

# **REACH Compliance Project “Availability of Health and Environmental Data for High Tonnage Chemicals under REACH” – Data Quality of Environmental Endpoints in Registrations**

Angelika Oertel, Jakob Menz, Anika Brüning, Agnes Schulte



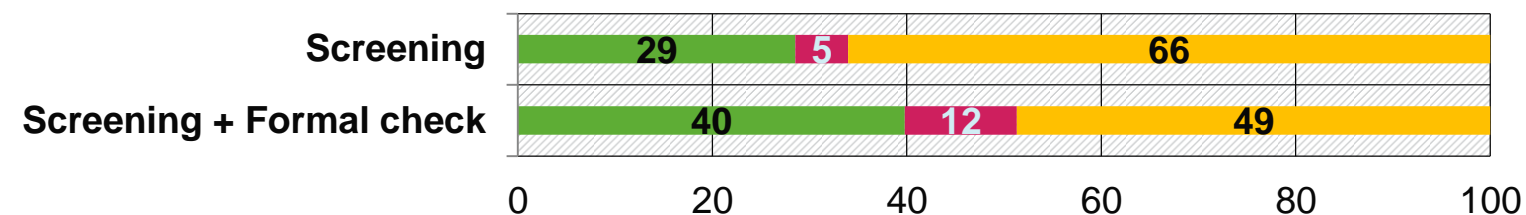
# Results

# Environmental Endpoints

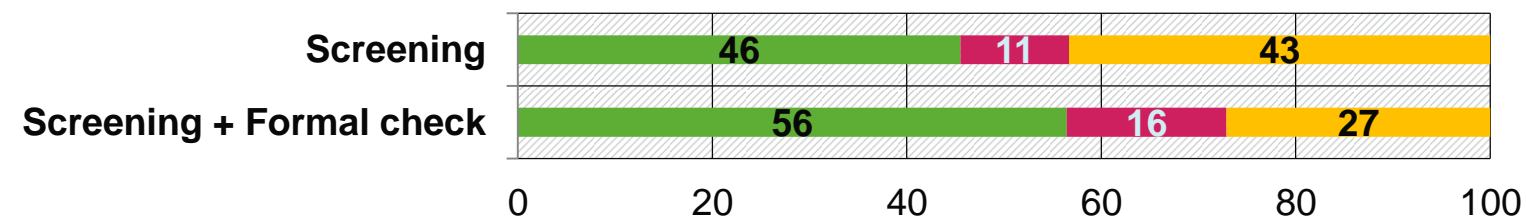
# Environmental endpoints – Results after screening, formal and refined check

≥1000 tpa

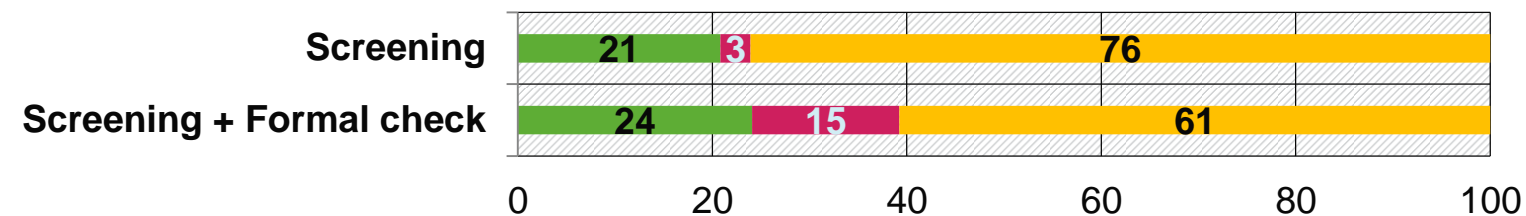
## Abiotic degradation



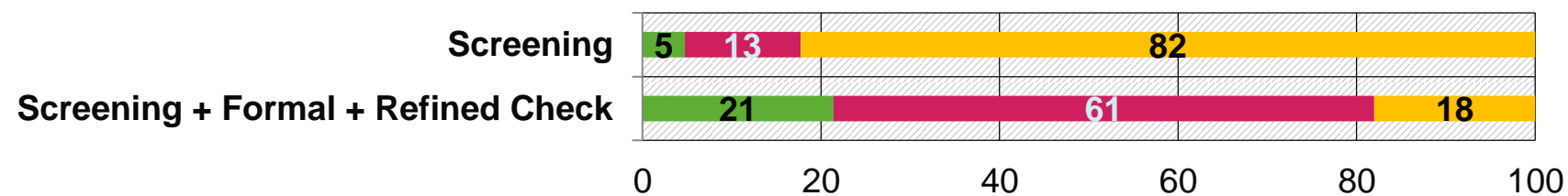
## Biotic degradation



## Bioaccumulation



## Ecotoxicity



■ "compliant" ■ "non-compliant" ■ "complex"

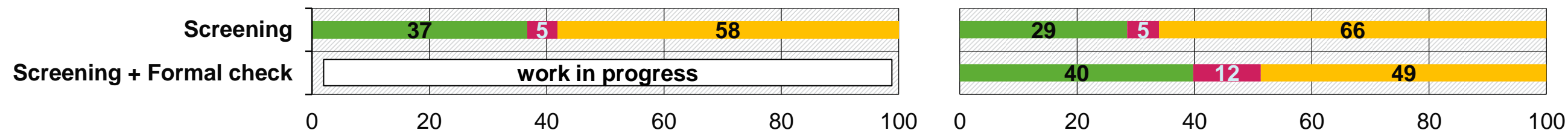
Percentage share [%]

# Environmental endpoints – Results after screening, formal and refined check

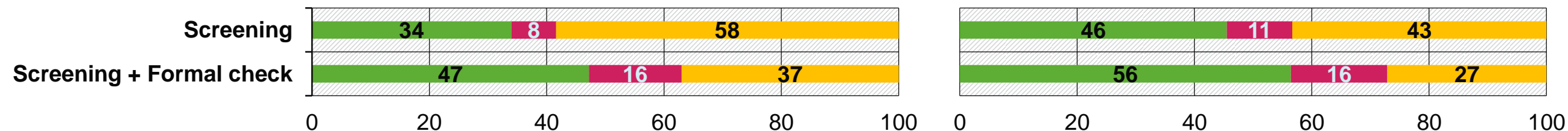
## 100-1000 tpa

## ≥1000 tpa

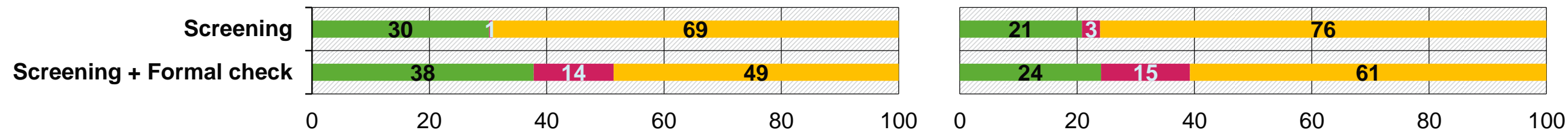
### Abiotic degradation



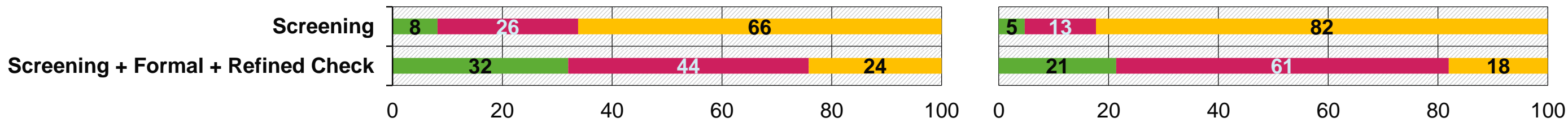
### Biotic degradation



### Bioaccumulation



### Ecotoxicity



Percentage share [%]

Percentage share [%]

■ "compliant" ■ "non-compliant" ■ "complex"

# Screening – Biotic degradation

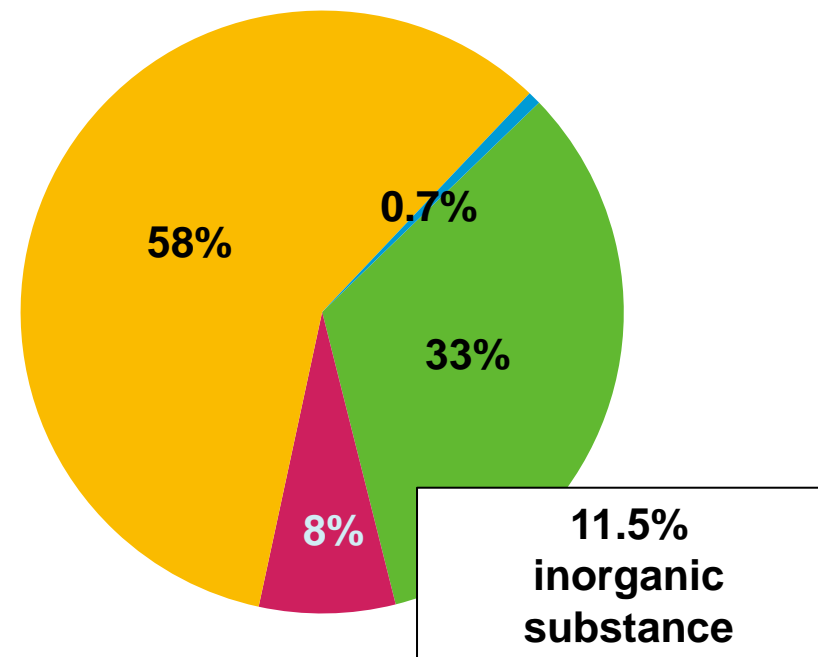
## Main assessment criteria

- Ready biodegradability (OECD TG 301; 310)
- Simulation testing in surface water (OECD TG 309) or in sediment/soil (OECD TG 308, 307)
- Waiving referring to Annex VII, column 2 (no test for inorganic substances)

## 100-1000 tpa

- Waiving/adaptation (69%)
- Less inorganic substances (11.5%)
  - Lower percentage of “compliant” decisions

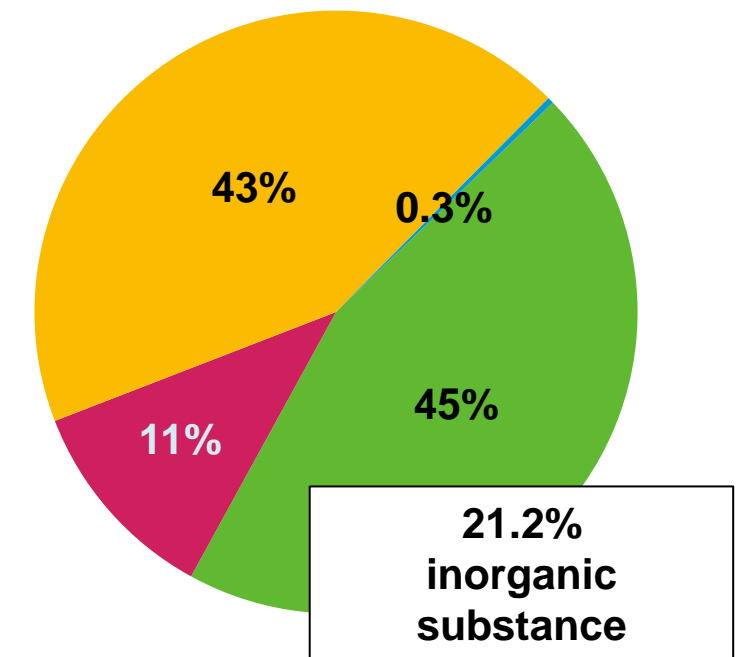
100-1000 tpa



N= 2053

■ "compliant"   
 ■ "non-compliant"   
 ■ "complex"   
 ■ "testing proposal"

≥1000 tpa



N= 1814

# Screening – Bioaccumulation

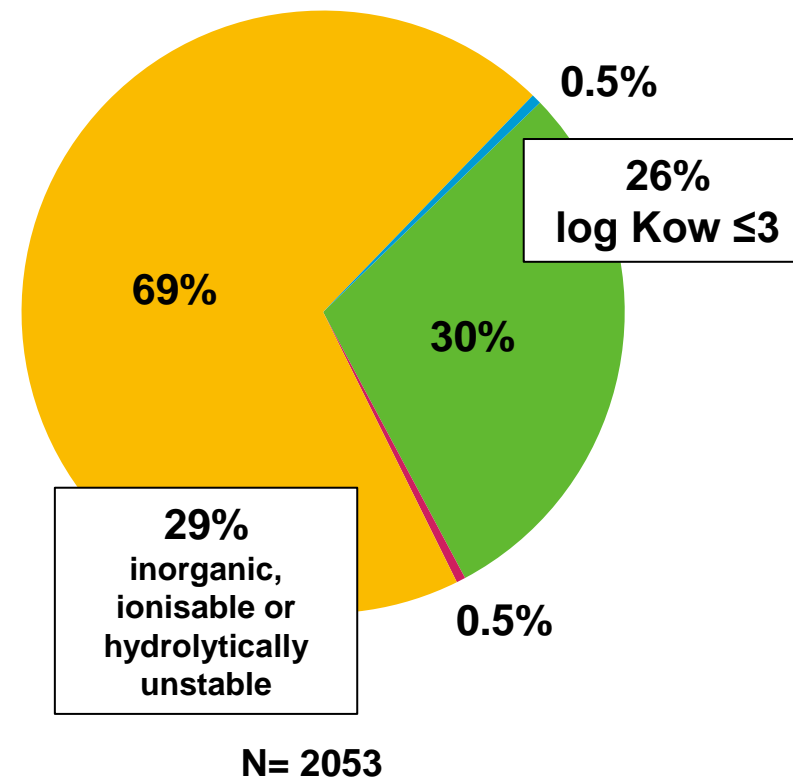
## Main assessment criteria

- Bioaccumulation study (OECD TG 305)
- Waiving referring to Annex IX, column 2 (log Kow ≤ 3)

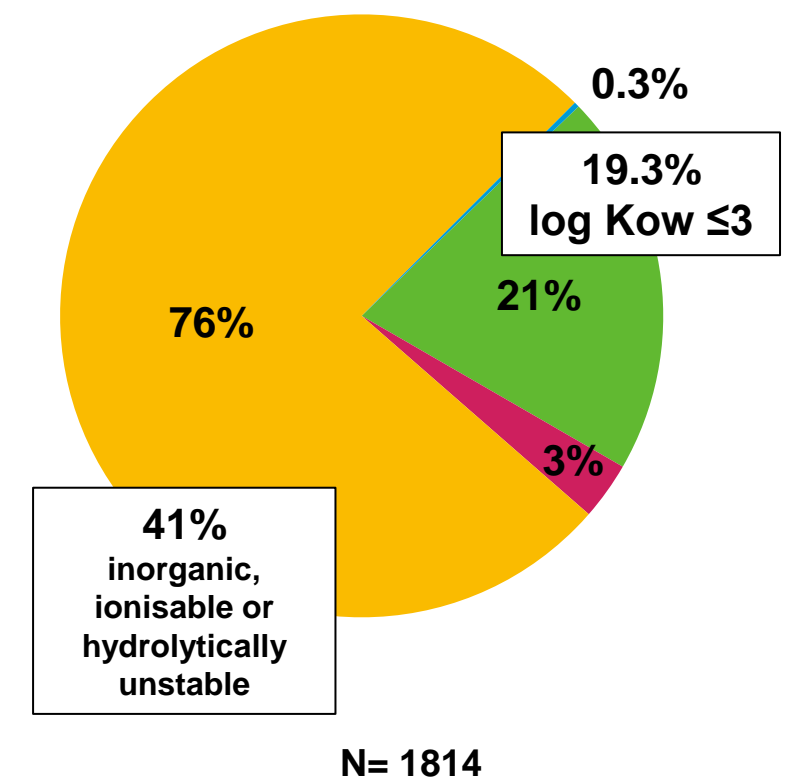
## 100-1000 tpa

- Less dossiers on inorganic, ionisable or hydrolytically unstable substances (29%)
  - lower percentage of “complex” endpoint decisions
- Waiving/adaptation
  - Majority of registrants used alternative methods to avoid animal testing

100-1000 tpa



≥1000 tpa



■ "compliant"   ■ "non-compliant"   ■ "complex"   ■ "testing proposal"

# Environmental exposure assessment: Screening

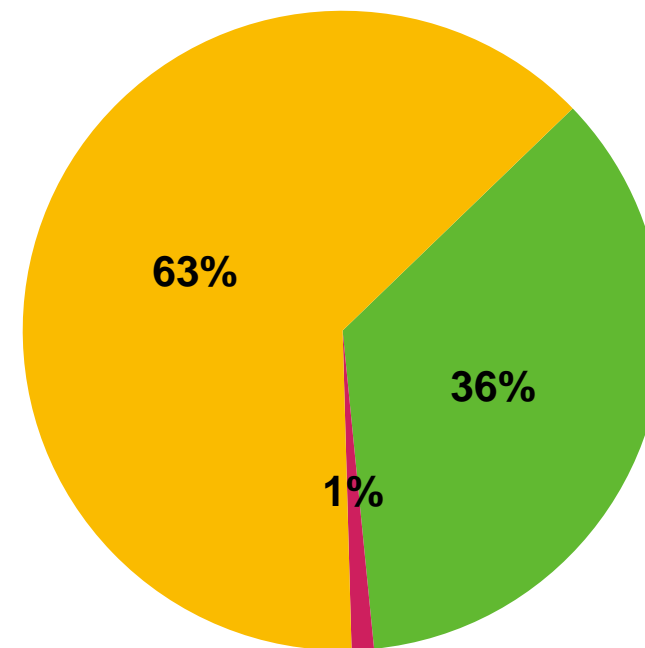
## Main assessment criteria

- Harmonised and/or self-classification
- Availability of environmental exposure scenarios for substances classified or PBT/vPvB (Art. 14(4) REACH)

## 100-1000 tpa

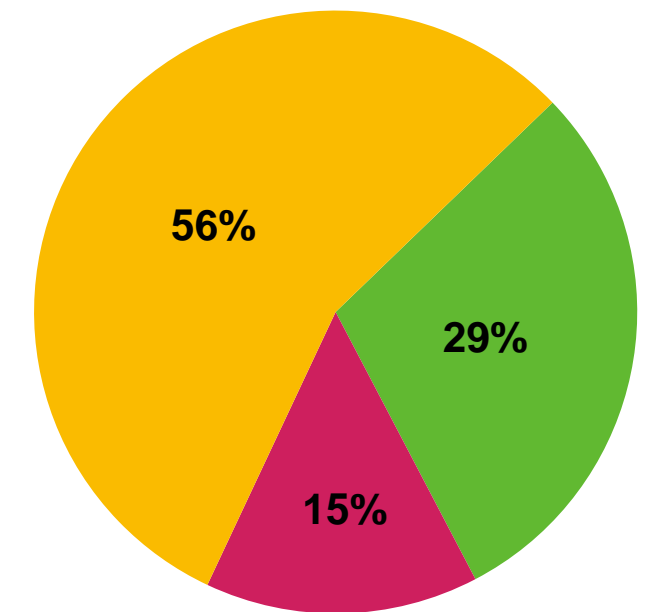
- “Compliant” exposure assessment not required
- “Non-compliant” classification-related exposure assessment missing
- “Complex” Available exposure scenarios need refined check

100- 1000 tpa



N= 2053

≥1000 tpa

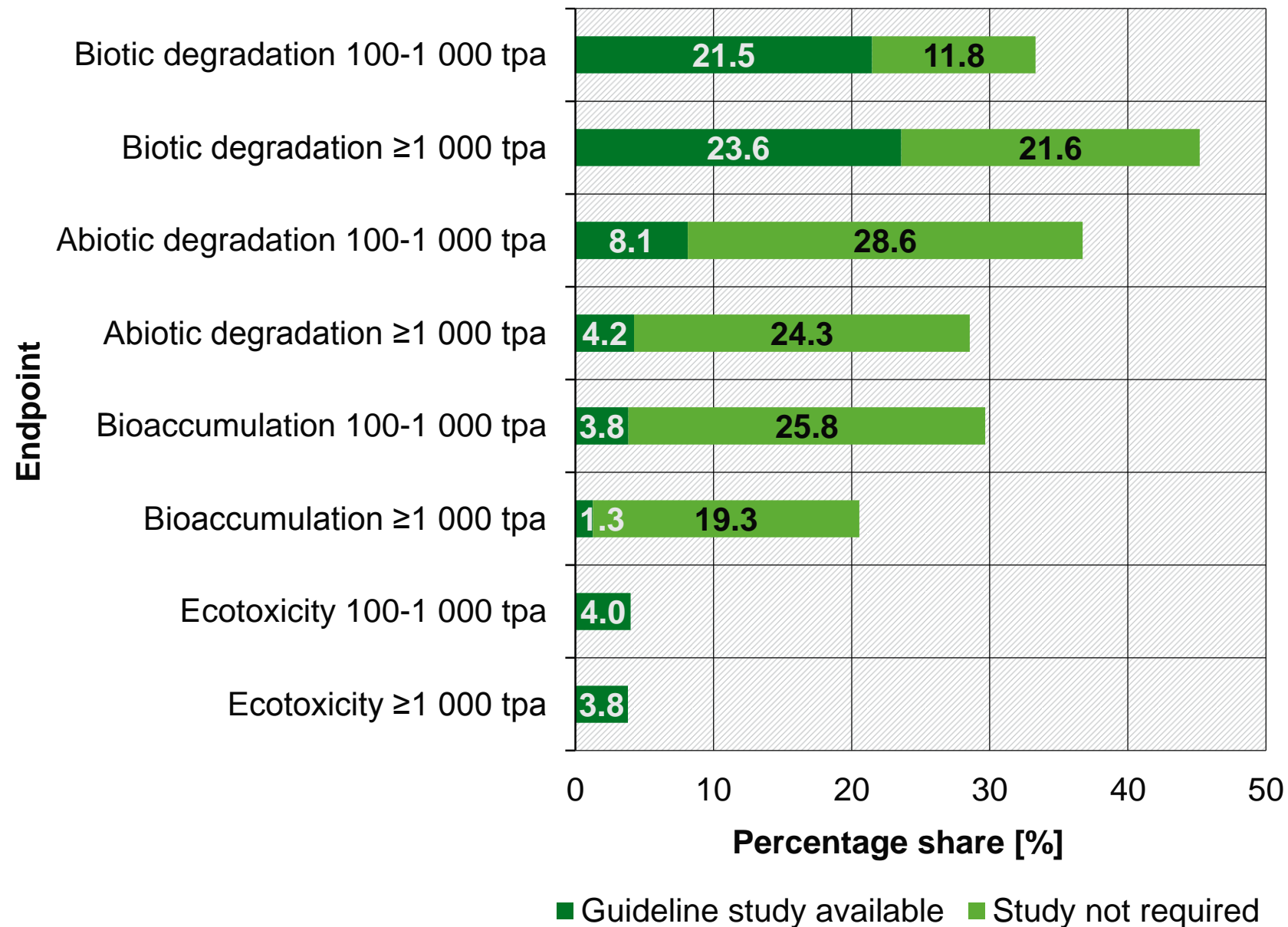


N= 1814

■ "compliant" ■ "non-compliant" ■ "complex"



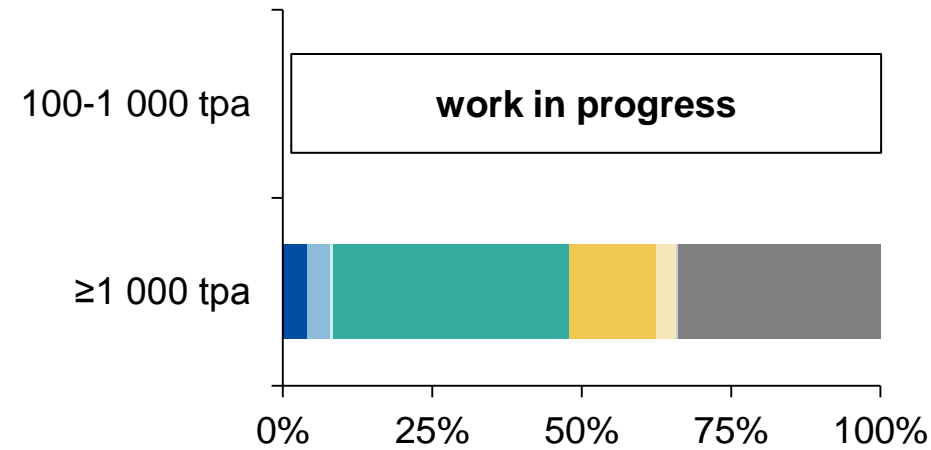
# “Compliant” decisions after screening



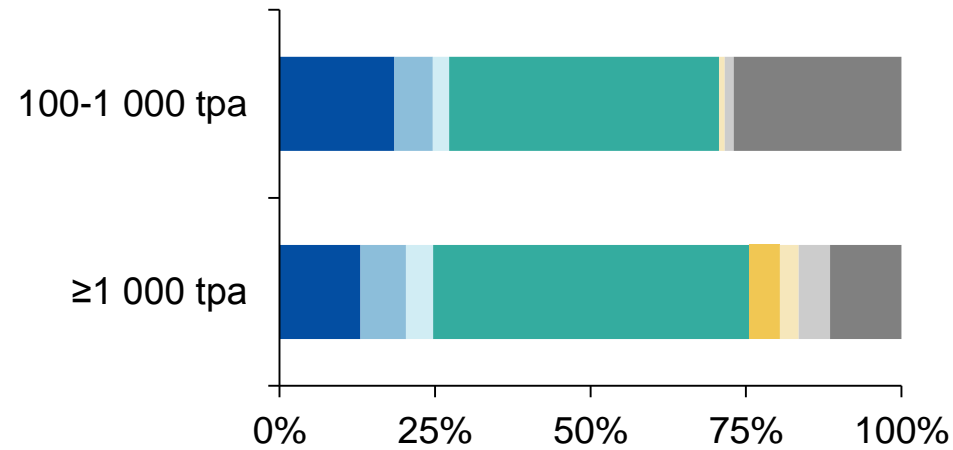
- Between **1.3 and 23.6% “compliant” by providing guideline studies**
- **Biodegradation:** “compliant” by providing guideline studies, either by
  - 21-23% readily biodegradable in TG 301 or
  - 0.5% studies for simulation testing
- **Abiotic Degradation / Bioaccumulation:**
  - mainly “compliant” because a study was not required (column 2)
- **Ecotoxicity:**
  - 4% “compliant” by providing guideline studies on chronic testing
- **Bioaccumulation/ Ecotoxicity: Animal testing**

# Frequency of documented data waiving/adaptation categories

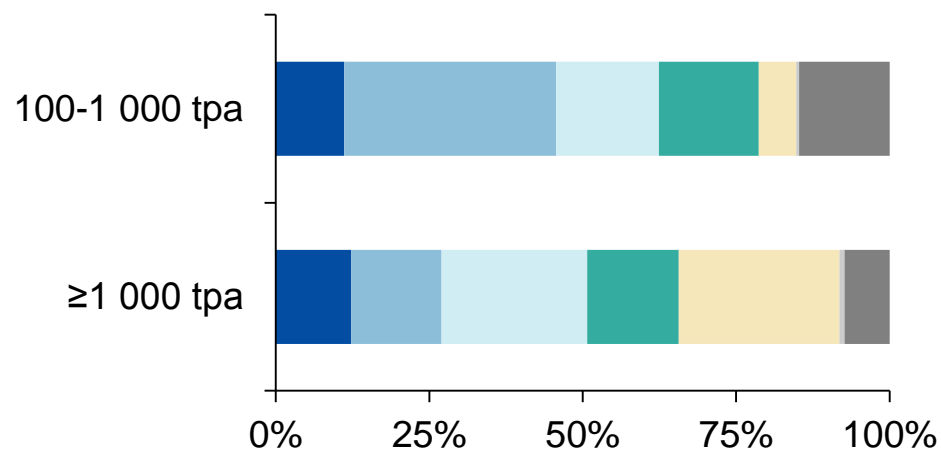
## Abiotic degradation



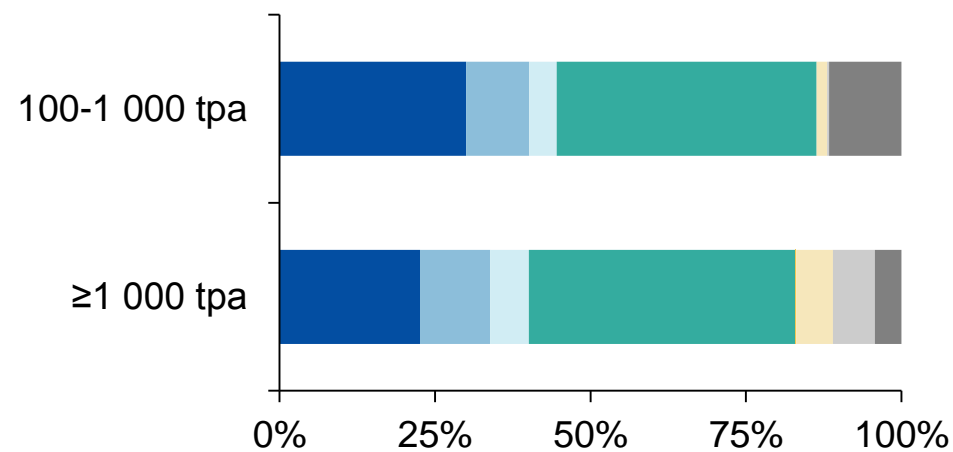
## Biotic degradation



## Bioaccumulation



## Ecotoxicity

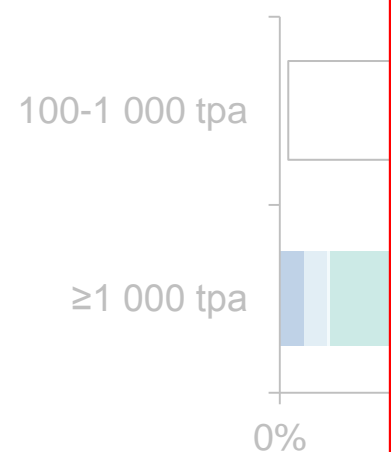


## Waiving/adaptation category

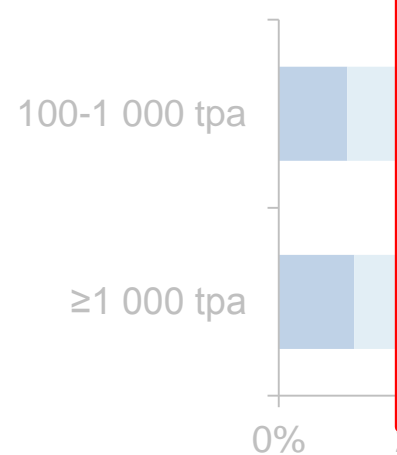
- Read Across
- Weight of Evidence
- Qualitative and Quantitative structure-activity relationship ((Q)SAR)
- Endpoint specific, column 2
- Scientifically unjustified
- Technically not possible
- Exposure-driven testing
- Other cases

## Frequency of documented data waiving/adaptation categories,

### Abiotic degradation



### Bioaccumulation



Data waiving/adaptation used in ca. **65-93%** of dossiers (depending on endpoint and tonnage band)

### Main categories used for data waiving/adaptation

1. Endpoint specific, Column 2
2. Read Across
3. Weight of Evidence
4. QSAR
5. Other cases (e.g. no reference to REACH Annexes VII-XI)

→ Only minor differences between tonnage bands

adaptation category

across

t of Evidence

ative and  
itative structure-  
/ relationship

oint specific, column 2

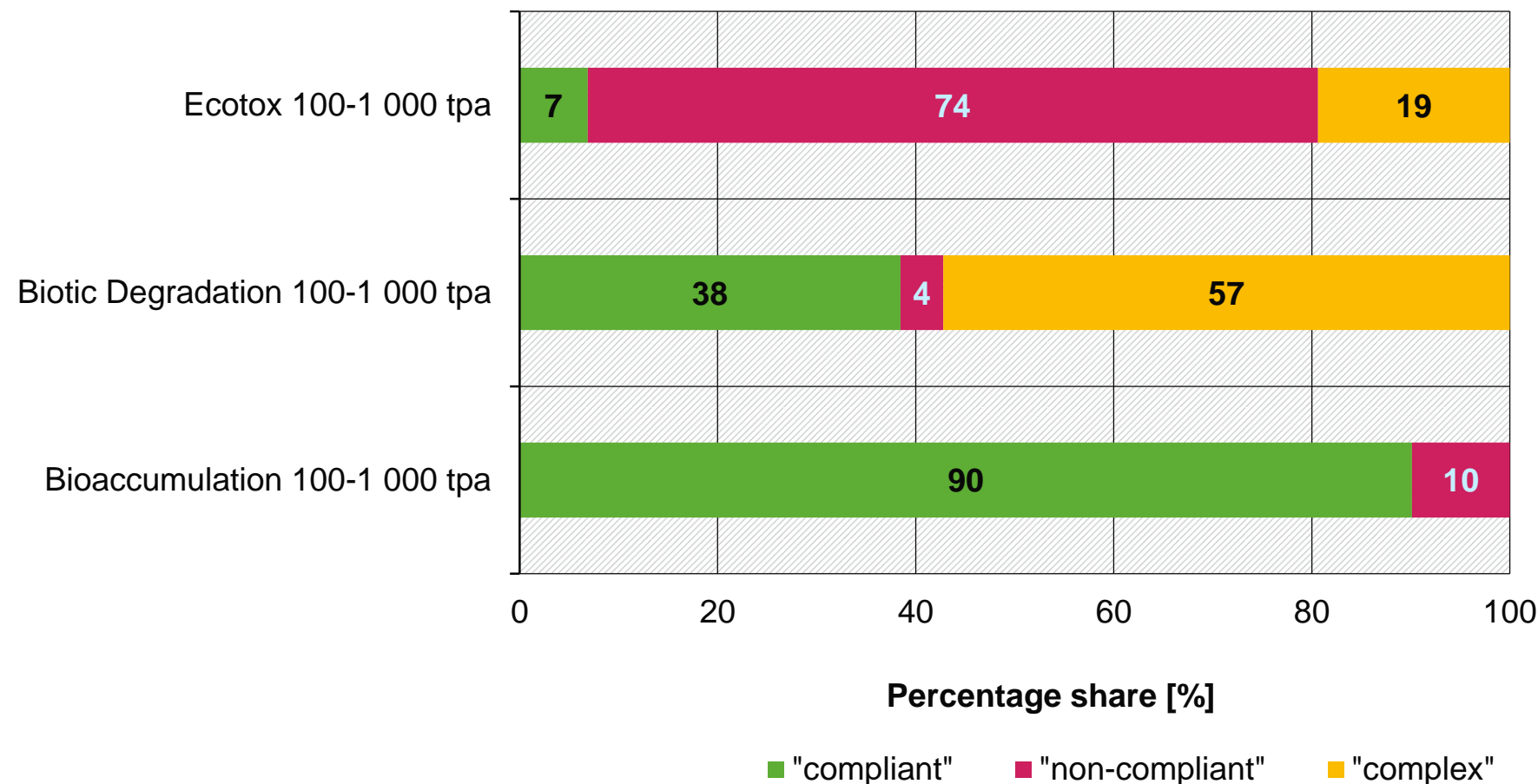
ificantly unjustified

cally not possible

ure-driven testing

Other cases

## Screening/Formal Check – Endpoint-specific waiving (Column 2)



### Main assessment criteria

- Endpoint specific rules, e.g.
  - Inorganic substance (BioDeg)
  - Direct or indirect exposure unlikely (BioDeg, Bioaccu)
  - Chemical safety assessment (BioDeg, Ecotox)
  - Log Kow (Bioaccumulation)
  - Water solubility (Ecotox, BioDeg)

### Annex VII-X, Column 2 – Specific rules for adaptation

→ Bioaccumulation mainly “compliant” because of  $\text{Log Kow} \leq 3$

→ Biotic Degradation mainly “complex” because of reference to chemical safety assessment

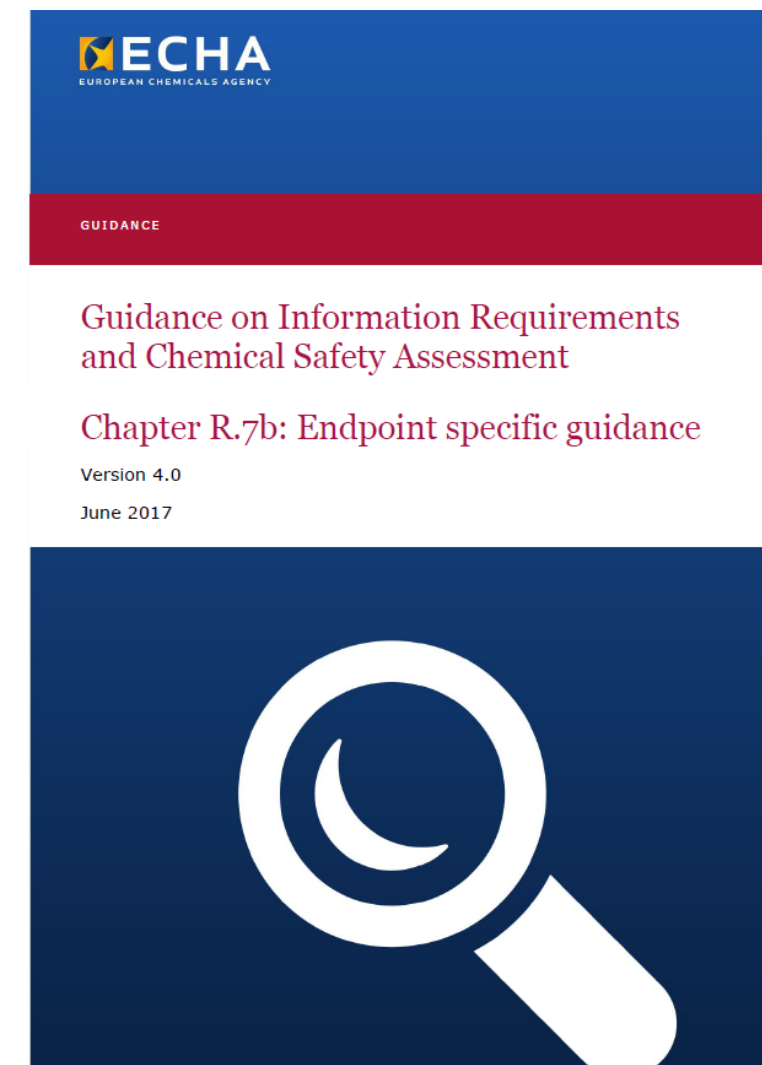
## Screening/Formal Check – Endpoint-specific waiving (Column 2)

### Reasons for non-compliance

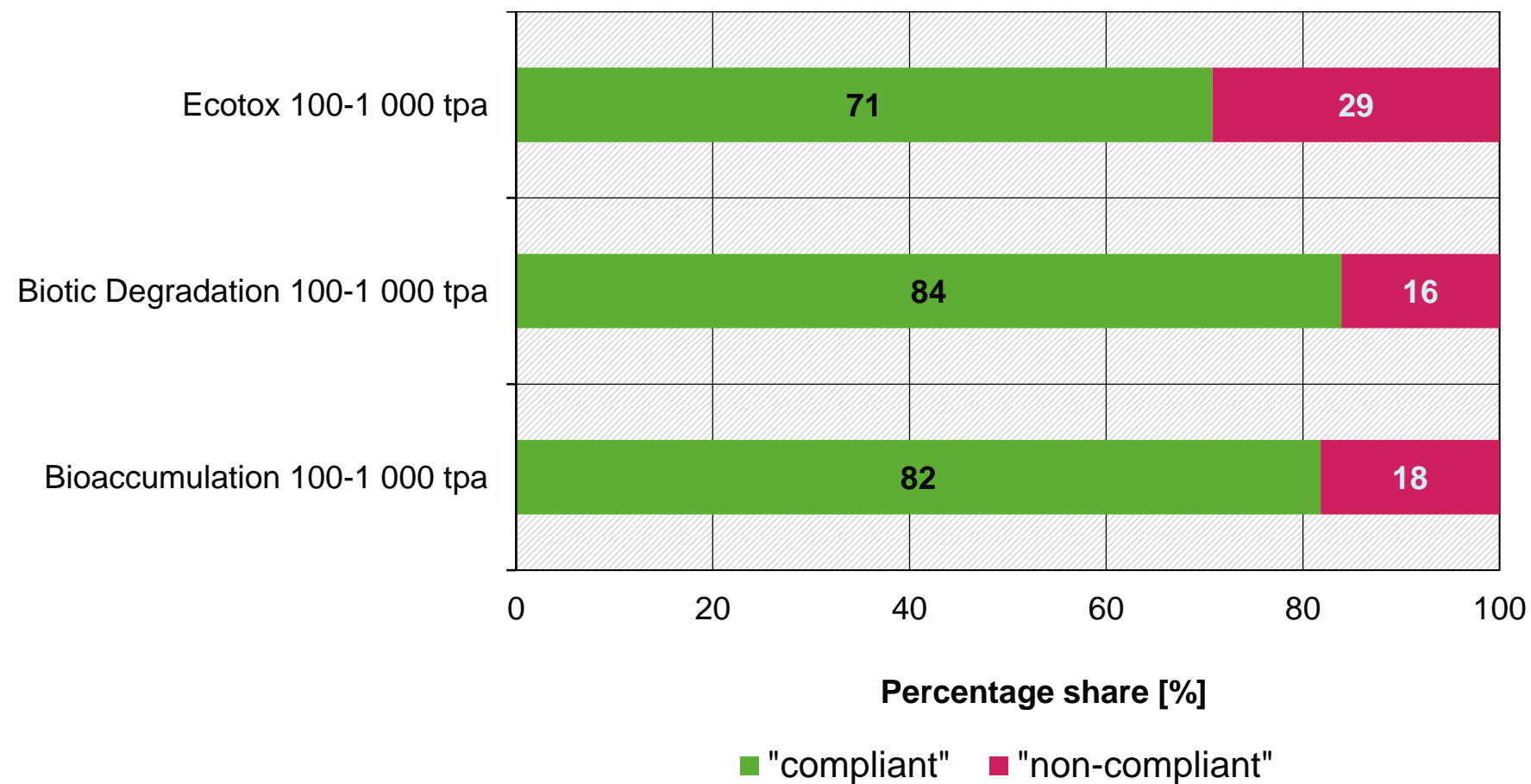
- Specific rules of REACH Annex VII to X column 2 were not met
  - Required information to justify the column 2 rules were either not provided or not adequately documented
  - Exposure assessment not available although required

### Recommendations

- Justification should meet specific rules of REACH Annex VII to X column 2
- Relevant information required to justify rules of column 2 should be available and adequately documented (e.g. log Kow)
- Exposure assessment should be available to demonstrate that exposure is unlikely



# Formal Check – Read Across



## Main assessment criteria

Is a justification according to Annex XI 1.5, paragraph 2 given? (or other adequate explanation)

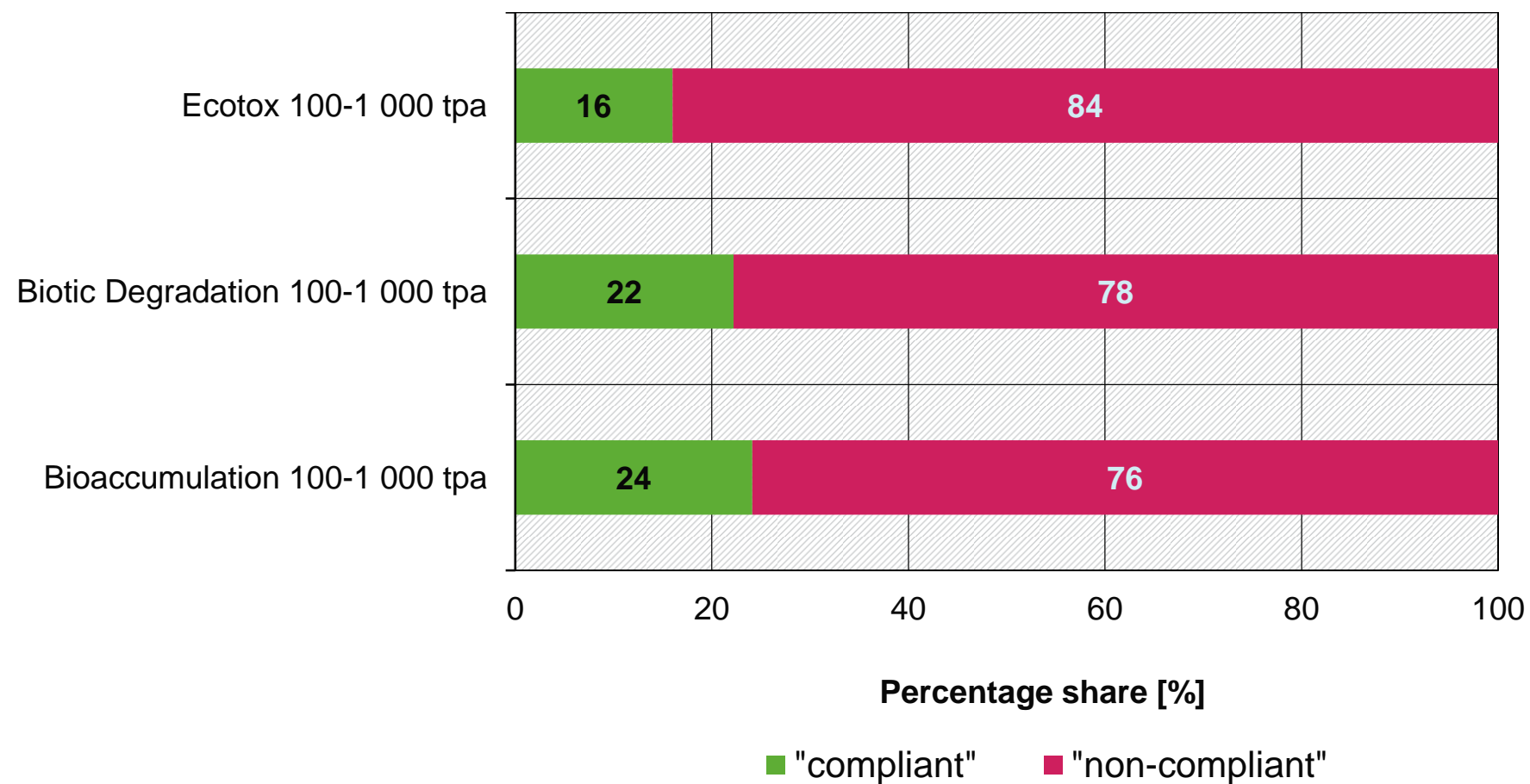
Similarities based on  
(1) functional group or  
(2) precursors, breakdown products or  
(3) constant pattern in the changing of potency

## Annex XI, 1.5 – Grouping of substances and read-across approach

→ 71-84% of evaluated Read Across approaches were formally “compliant”

→ Recommendations for human health endpoints apply here as well

# Formal Check – (Q)SAR



## Main assessment criteria

- (Q)SAR Model Reporting Format (QMRF)
- (Q)SAR Prediction Reporting Format (QPRF)
- Scientific validity
- Applicability domain

## Annex XI, 1.3 – Qualitative or Quantitative structure-activity relationship ((Q)SAR)

→ 76-84% of evaluated (Q)SAR approaches were formally “non-compliant”

## Formal Check – (Q)SAR

### Reasons for “non-compliant”

- QMRF/QPRF (or equal information) is not available
- Scientific validity of the model is not documented
- Evaluation whether substance falls within the applicability domain is missing

### Recommendations

- The study summary for a (Q)SAR prediction should be created exactly according to ECHA’s practical guide
- The QMRF and QPRF should be attached to the study summary
- A (Q)SAR prediction should not be used if the model is not scientifically validated or if the substance does not fall within the applicability domain



## Practical guide

## How to use and report (Q)SARs

[https://echa.europa.eu/documents/10162/13655/pg\\_report\\_qsars\\_en.pdf](https://echa.europa.eu/documents/10162/13655/pg_report_qsars_en.pdf)



# Ecotoxicity – Results after screening, formal and refined check

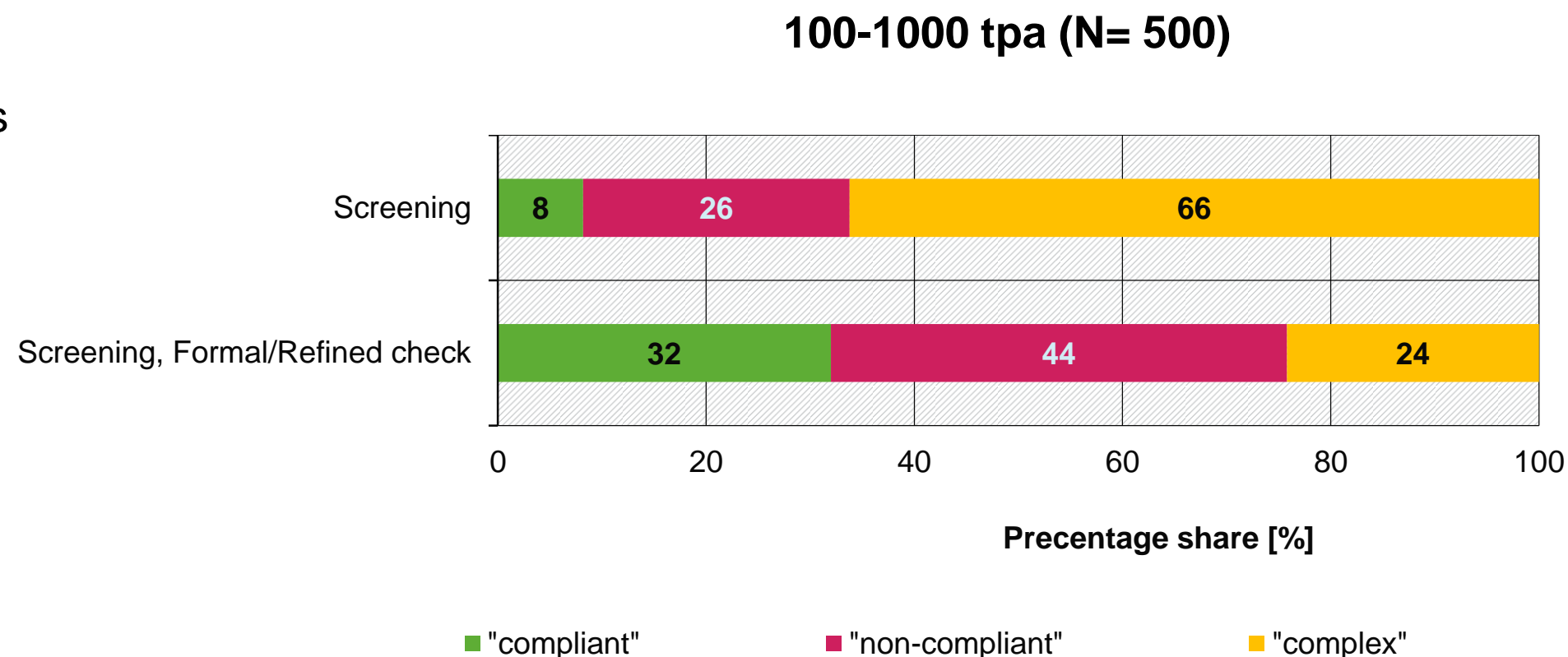
## Main assessment criteria

### Screening

- Long-term tests fish & invertebrates (e.g. OECD TG 210, 211)
- Short-term tests fish & invertebrates (e.g. OECD TG 203, 202)
- Water solubility
- Ratio EC50/LC50

### Refined Check

- Chemical Safety Assessment



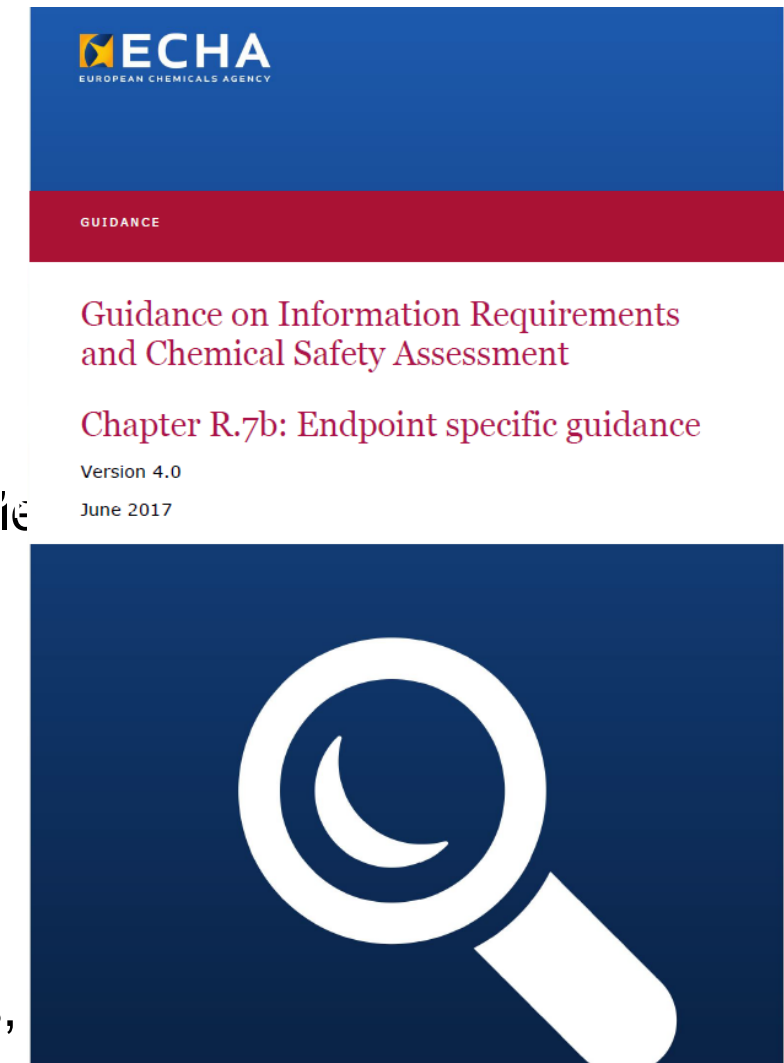
# Refined Check – Ecotox – Column 2

## Reasons for “non-compliant”

- Test method not suitable as a chronic test
- Water solubility <1 mg/L requires chronic testing unless the substance is highly insoluble
- Assessment factor for PNEC derivation not appropriate
- Environmental exposure assessment not performed although required
- Risk is indicated by PEC/PNEC > 1

## Recommendations

- Long-term fish tests (e.g. OECD TG 210) should include sensitive life-stages (juveniles, eggs, and larvae)
- Chronic testing if water solubility <1 mg/L or evidence of highly insolubility
- For derivation of PNECs all available hazard information needs to be evaluated
- Environmental exposure for classified or PBT/vPvB-substances (REACH Art 14(4))
- Risk > 1 should not be indicated



# Conclusions on environmental endpoints

## Overall results on 100-1000 tpa and $\geq 1000$ tpa after screening

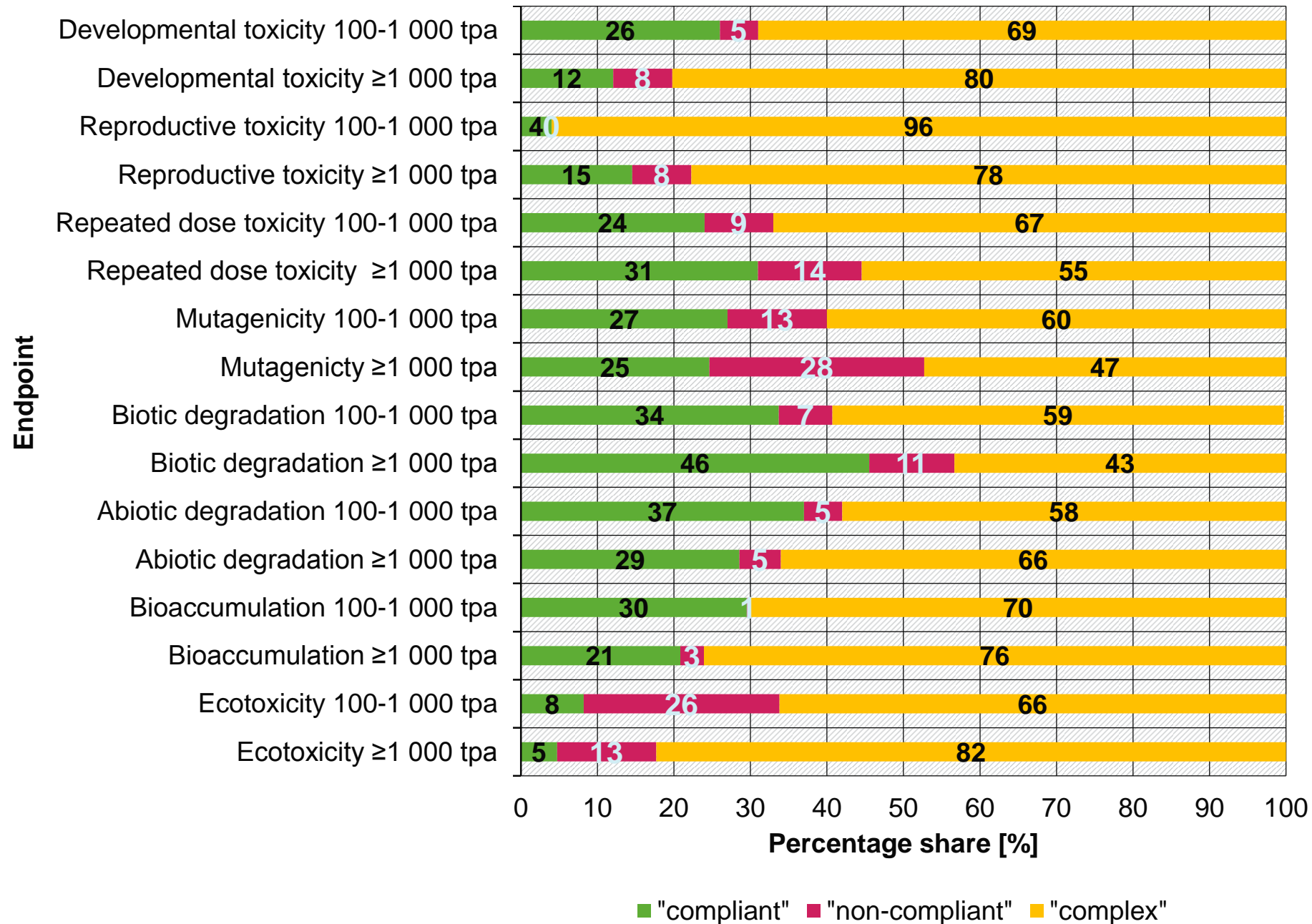
- No general trend on dossier quality
- Intensive use of data waiving / adaptation → **Low availability of guideline studies**
- Endpoint specific waiving (column 2) most frequently used

## After screening and formal check (and refined check for Ecotox)

- $\geq 1000$  tpa: on average 34% compliant ; 31% non compliant (AbioDeg excluded)
- 100 -1000 tpa: on average **39% compliant**; 24% non compliant (AbioDeg excluded)
  - Data quality slightly improved for particular endpoints (Bioaccumulation, Ecotox)
- On average 36% of endpoints remained “complex”
  - Waiving justifications without reference to REACH Annexes VII-XI
  - Waiving justifications with reference to chemical safety assessment

# Overall results and conclusions

# Human health and environmental endpoints – Screening results



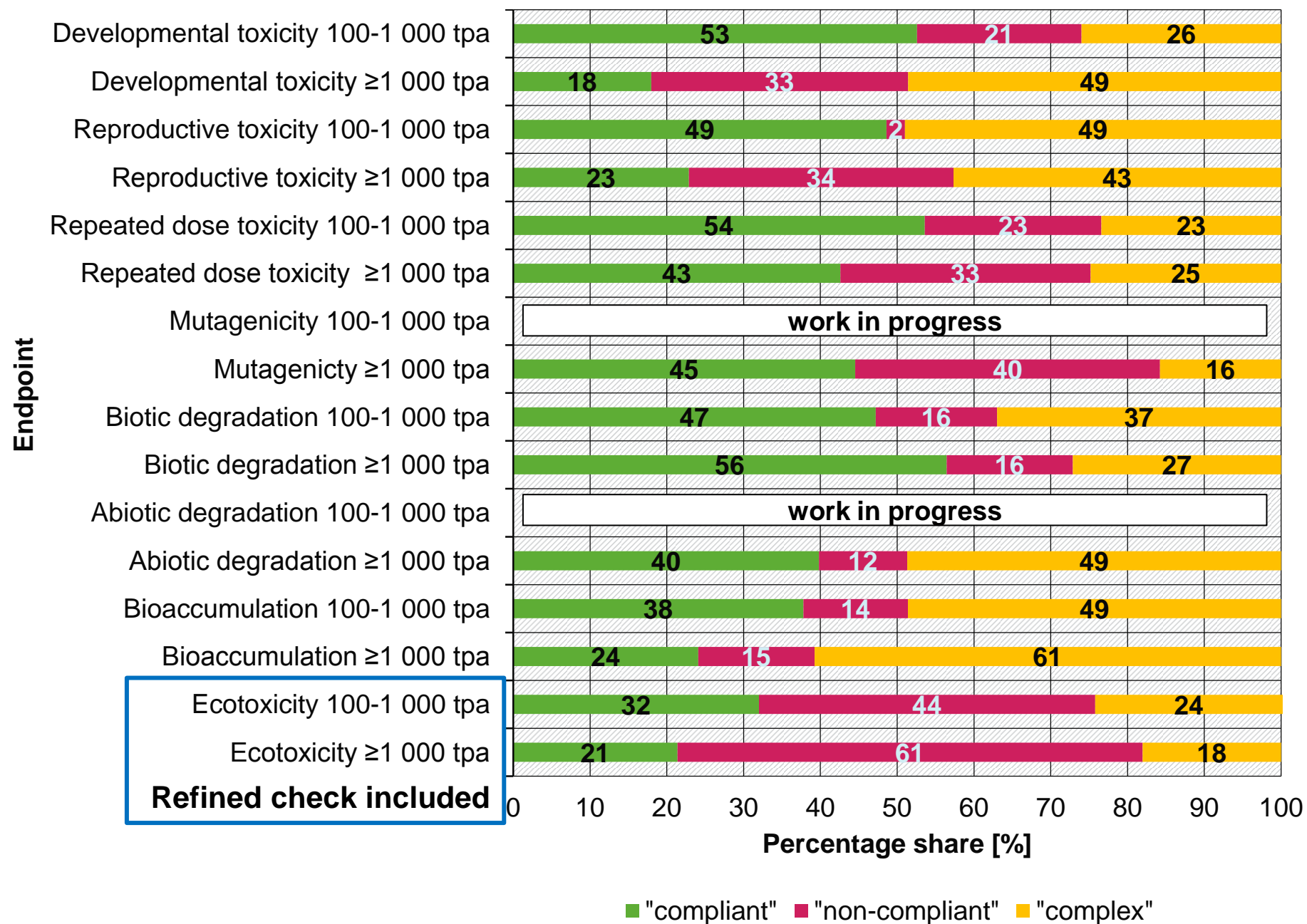
## Results after screening (both tonnage bands)

- 43-96% of dossiers “complex”
- 4-46% of dossiers “compliant”
- 0-28% of dossiers “non-compliant”

→ High rates of “complex” cases

→ **Further evaluation of waiving / adaptation needed to increase decision rates**

# Human health and environmental endpoints – Results after screening and formal check



## Results after screening and formal check (both tonnage bands)

- 16-61% of dossiers “complex”
- 18-56% “compliant”
- 2-61% “non-compliant”

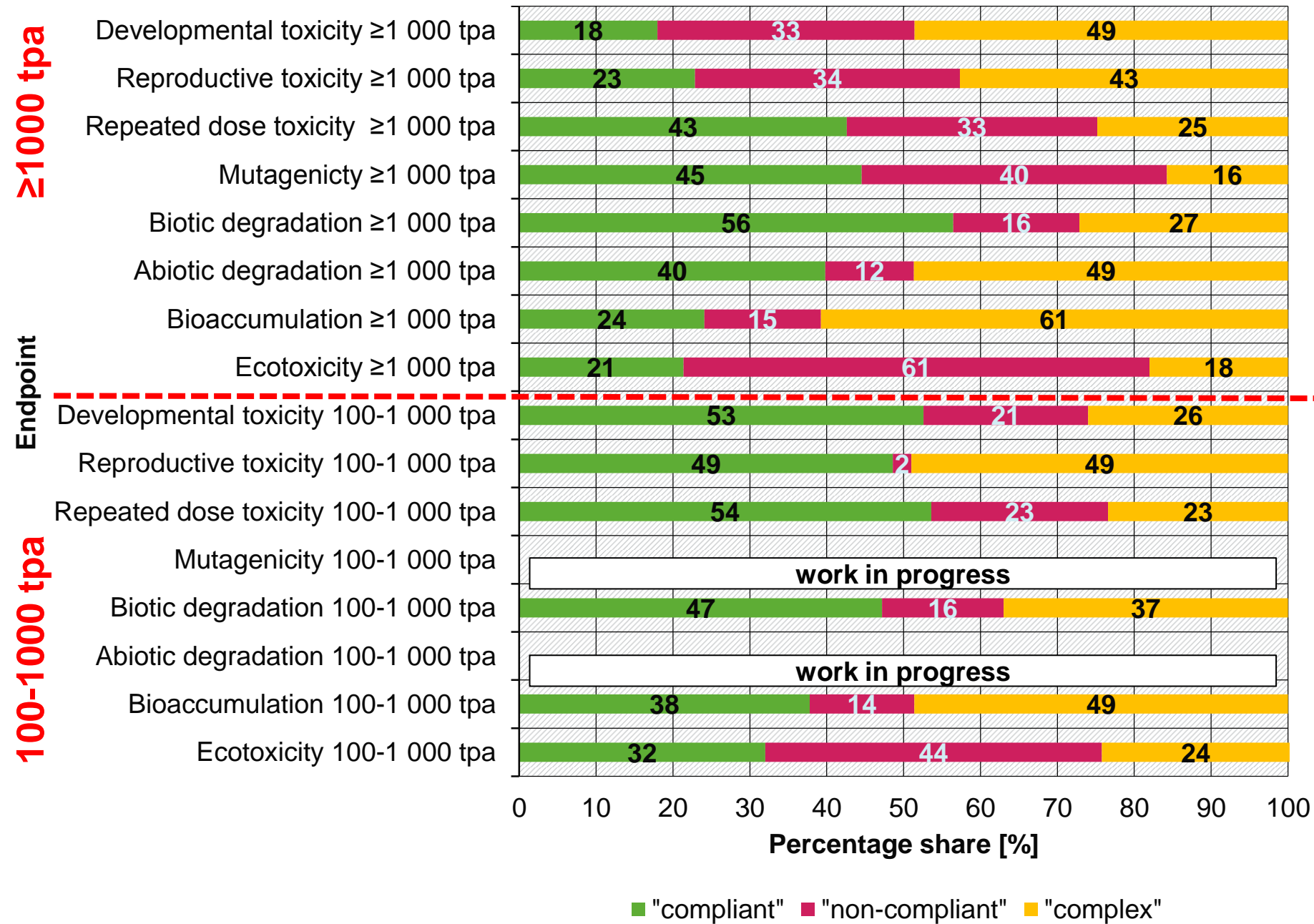
→ Still high rates of “complex” cases

→ **Further evaluation needed to solve all complex cases**

→ Refined check

- Groups of similar cases
- “Weight of evidence” case group
- Other case groups: Aim to identify frequent errors/problems

# Human health and environmental endpoints – Results after screening and formal check



## Average on all endpoints

(except Muta & AbioDeg)

### ≥1000 tpa

- 31% “compliant”
- 32.% “non-compliant”
- 37% “complex”

### 100-1000 tpa

- 44% “compliant”
- 19% “non-compliant”
- 37% “complex”

### → Higher rate of compliance at 100-1000 tpa

- DevTox / ReproTox lower requirements
- RDT / Ecotox improved compliance

# Conclusions

**Mean average of compliant endpoints higher in 100-1000 tpa (44%) compared to  $\geq 1000$  tpa (31%)**

Potential reasons

- Requirements less comprehensive for DevTox and ReproTox
- Higher frequency of compliant justifications on data waiving / adaptations (RDT, Ecotox)

→ Indicates improvement of data quality

**Data gaps and inappropriate waiving/adaptations identified in registrations**

- $\geq 1000$  tpa: 12-61% of the examined endpoints “non-compliant”
- 100-1000 tpa: 2-44% of the examined endpoints “non-compliant”

→ There is a need for improvement of registrations.

Conclusions on the examined endpoints not possible for all dossiers (remained “complex”)

Note on project results

- Do not represent the Compliance Check done by ECHA
- “Compliant” endpoints may still require an in-depth (scientific) analysis of studies and justifications (e.g. Read Across)



# Recommendations to registrants $\geq 1000$ tpa

## Aim

- Evidence-based assistance to registrants

## Structure

- **General recommendations**, e.g.:
  - for identity/similarity of substance and test material
  - Data adjustments according to REACH Annex XI
- **Endpoint specific recommendations**
  - Human health
  - Environmental endpoints

→ 33 recommendations published soon

→ Recommendations also applicable to 100-1000 tpa



# Example Bioaccumulation – Reasons for “non-compliance” and development of recommendations

## Report on $\geq 1000$ tpa

Waiving/adaptation category	Main reason(s)
(Q)SAR (28 %)	Insufficient model was used
	ESR not provided
	Reporting of model and prediction were insufficient
Technically not feasible (21 %)	Substance is UVCB



## Recommendations on $\geq 1000$ tpa

Problems	Recommendations
Validation data on the (Q)SAR model and prediction results are not available	<ul style="list-style-type: none"> <li>• OCED validation criteria should be met</li> <li>• Model and prediction reporting formats should be used</li> <li>• ESR for each (Q)SAR required</li> </ul>
Testing is not required because the substance is a UVCB substance	<ul style="list-style-type: none"> <li>• UVCB could contain CMR substances and/or PBT- substances, e.g. PAHs, and should be analysed</li> <li>• Deficiencies in substance identity should be tackled or justified</li> <li>• Validation of analytical methods for UVCB but also for UVCB in environmental matrices</li> </ul>

# Outlook – Publications and information

## ≥1000 tpa

- Final Report part 1 and part 2 (soon available)
- Recommendations to registrants (soon available)

## 100-1000 tpa

- Final report (in preparation)

## ECHA-Newsletter

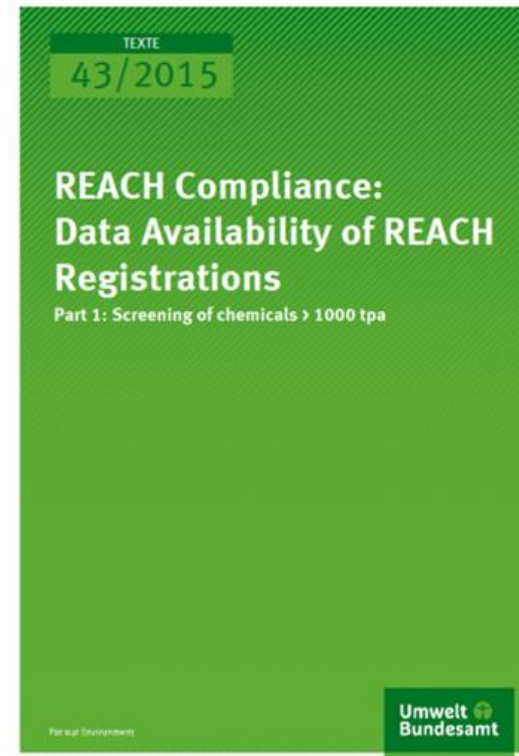
<https://newsletter.echa.europa.eu/home/-/newsletter/entry/guest-column-are-reach-data-appropriate-for-hazard-identification-and-risk-assessment->

## Information and downloads on the project

[http://www.bfr.bund.de/de/verfuegbarkeit\\_von\\_gesundheits\\_und\\_umweltdaten\\_fuer\\_hochtonnagige\\_chemikalien\\_unter\\_reach\\_reach\\_iii\\_-202836.html](http://www.bfr.bund.de/de/verfuegbarkeit_von_gesundheits_und_umweltdaten_fuer_hochtonnagige_chemikalien_unter_reach_reach_iii_-202836.html)

<https://www.umweltbundesamt.de/publikationen/reach-compliance-data-availability-of-reach>

<http://www.reach-info.de/reach-compliance.htm>



# Thank you for your attention

Angelika Oertel

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- Former project colleagues Andrea Springer, Dana Sittner, Henning Hermann, Anna Lena Kronsbein, Katrin Maul, Anne-Katrin Müller, Uta Herbst

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