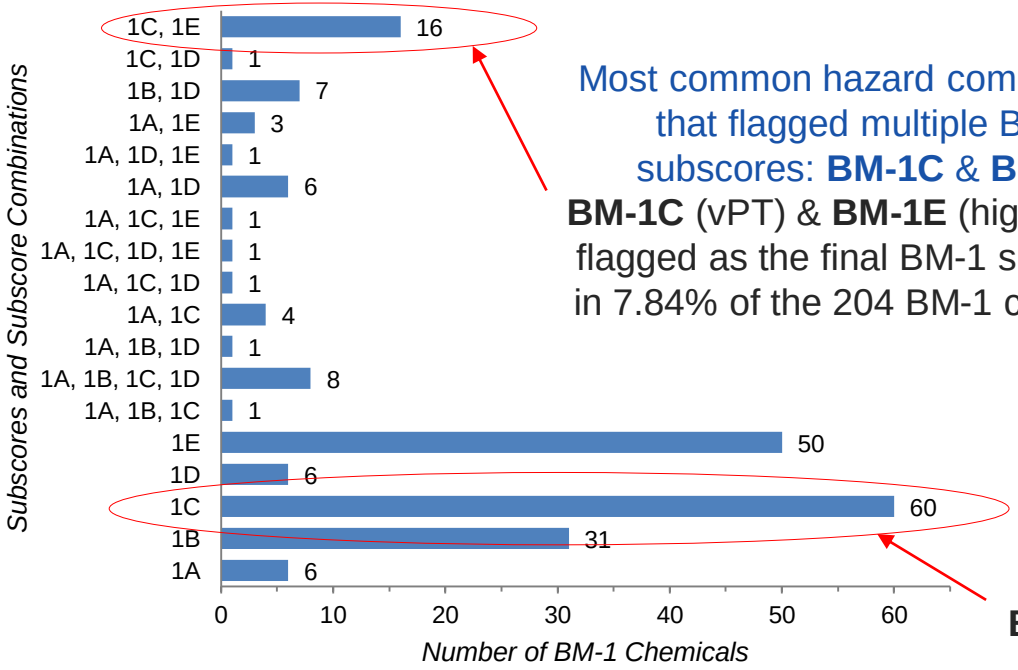


- ClassyFire identified 57 different chemical classes for these 204 BM-1 chemicals
- For simplicity, these 57 chemical classes were further grouped into 22 different categories
- The most common chemical class for BM-1 chemicals are benzene and substituted derivatives, and transition metal compounds
- As the BM-1 chemicals span a wide range of classes, there is no singular chemical class to avoid

** Other represents any chemical class only present once among the 204 BM-1 chemicals*

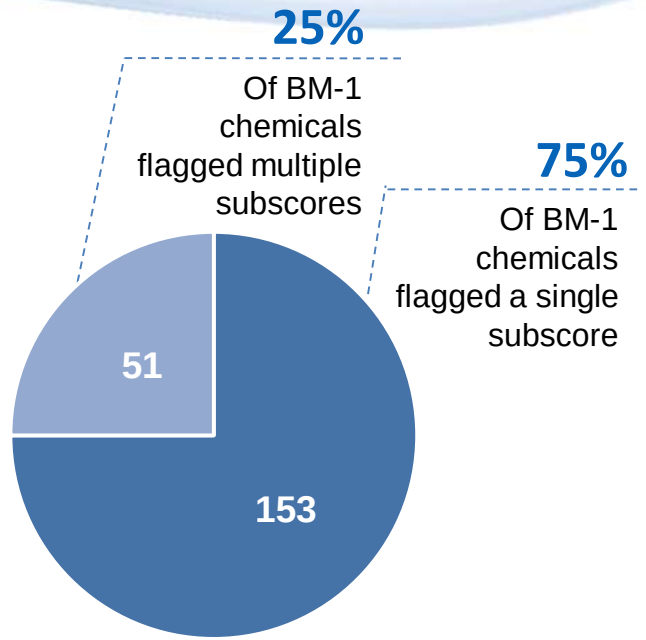
Benchmark-1 Analysis

Breakdown of BM-1 Chemicals by Final Subscore/Subscore Combinations



Most common hazard combinations that flagged multiple BM-1 subscores: **BM-1C** & **BM-1E**

BM-1C (vPT) & **BM-1E** (high T) were flagged as the final BM-1 subscores in 7.84% of the 204 BM-1 chemicals

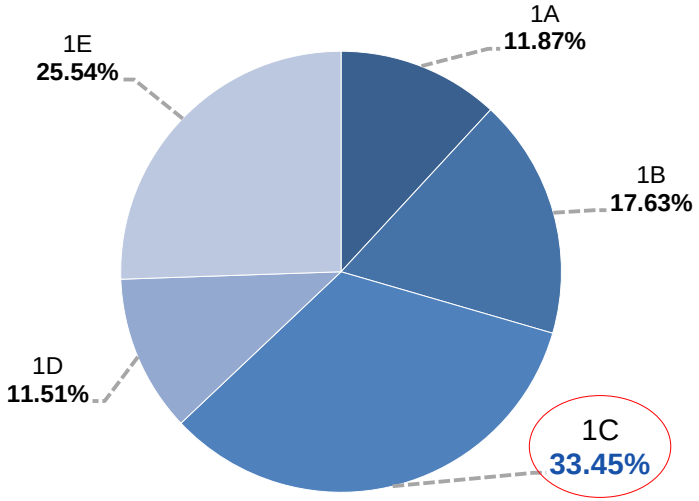


Most common hazard combination that flagged a single BM-1 subscore: **BM-1C**

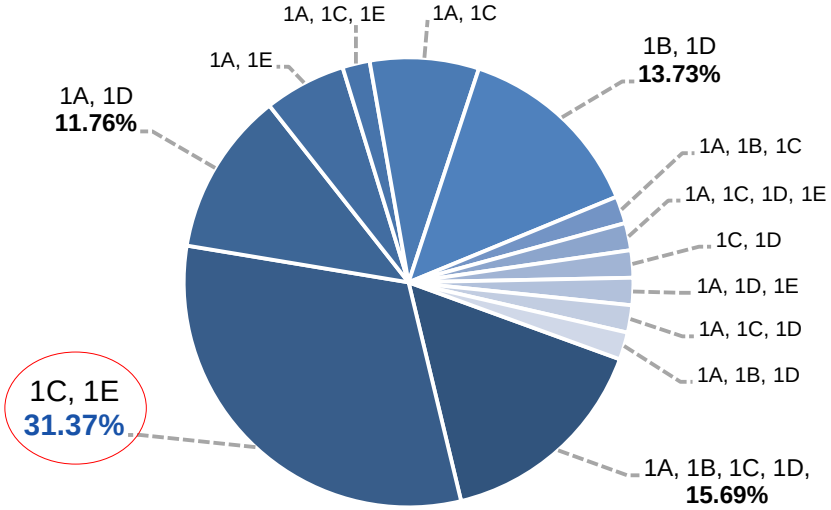
BM-1C (vPT) was flagged as the final subscore in 29.41% of the 204 BM-1 chemicals

Benchmark-1 Analysis

BM-1 Chemicals by Singular Subscore Only



BM-1 Chemicals by Subscore Combinations Only



Most common hazard combination that flagged a BM-1 subscore: **BM-1C**

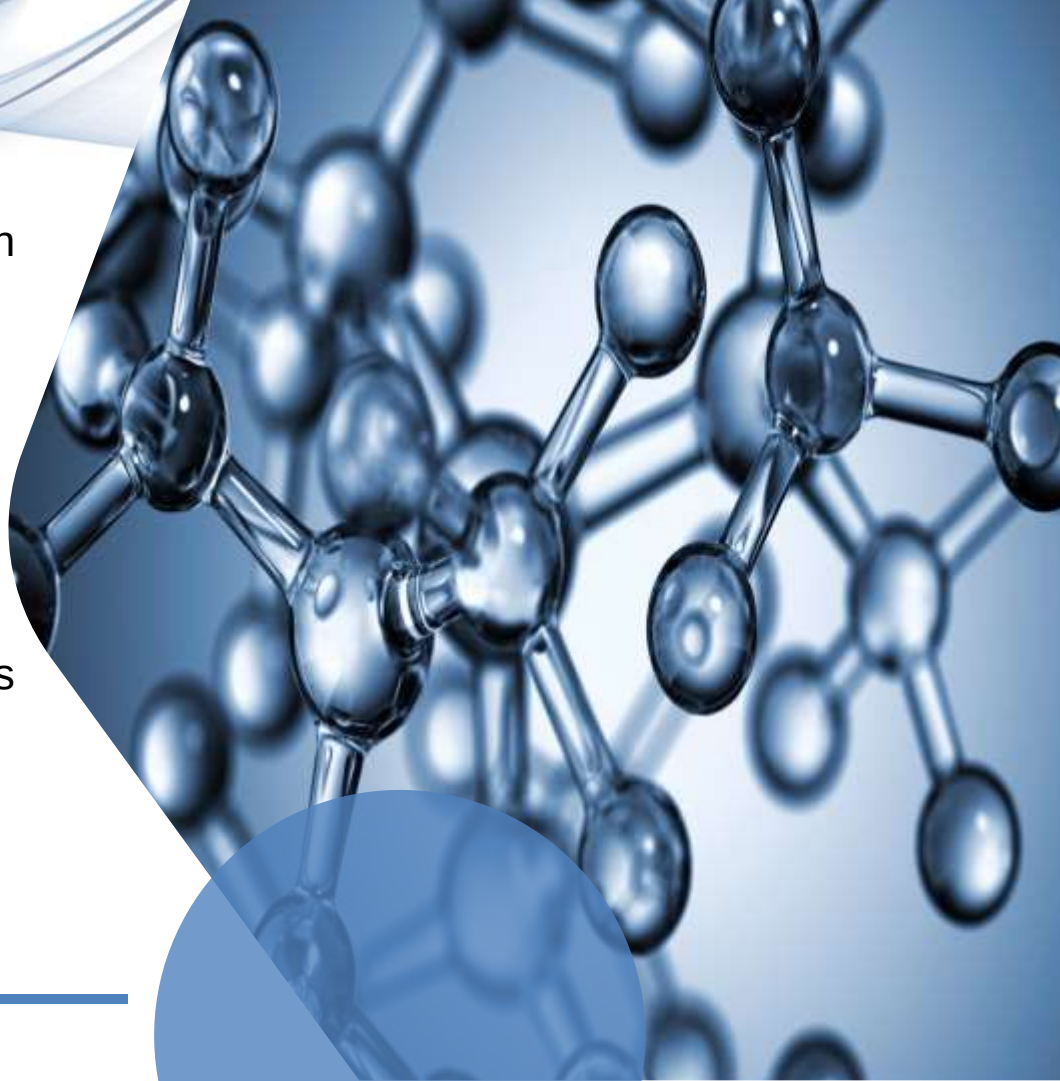
BM-1C (vPT) was flagged as a subscore in 93 of the 278 subscores flagged across the 204 BM-1 chemicals (33.45%)

Most common hazard combinations that flagged multiple BM-1 subscores: **BM-1C** & **BM-1E**

BM-1C (vPT) & **BM-1E** (high T) were flagged as the final BM-1 subscores in 16 of the 51 BM-1 chemicals with multiple subscores (31.37%)

Conclusions

- Many BM-1 chemicals pose both human health and environmental concerns
- BM-1 classifications effectively identify chemicals of concern and as well as identify candidates for chemical substitution.
- Chemicals from many different classes can be BM-1 chemicals
    - There is no singular chemical class to avoid
    - The implementation of CHAs to guide decision-making is more useful for eliminating chemicals of high concern



TOXSERVICES
TOXICOLOGY RISK ASSESSMENT CONSULTING

Thank You

Margaret H. Whittaker, Ph.D., M.P.H., CBiol., F.R.S.B., E.R.T., D.A.B.T.
Managing Director and Chief Toxicologist
ToxServices LLC
Email: mwhittaker@toxservices.com

Samantha Vaccaro
Sustainability Project Manager
ToxServices LLC
Email: svaccaro@toxservices.com