

Biodegradation of Fragrances

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January 31, 2024

Overview

- Biodegradation in NCD's environmental fate assessments
- Biodegradation data for recent fragrance PMNs
- Biodegradation data sources:
 - Submitted data
 - Publicly available data
 - Models or QSARs
- Summary
- Looking forward
- Challenges

Environmental Fate Assessments

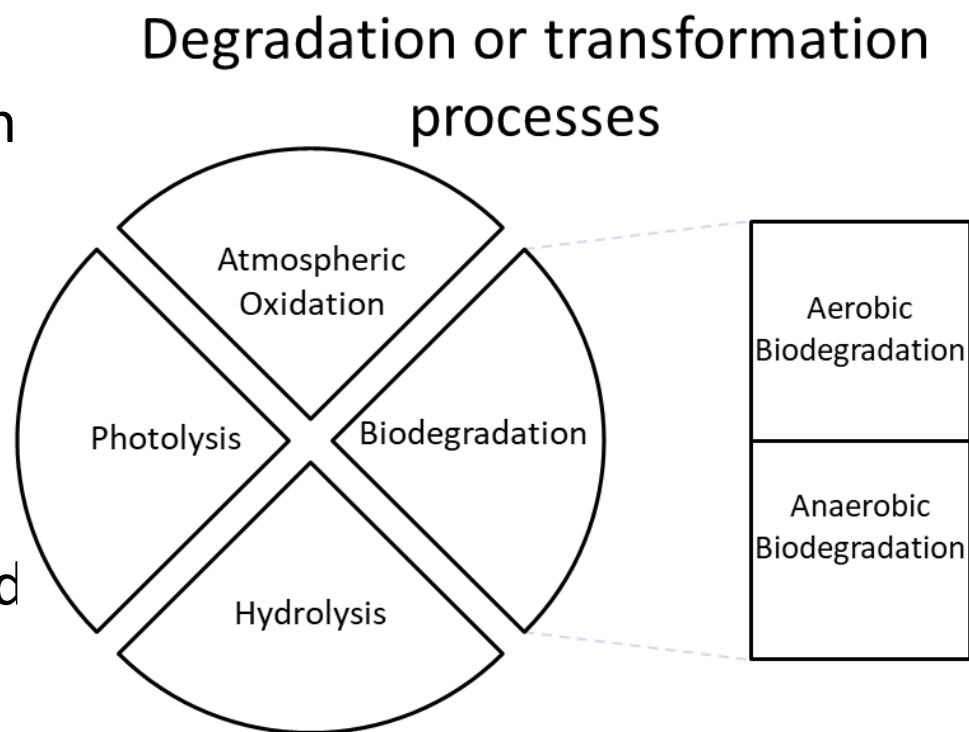
- NCD's environmental fate assessments take into consideration:
 - Environmental half-lives from degradation processes such as hydrolysis, photolysis, atmospheric oxidation, and/or **biodegradation**.

Rating and Concern Level	P1 (Limited Persistence)	P2 (Persistent)	P3 (Very Persistent)
Water, Soil, or Sediment Half-life	< 2 months	2 to 6 months	> 6 months
Atmospheric Half-life	< 2 days		≥ 2 days

- Bioconcentration Factors (BCFs) and Bioaccumulation Factors (BAFs).
- P-chem and fate properties (HLC, Log K_{OC}, Log P, etc.) and fugacity modeling.
- Measured and modeled data can be used to predict these endpoints.

Biodegradation in an Environmental Fate Assessment (1)

- Biodegradation is a degradation or transformation process that influences how long a chemical will remain in the environment.
- Environmental half-lives from aerobic and anaerobic biodegradation are considered when evaluating persistence.



Biodegradation in an Environmental Fate Assessment (2)

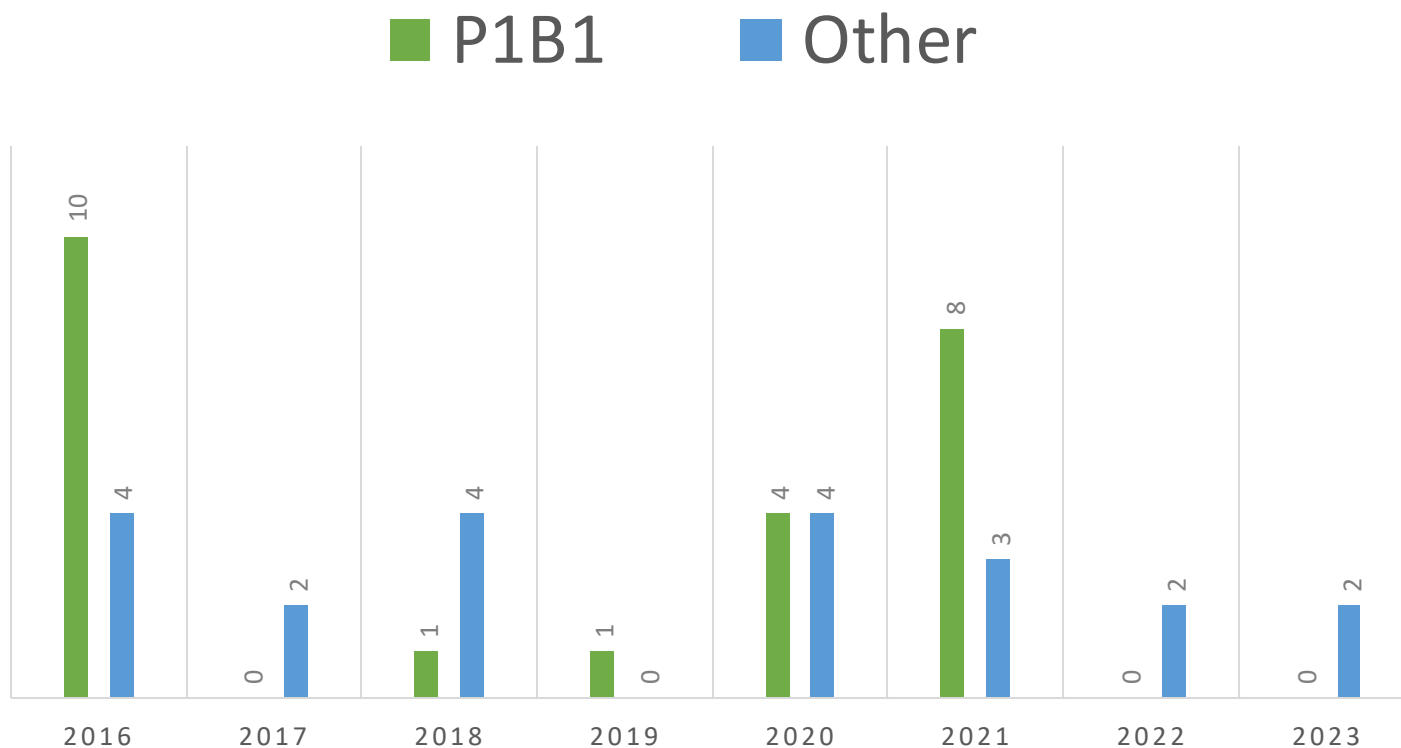
- Ready and inherent biodegradation test results from EPA and OECD guidelines are used to estimate aerobic and anaerobic biodegradation half-lives.
- **Ready biodegradation** – the ability of a substance to biodegrade quickly and completely.
- **Inherent biodegradation** – the characteristic of a product to be consumed by naturally occurring organisms in nature over an indefinite period.

Biodegradation of Fragrances (1)

- Of **45** Premanufacture Notices (PMNs) for Fragrances from 2016 to 2023, **24** were rated P1B1 and **21** received other scores (See Appendix for P and B scoring)
- **38** of the 45 PMNs included submitted, measured data using at least one OECD test guideline.
- There was a wide variety of OECD guidelines and results:
 - 11 OECD 301C studies
 - 12 OECD 301D studies
 - 19** OECD 301F studies
 - 8 OECD 310 Studies
 - 1 OECD 309 study
 - 2 OECD 302C studies
- **16** fragrances met the criteria for ready biodegradation, **20** fragrances did not meet the criteria for ready biodegradation, and **2** had mixed results.
- EPA Fate Assessors used all submitted data in the evaluation of all 38 substances.

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Biodegradation of Fragrances (2)



Biodegradation Data Sources for Fragrances

- NCD Fate Assessors do not evaluate fragrances differently than any other new chemical substance.
 - All the 38 fragrances had submitted, measured biodegradation data on the new chemical substance.
- Data sources include:
 - Submitted biodegradation data for the new chemical substance or analogue(s).
 - Publicly available data on the new chemical substance or analogue(s).
 - Modeling or QSAR data.
- NCD Fate Assessors will use a combination of data sources to fill in data gaps.

Preference: Chemical-specific test data >> Analogue data > Modeled data

Submitted Biodegradation Data

- NCD Fate Assessors review submitted environmental biodegradation test data for all new chemical substances and analogues, including fragrances, to analyze:
 - If the study is on the new chemical substance or an analogue.
 - If the study follows a specific guideline or similar method.
 - If there are any major deviations to the guidelines.

Publicly Available Biodegradation Data

- NCD Fate Assessors look for measured data that follow OECD and EPA guidelines or similar methods in:
 - ECHA: <https://echa.europa.eu/search-for-chemicals>
 - PubChem: <https://pubchem.ncbi.nlm.nih.gov/>
 - NITE/J-Check:
https://www.nite.go.jp/chem/jcheck/search.action?request_locale=en
 - ChemView: <https://chemview.epa.gov/chemview>
 - ATSDR: <https://www.atsdr.cdc.gov/>
 - Danish EPA
 - Peer-reviewed literature
 - Other reliable sources

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Modeling of Biodegradation Data

- EPISuite™ is our main estimation program:
 - STPWIN: Estimation of removal in a WWTP
 - BOWIN1-6 Models: Aerobic biodegradation
 - BOWIN1 (Linear Model Prediction) and BOWIN2 (Non-linear Model Prediction) – predicts whether a chemical is expected to biodegrade quickly.
 - BOWIN3 (Ultimate Survey Model) and BOWIN4 (Primary Survey Model) – estimates the time required for a chemical to undergo ultimate and primary degradation.
 - BOWIN5 (MITI Linear Prediction) and BOWIN6 (MITI Non-linear prediction) – predicts whether a chemical would pass an OECD 301C test and be readily biodegradable.
 - BOWIN 7 Model: Anaerobic biodegradation – predicts whether degradation of a chemical will be fast or slow.

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Summary

- EPA welcomes guideline and non-guideline biodegradation data on fragrances and other substances.
- NCD Fate assessors utilize quality measured biodegradation data on the new chemical substance or analogue(s) in our assessment of Persistence.
- EPA utilizes EPISuite™ to characterize ready biodegradation in the absence of data.

Looking Forward

- EPA is looking forward to continuing collaboration with:
 - Research Institute of Fragrance Materials (RIFM)
 - RIFM has initiated talks with EPA and has offered to provide data sets on fragrances.
 - EPA would like to increase our training set for BLOWIN5-6 using RIFMs OECD 301C data set.
 - EPA would like to create new models in EPISuite™ to consider RIFMs OECD 301F and/or OECD 301B data set.
 - Office of Research and Development (ORD)
 - New Chemical Collaborative Research Program (NCCRP).
 - ORD has partnered with NCD to help refine our processes and update our models.

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Challenges

- All the 38 fragrances had quality measured biodegradation data.
 - However, NCD sometimes finds:
 - Limited biodegradation data on the new chemical substance and analogues.
 - Increases the reliance on models
 - Poor quality biodegradation data
 - Results in rejection of the data
 - Limits the ability to use data in the assessment
- BOWIN5-6 Models use training sets of OECD 301C data.
 - No other guidelines are used.
 - Unclear if there are other guidelines that are better suited for fragrances.

Questions



Thank You!

Contact me:
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Appendix

PBT Scoring

- Identify the persistence and bioaccumulation potential:

	Limited Persistence (P1)	Persistent (P2)	Very Persistent (P3)	
Persistence	< 2 months	2 to 6 months	≥ 6 months	Half-life
	Low (B1)	Moderate (B2)	High (B3)	
Bioaccumulation potential	< 1000	1000 to 5000	≥ 5000	BCF and/or BAF