Identifying Persistent, Bioaccumulative and Toxic Chemicals among the Chemicals on the EU Market

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Overview

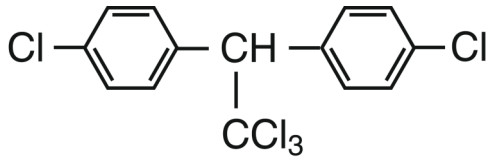
- PBT chemicals: the problem
- Chemicals and property data
- Potential PBT chemicals among existing and new chemicals
- Conclusions: persistence matters!

PBT Chemicals: the Problem

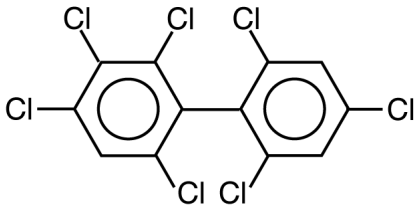
- PBT chemicals: persistence, bioaccumulation potential, and toxicity all particularly high

UNEP/AMAP Expert Group (2011)
Climate Change and POPs: Predicting the Impacts, p. 17

- Typical PBT chemicals:



DDT



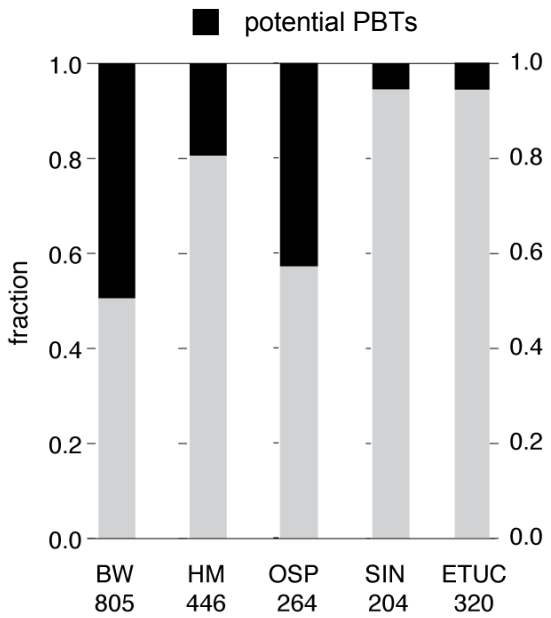
PCBs

- How many are there in total?
- How can they be identified?

PBT Chemicals: Current Approaches

- Various **lists of priority chemicals**:
  - Substitute It Now (SIN) list
  - ECHA SVHC candidate list
  - list of the European Trade Union Confederation (ETUC)
  - Howard & Muir (2010): 610 priority chemicals (focus: P and B)
  - Brown & Wania (2008): list of 810 chemicals with high Arctic Contamination Potential
  - OSPAR Convention, substances of possible concern

- But: **lists differ** with respect to
  - criteria for chemicals of concern
  - threshold values for the criteria



S. Strempel et al., Environ. Sci. Technol. 46 (2012), DOI: 10.1021/es3002713

Our PBT Screening Approach

- Step 1: set up database of CAS and SMILES codes
- Step 2: compile property data for P, B and T and compare them to the REACH thresholds
  - P: $t_{1/2}$ in marine water > 60 days
  - B: BCF > 2000
  - T: $NOEC_{chronic}$ < 0.01 mg/L, EC_{acute} < 0.1 mg/L

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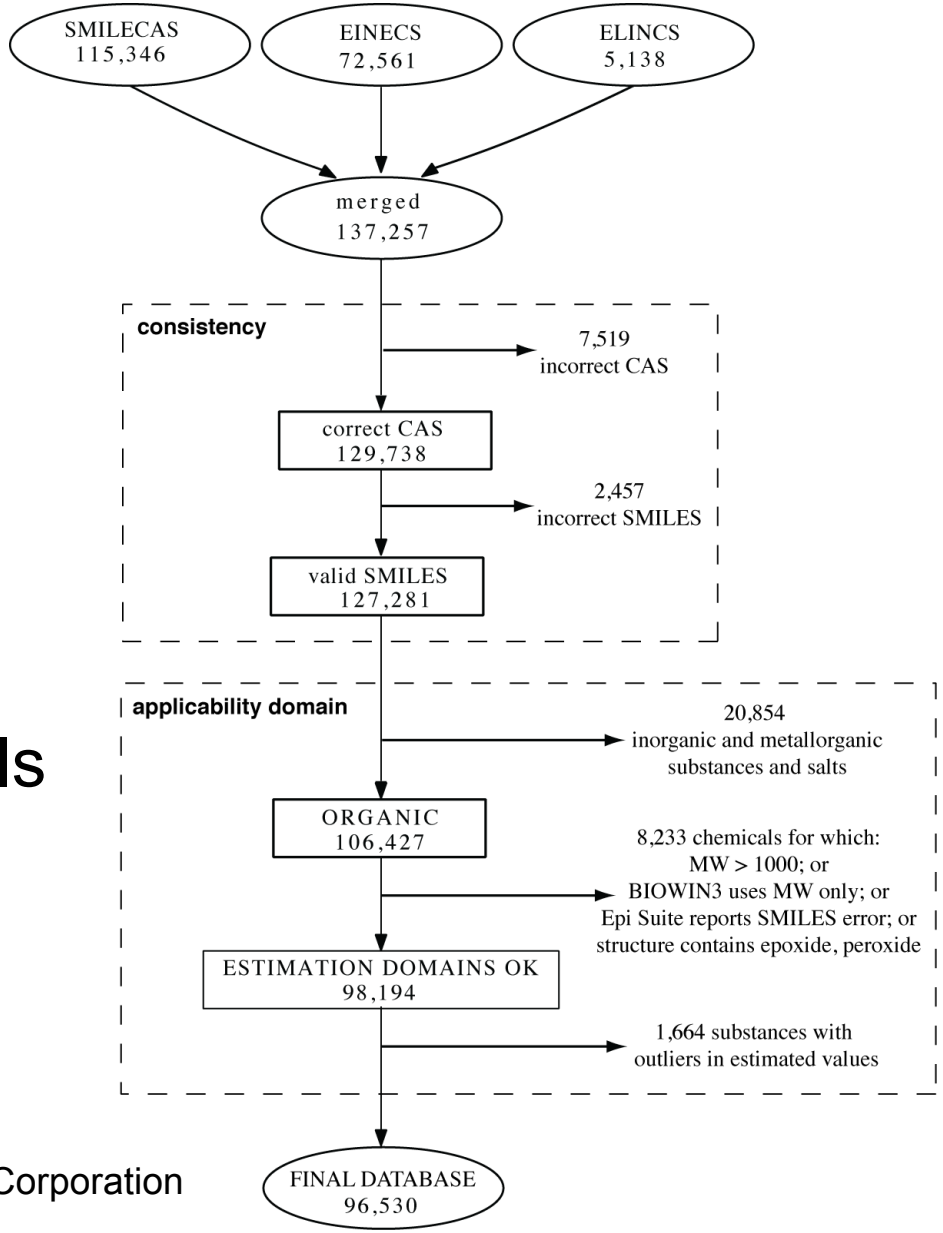
Step 1: Database of Chemicals

- Existing chemicals: EINECS, SMILECAS[1]
- New chemicals: ELINCS
- remove incorrect CAS and SMILES
- remove inorganic, ionic and metallorganic chemicals
- remove chemicals outside applicability domain
- total: 96,530



1: Syracuse Research Corporation

Step 2: The PBT Score

- For P, B, T individual subscores:
  - ratio of chemical property value and REACH threshold, truncated at 1.0 and divided by 3
- PBT score, S_{PBT}: sum of the three subscores
- S_{PBT} = 1.0 indicates that all three thresholds are exceeded

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- PBT score, S_{PBT}: sum of the three subscores
- S_{PBT} = 1.0 indicates that all three thresholds are exceeded
- Four hazard classes:
  - PBT with S_{PBT} = 1.0
  - nonPBT2: two thresholds exceeded, 0.667 < S_{PBT} < 0.999
  - nonPBT1: one threshold exceeded, 0.333 < S_{PBT} < 0.999
  - nonPBT0: no threshold exceeded, 0 < S_{PBT} < 0.999

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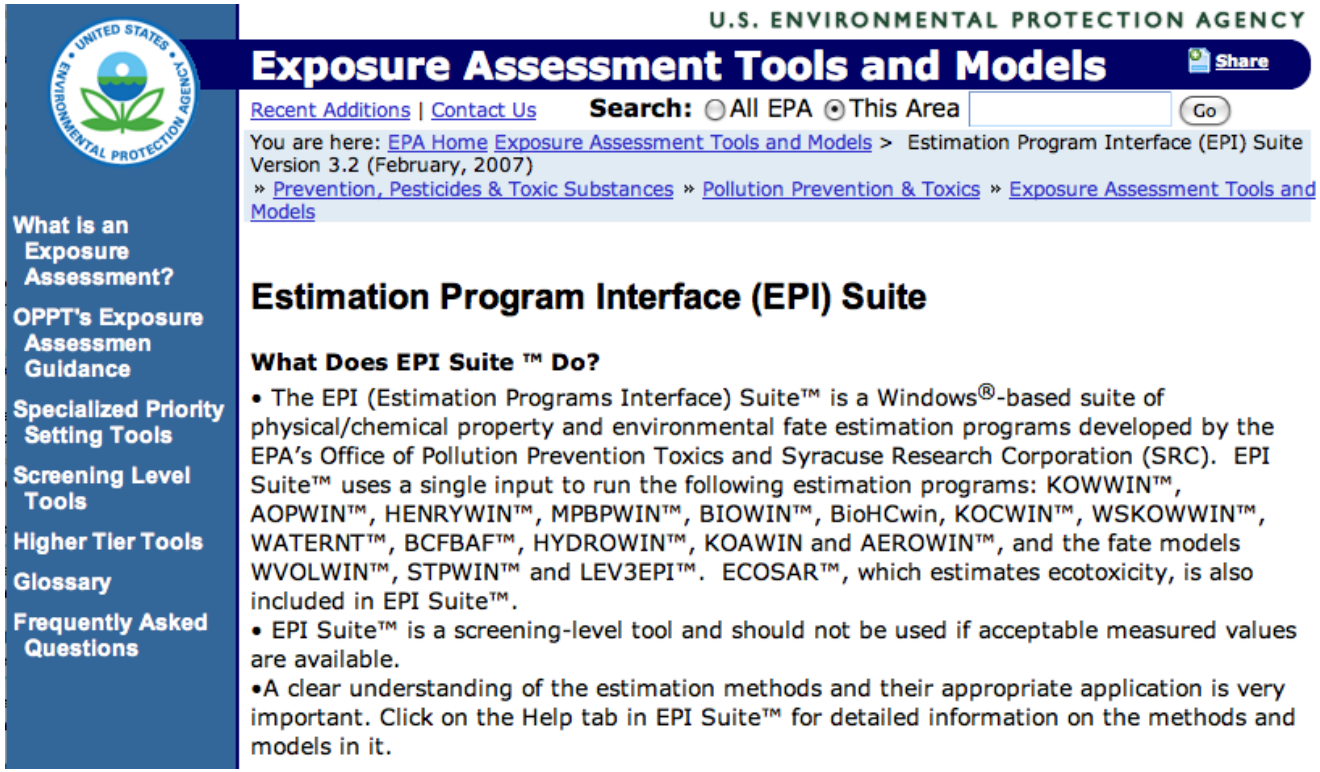
Experimental Property Data

- Half-life:
  - aerobic biodegradation
  - 222 measured data (source: BIODEG database)
- BCF:
  - 1,213 measured BCF values, 13,731 K_{ow} values (sources: CHEMFATE database, BCF gold standard database, others)
- Aquatic toxicity:
  - 2,245 acute effect concentrations in daphnia or fish (sources: ECOTOX database, others)

Tiny fraction!

Property Estimation Methods Used

- Estimation methods:
  - half-life of aerobic biodegradation: BIOWIN3
  - BCF: BCFBAF
  - aquatic toxicity: ECOSAR



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OPPT's Exposure Assessmen Guidance
Specialized Priority Setting Tools
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Frequently Asked Questions

Estimation Program Interface (EPI) Suite

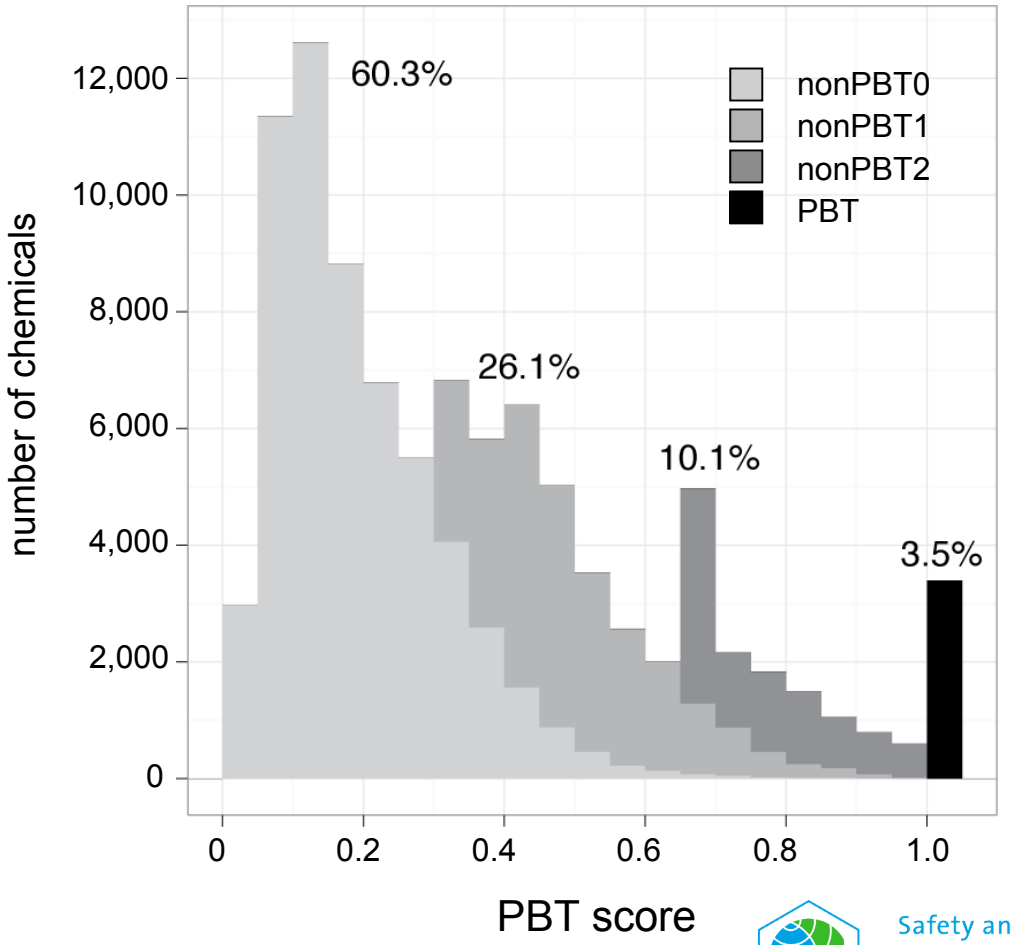
What Does EPI Suite ™ Do?

• The EPI (Estimation Programs Interface) Suite™ is a Windows®-based suite of physical/chemical property and environmental fate estimation programs developed by the EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC). EPI Suite™ uses a single input to run the following estimation programs: KOWWIN™, AOPWIN™, HENRYWIN™, MPBPWIN™, BIOWIN™, BioHCwin, KOCWIN™, WSKOWWIN™, WATERNT™, BCFBAF™, HYDROWIN™, KOAWIN and AEROWIN™, and the fate models WVOLWIN™, STPWIN™ and LEV3EPI™. ECOSAR™, which estimates ecotoxicity, is also included in EPI Suite™.
• EPI Suite™ is a screening-level tool and should not be used if acceptable measured values are available.
•A clear understanding of the estimation methods and their appropriate application is very important. Click on the Help tab in EPI Suite™ for detailed information on the methods and models in it.

http://www.epa.gov/oppt/exposure/pubs/episuite.htm

PBT Score: Results for 96,530 Chemicals

- hazard classes:
  - 3.5% (3,404) PBT
  - 10.1% (9,730) nonPBT2
  - 26.1% (25,223) nonPBT1
  - 60.3% (58,173) nonPBT0



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Uncertainties of PBT Classification

- Uncertainty factors of P, B and T properties
  - half-life of aerobic biodegradation: $f = 4$
  - K_{ow} and BCF: $f = 4$
  - toxicity data: $f = 45$
- Corresponding changes in number of PBT chemicals?
  - upper limit: 13,050 instead of 3,404
  - lower limit: 254 instead of 3,404
- By far most important contribution is from uncertain P data

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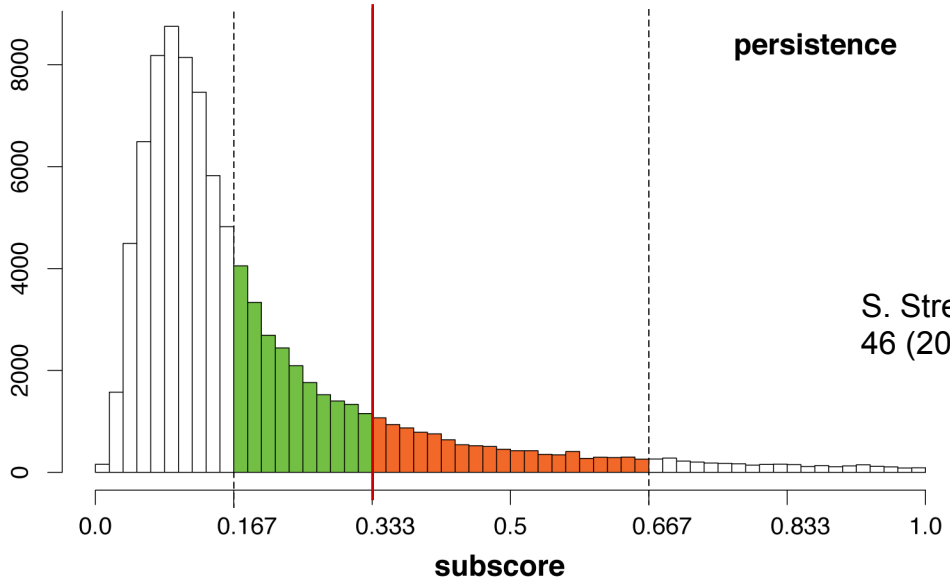
Distributions of Individual Subscores

REACH threshold

colored regions:
factor of 2 around threshold



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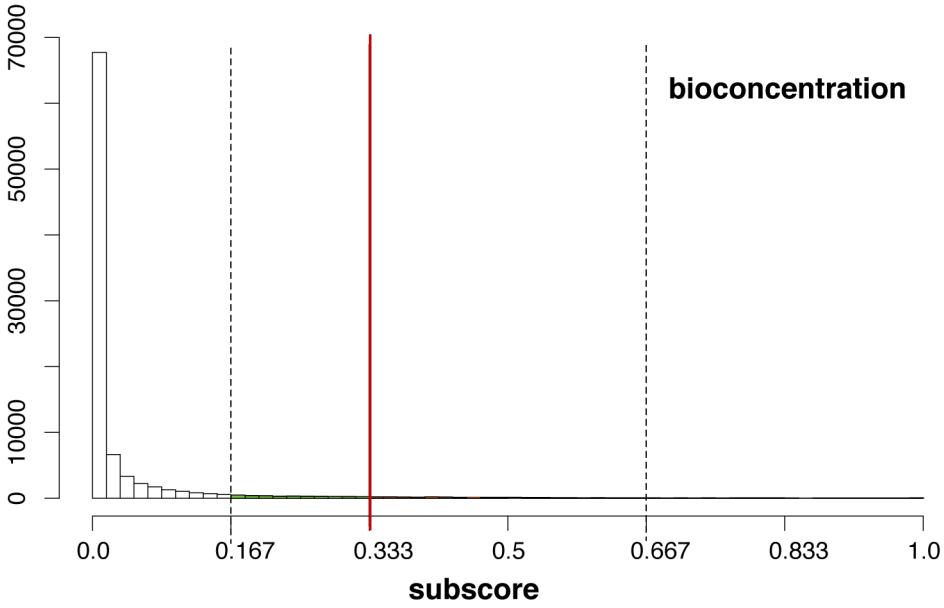
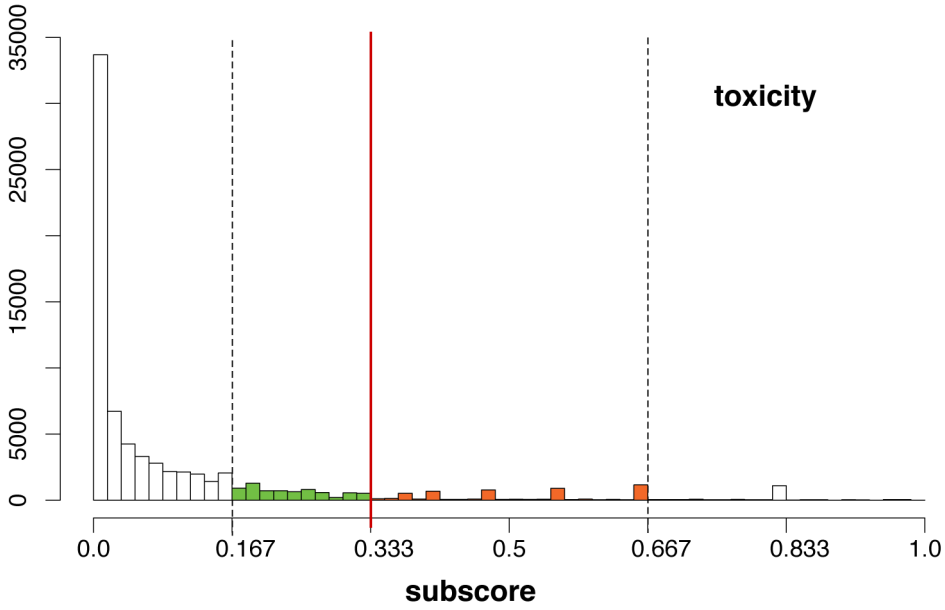
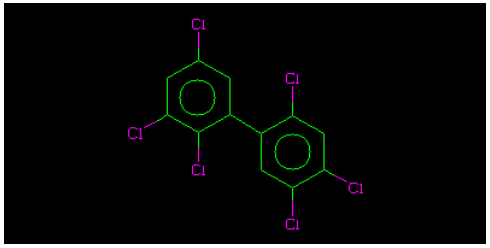
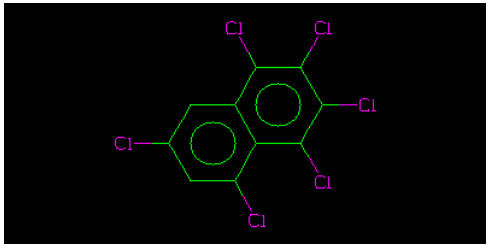
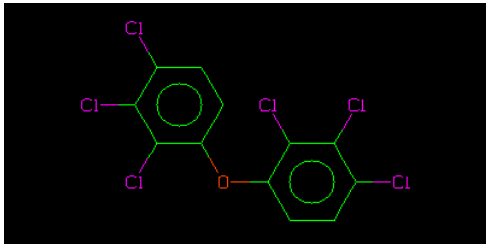
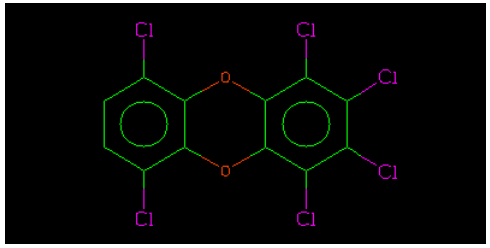




Chemical Structures in the PBT Class

- chlorinated, brominated aromatic systems
  - benzenes, naphthalenes, biphenyls, diphenylethers, dibenzodioxins and -furans

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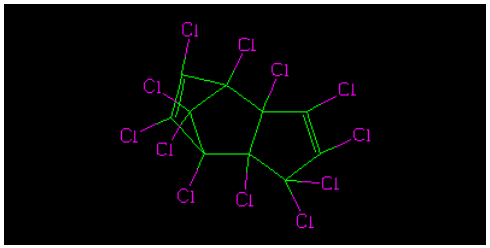
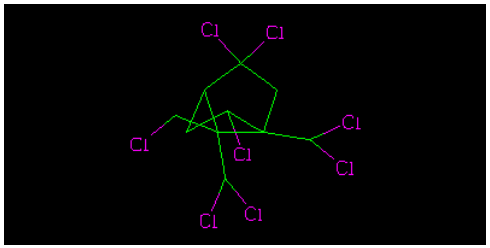
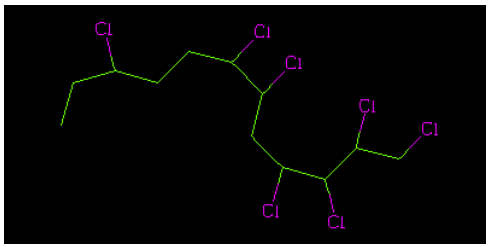
- chlorinated, brominated (cyclo-)aliphatic compounds







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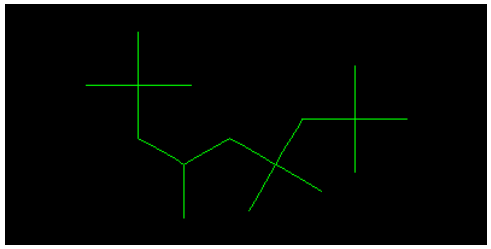
- highly branched alkyl substances



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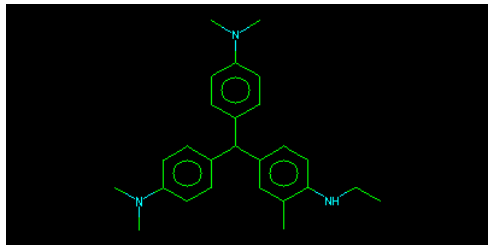
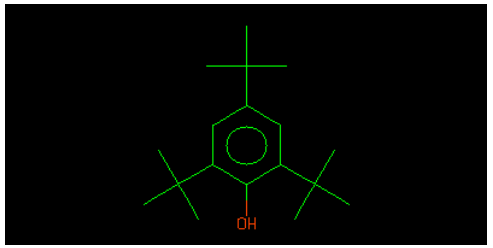
- aromatic substances with several highly branched alkyl, ether, or tertiary amine groups





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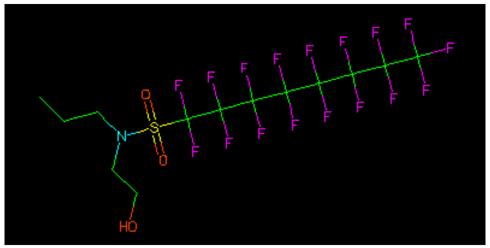
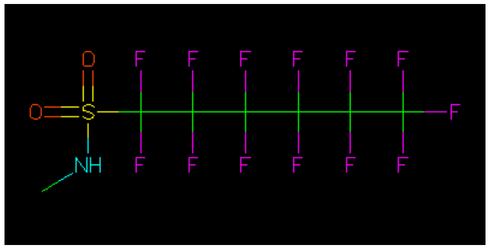
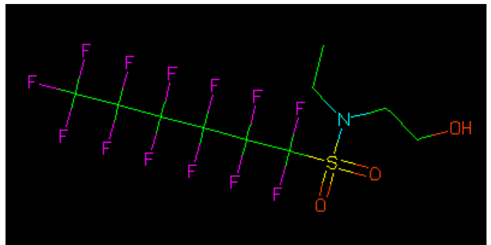
- aromatic substances with several highly branched alkyl, ether, or tertiary amine groups
- per- and polyfluorinated alkyl substances







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- highly branched alkyl substances
- aromatic substances with several highly branched alkyl, ether, or tertiary amine groups
- per- and polyfluorinated alkyl substances
- PAHs
- combinations of all these elements...

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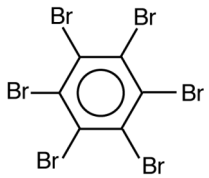
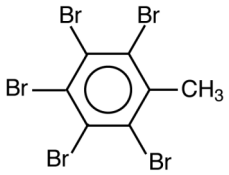
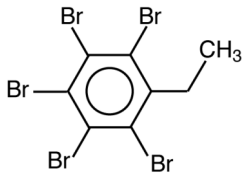
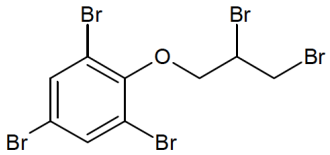
Results for non-BDE BFRs and DP

- HBB
- PBT
- PBEB
- DPTE
- DBDPE
- BTBPE
- EBTPI
- DP

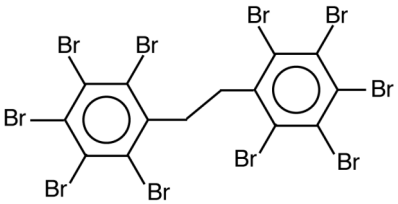


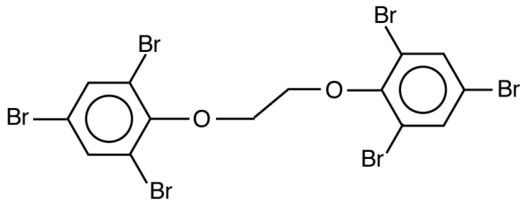




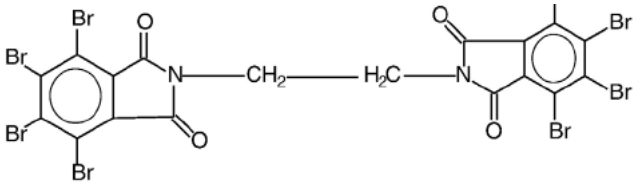


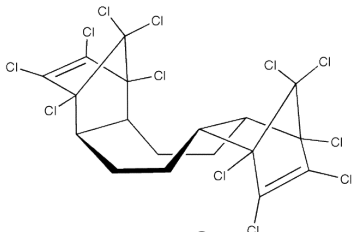
all four: PBT





all four: P and T;
B not clear





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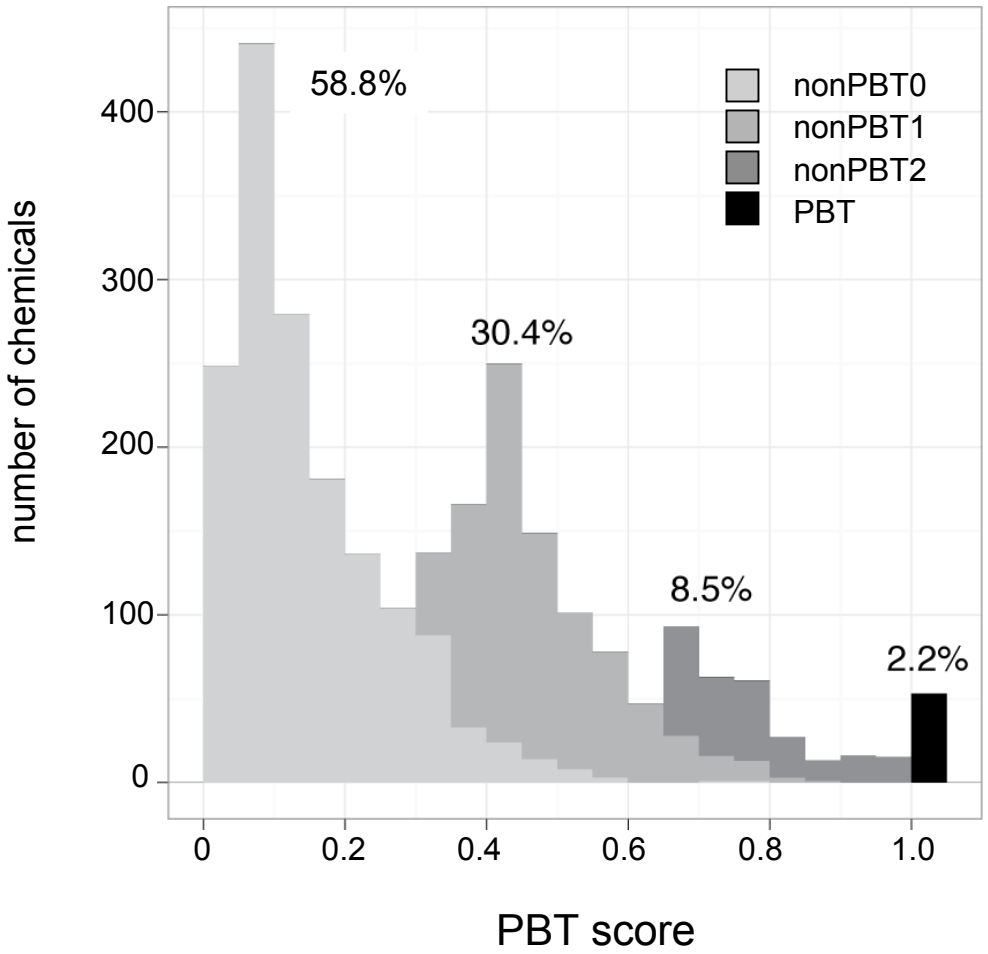
PBT Scores of 2,659 HPVCs

- all four hazard classes populated
- numbers of chemicals:
  - 2.2% (58) PBT
  - 8.5% (225) nonPBT2
  - 30.4% (808) nonPBT1
  - 59% (1,568) nonPBT



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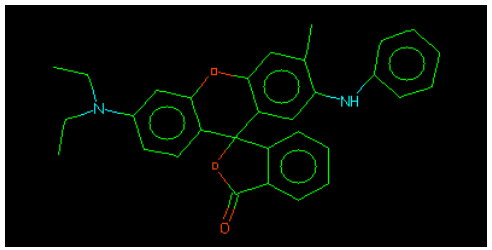
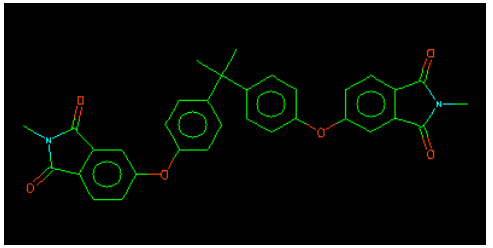
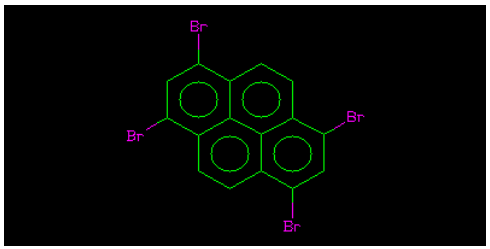
58 HPVC CAS in the PBT Class

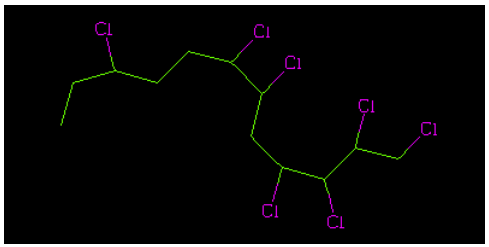
- 24 CAS related to heavy fractions of petroleum, used, e.g., as lubricating oils
- 34 chemicals from various classes:
  - several compounds used as antidegradants (UV absorbers) in synthetic rubber



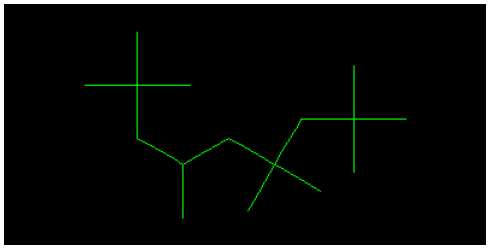


  - several fluorinated, chlorinated and brominated compounds



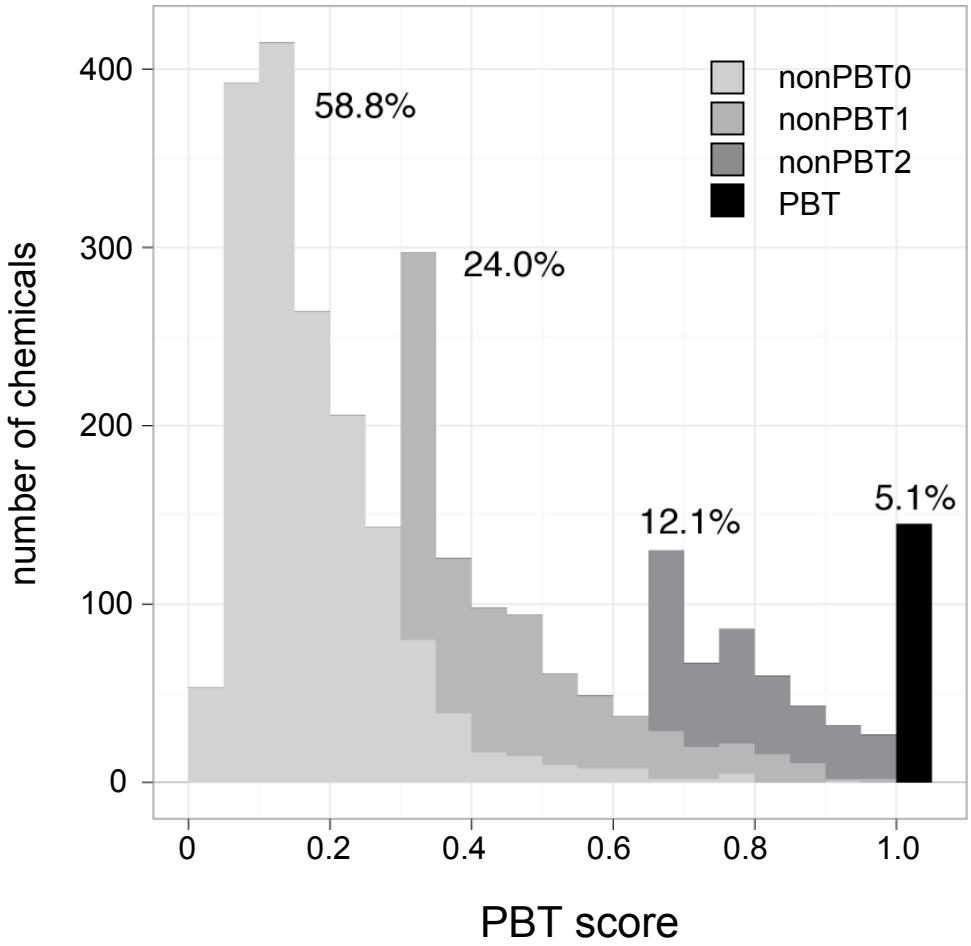


  - highly branched alkyl compounds



PBT Scores of 2,825 ELINCS Chemicals

- high fraction of chemicals in the PBT class: 5.1% (142)
- higher fraction of fluorinated chemicals 30% vs. 12% in full set
- individual structures confidential!



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Conclusions

- Around 2% of potential PBT chemicals
  even among HPVCs: 20–60 chemicals
- Around 3000 potential PBT chemicals in the full set

- ELINCS chemicals do not show a trend towards „Green Chemistry“
- Persistence matters most:
  more and better degradation data needed!

Are these potential PBT chemicals “emerging”?!

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and
by the German Federal Environment Agency (UBA)

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