

Building Knowledge from Available Degradation Simulation Studies to Improve Use in Regulatory Persistence Assessments

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Camenzuli L, Earl M, Endersby K, Gibson R, Golombek P, Hafner J, Helbling D, Hughes CB, Lapczynski A, Peter S, Saunders D, Tamasi B, Vitale CM, Wang N, Wilmot L, Leon Paumen M, Lemaire P, Tolls J, Collard M

Scope

The OECD TG 309 is an OECD standard test
with high potential for variability

Inoculum variability

Surface water: river, pond, lake, marine
Geographical location: urban, remote
Amount of organic carbon
Amount of nutrients
Cell concentration/ microbial community

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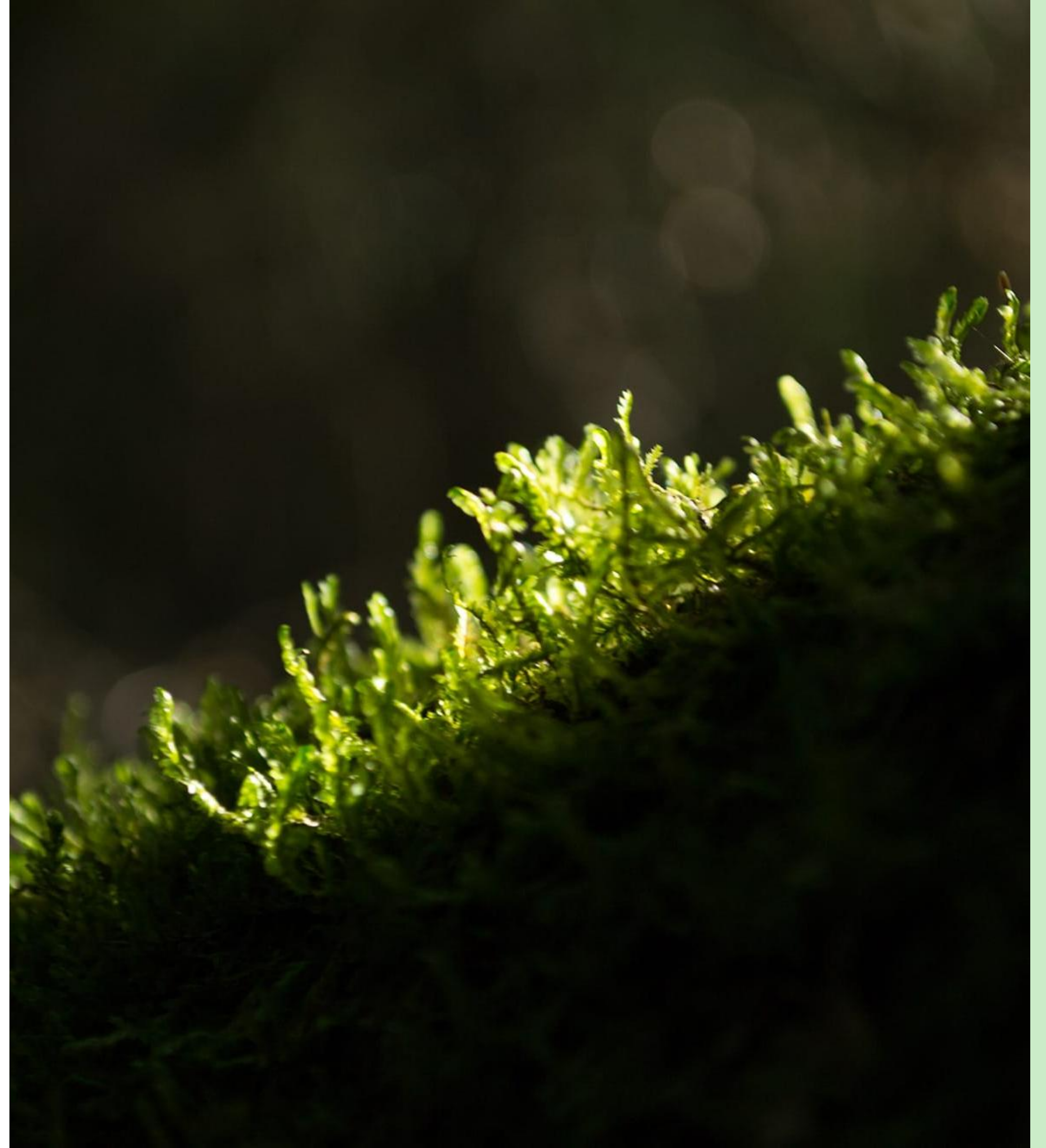
Test set up variability

Test concentration
Test vessel dimensions
Suspended sediment concentration
Open vs closed test set up
Water volume

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**Metadata analysis from studies used for
regulatory compliance**

Data collection.



Data collation from OECD 309

1. Data sources:

- ECHA
- EFSA
- KWR published studies
- Unpublished studies from company R&D programs

2. Database development

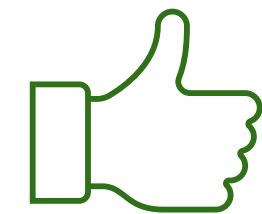
- Relevant parameters extracted based on PAT*
- Biowin fragments (EPISuite)
- Ecosar chemical classes
- enviPath predicted pathways

3. Data curation

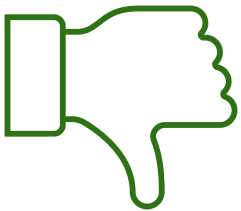
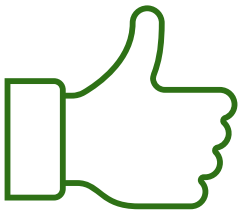
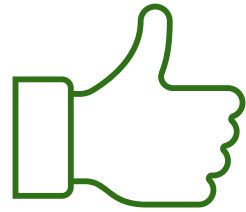
- Manual evaluation
- Confirmation of test material
 - *UVCBs*
 - *Read across*
- Missing Phys-chem data
- Harmonisation of half-life
 - *Definition for “>”*
 - *Removal of entries < 1d*

Available OECD 309 TG studies

	Substances	Data points
REACH	69	140
PPP	77	256
Other	20	31
Total	166	427



Test substance information	range
Water solubility (mg/L)	2.0E-4 – 1.6E+6
Henry's Law constant (Pa.m ₃ /mol)	2.3E-16 – 2.4E+4
Log Kow	-6.4 – 8.4



Test system parameters	range	coverage
Test substance conc (µg/L)	0.005-7400	100%
closed ; open system	36% ; 64%	96%
Information on mass balance		92%
Water temperature at sampling (°C)	3 – 24	69%
Agitated ; stagnant system		69%
Studies with biomass meas.	CFU & other	12%
Inoculum storage before test (days)	0 – 29	35%
Oxygen conc. at test end (mg/L)		26%

Results.

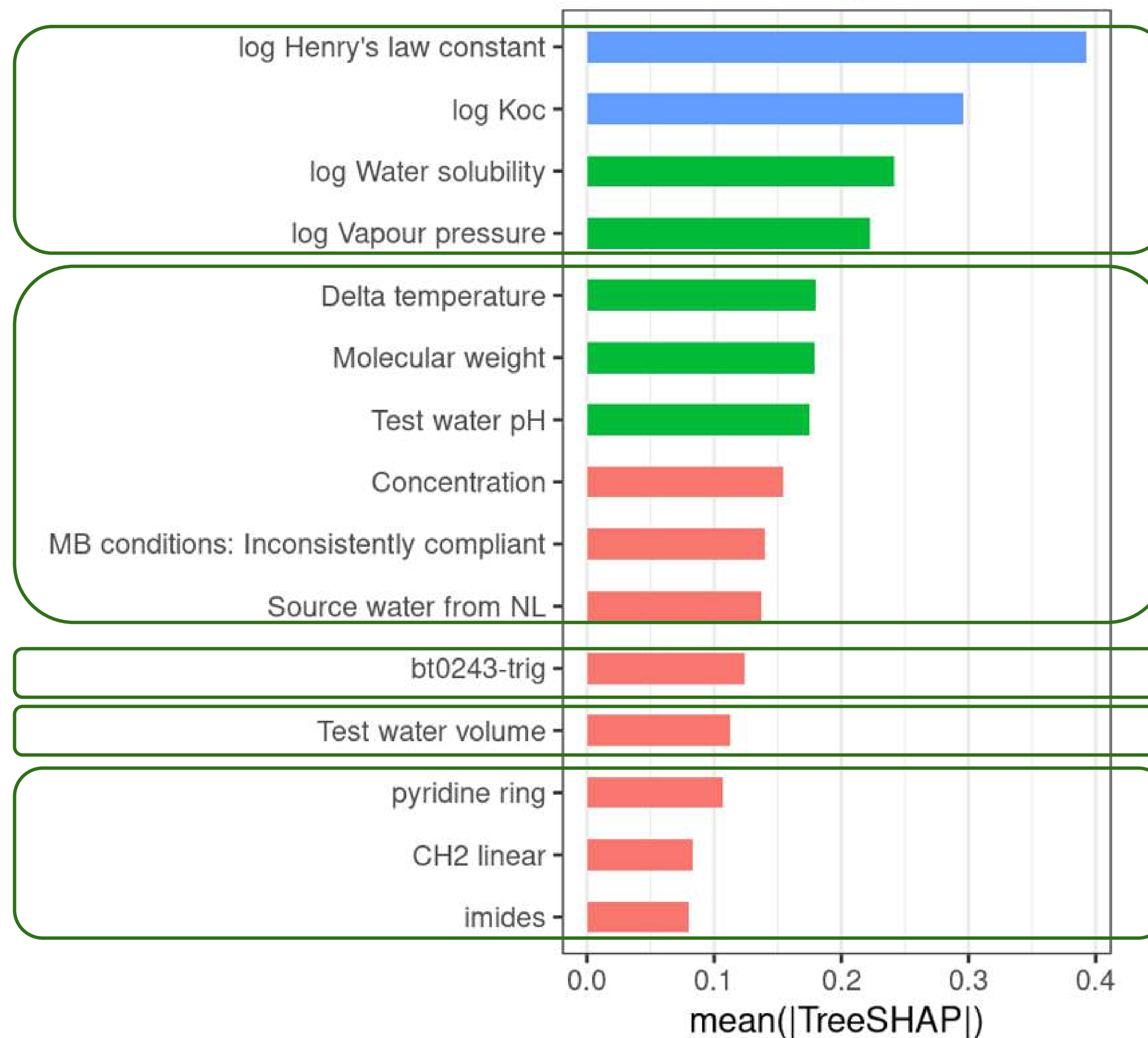


Results

Gradient boosted regression tree analysis

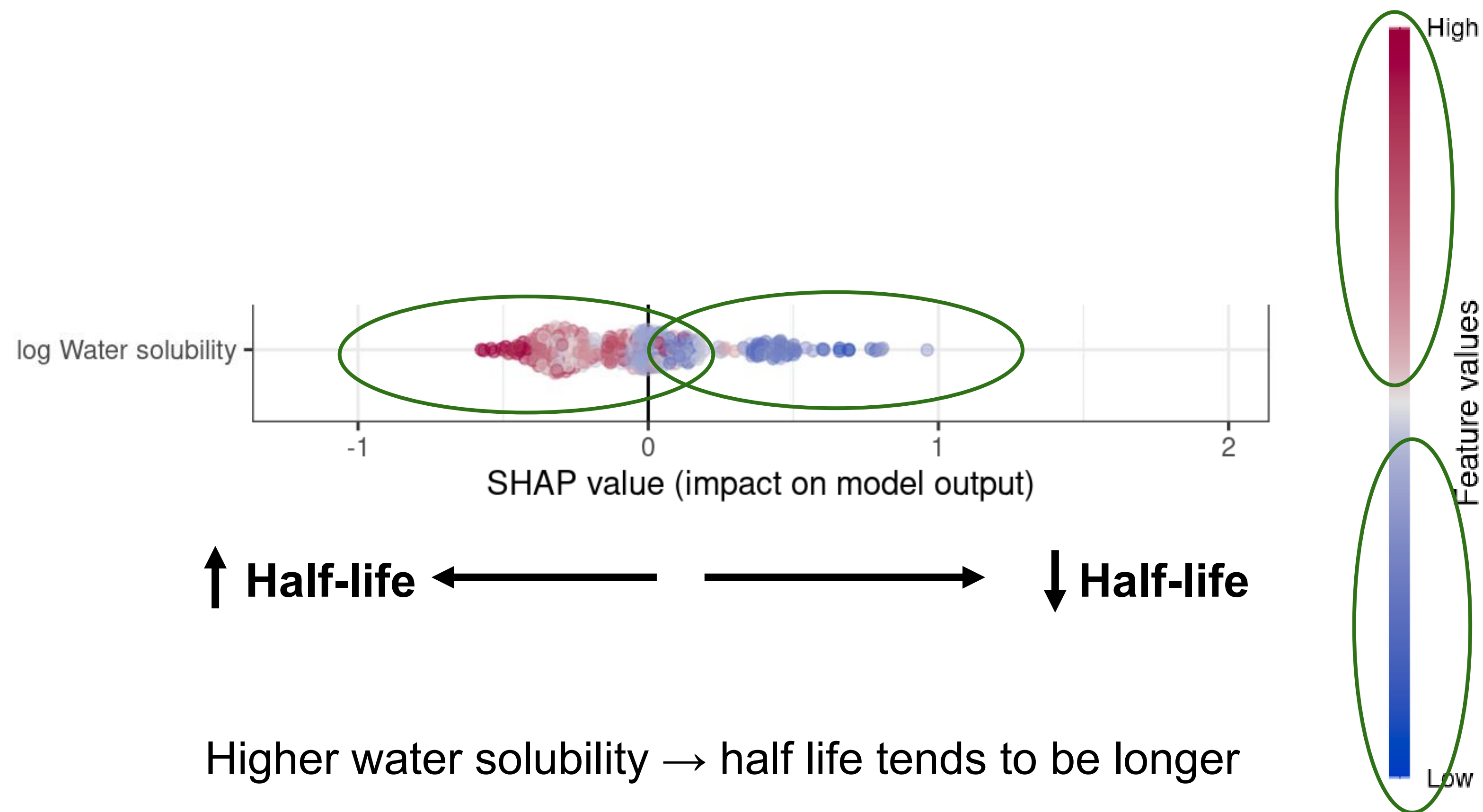
- Tree-based model
- Captures complex interaction
- Ideal to deal with missing values
- Hard to interrogate

SHAP summary



Results:

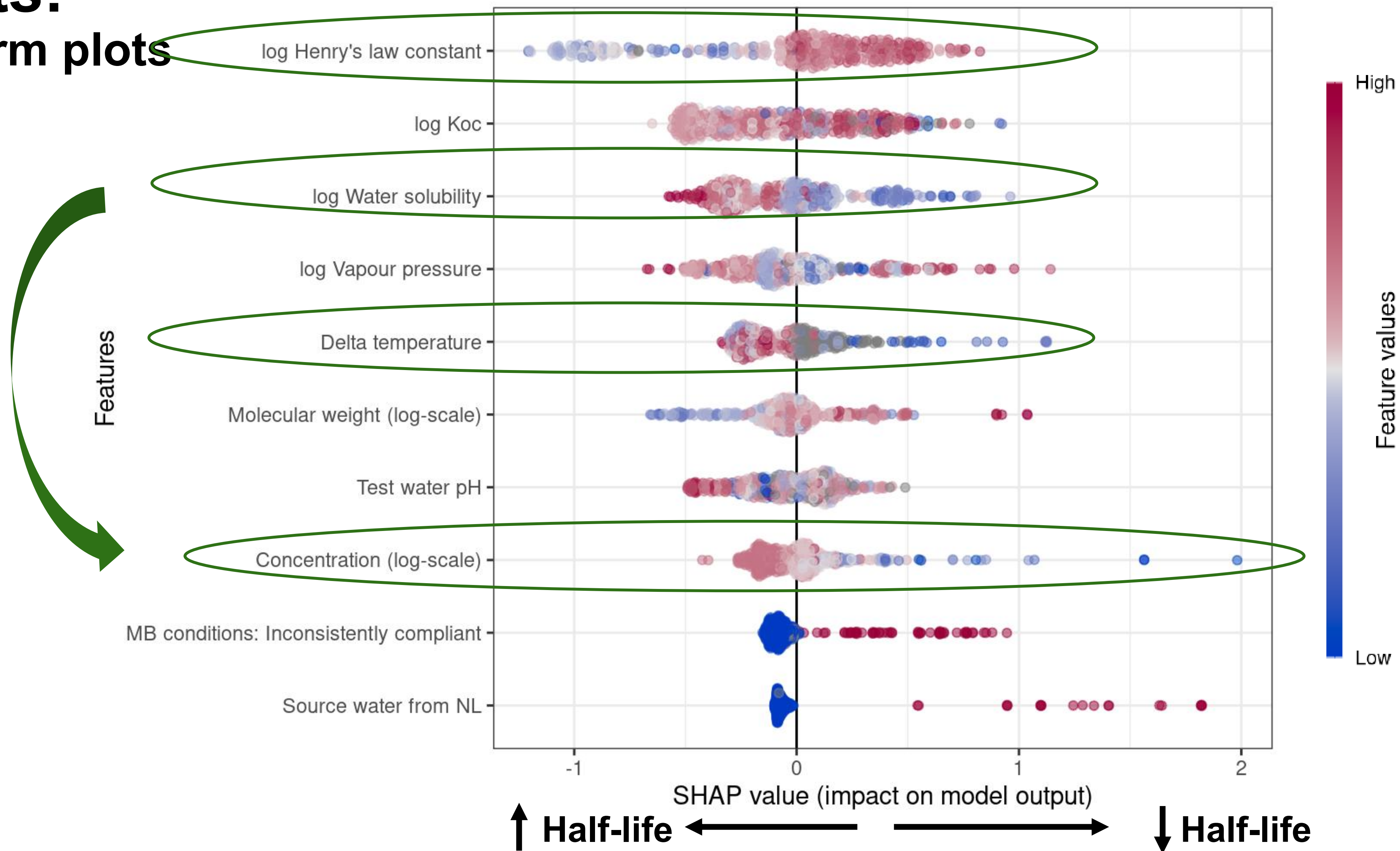
Beeswarm plots



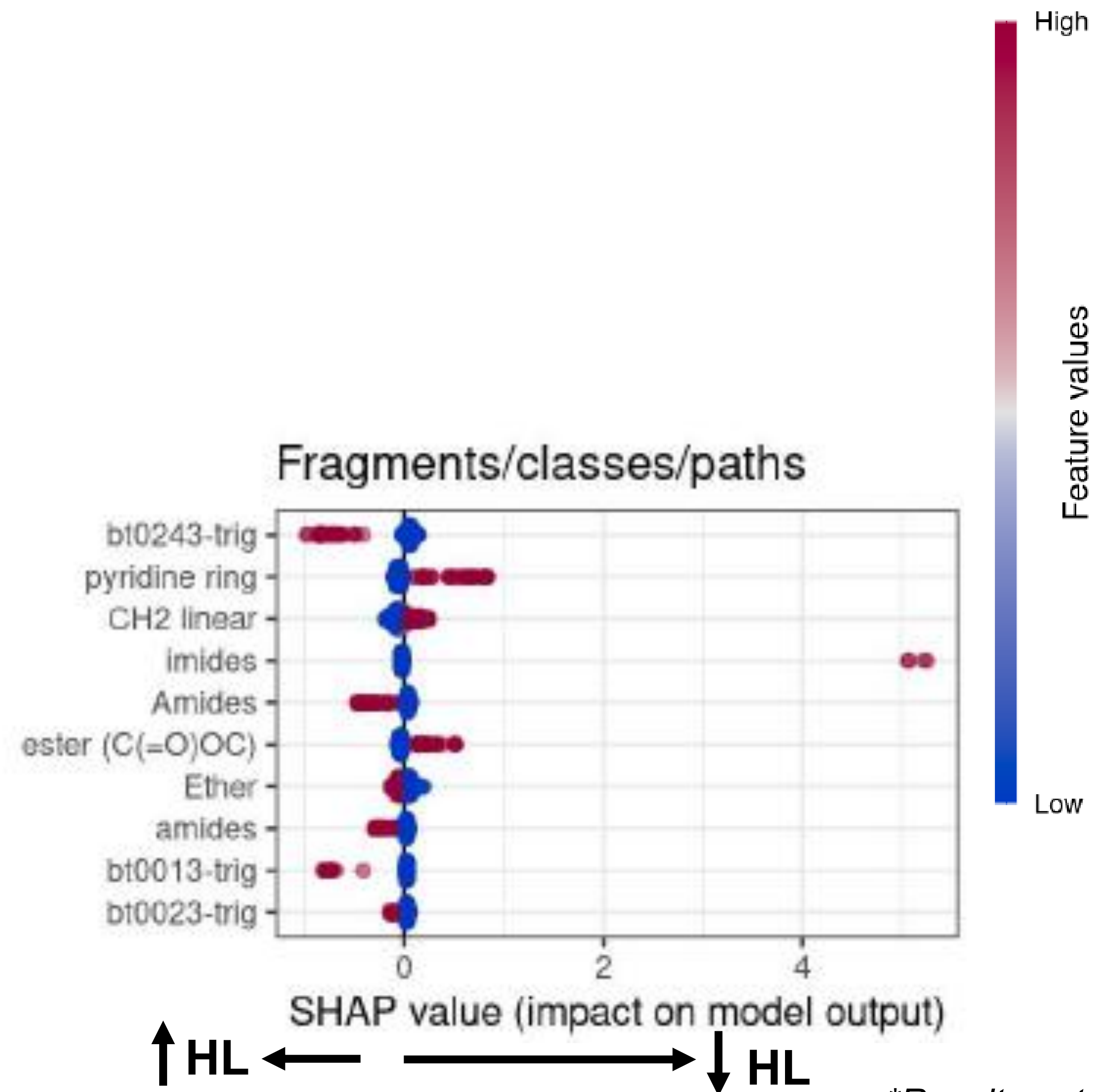
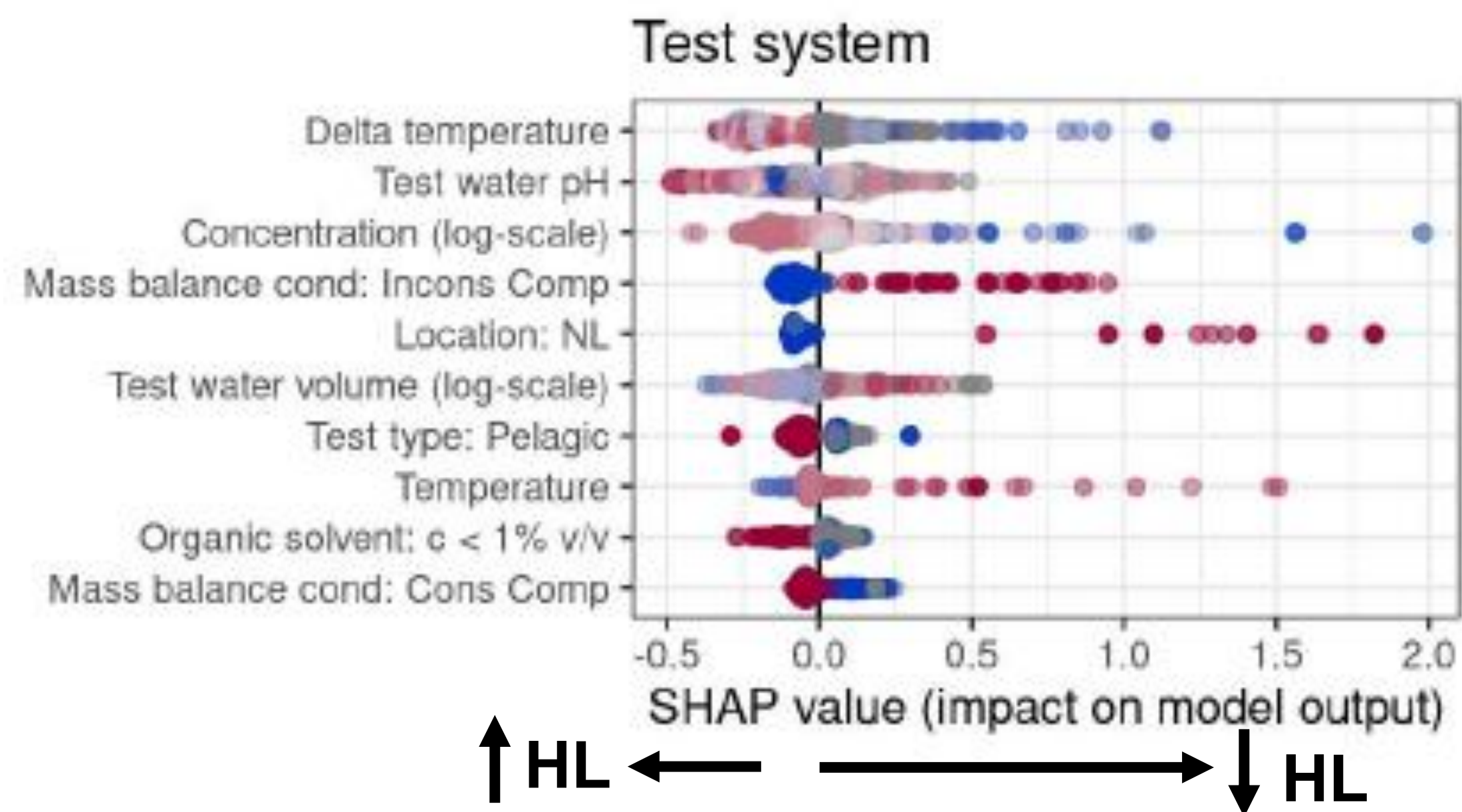
Higher water solubility → half life tends to be longer

Lower water solubility → half life tends to be shorter

Results: Beeswarm plots



Results: Beeswarm plots



**Results not yet finalised*

Results

Can the OECD 309
ever be considered
a standard test?

Metadata analysis confirms **high variability**

- Test system and physico-chemical parameters **influential predictors of HL**
 - Impact should be understood to be minimised
 - Potential other factors not tested here
- Fragments, chemical classes and degradation pathways seem generally **less relevant**
 - **Biodegradation HL should mostly be dependent on the test chemical**

So what?



So what?

Building knowledge from available degradation simulation studies to improve use in regulatory persistence assessments

How can this information help to improve regulatory persistence assessment and exposure / risk assessment?

Recognising that the outcome of simulation testing is not standardized as the test guidance allows for too many variables that potentially influence the outcome of the test

How should the potential influential factors be considered when assessing the results of this test?



Thank you.