Anthropogenic chemicals that are environmentally stable and highly polar (mobile in water) have the potential to break through natural and technical barriers in the aquatic environment and thus threaten the quality of our raw water resources (Reemtsma et al., 2016). Such substances are called persistent (P) and mobile (M) organic chemicals (PMOCs).

In order to identify PMOCs among the wealth of anthropogenic chemicals it is of vital scientific and regulatory interest to predict and assess P and M of substances in commerce. P and M can be assessed based on degradation test results and chemical property data, respectively, which are available from the open or grey literature, either experimentally derived or based on QSAR modeling.

A total of 167 industrial chemicals (registered under REACH) that were suspected to be PMOCs were initially chosen for this study. Three different approaches were used to assess the intrinsic chemical property data, respectively, which are available from the open or grey literature, either experimentally derived or based on QSAR modeling.

Of the 167 target chemicals 15 were eliminated because either P or M could not be assessed by at least one of the approaches, leaving a total of 152 assessed substances.

### Methods

#### Approaches, evaluation criteria and data sources

**Kalberlah approach** (Criteria by Kalberlah et al. (2014); data sources and interpretation of data with respect to the criteria by the present study)
- **Criteria**
  - P: An environmental half-life >40 d in freshwater (red)
  - M: Water solubility >150 µg/L and log Koc <4.5 in the pH range 6-8 (red)
- **Data sources**
  - Manually collected data from
  - Public dossiers on the ECHA website
  - Chemical safety reports obtained from the German Environment Agency
  - Scientific literature
  - QSARs

**PROMOTE approach** (Arp et al., submitted; translation of the results by Arp et al. into the color scheme by the present study)
- **Criteria**
  - P: An environmental half-life >60 d in freshwater (red);
  - >40 d but <60 d (yellow)
  - M: log Koc <2 or water solubility >1 g/L (red);
  - log Koc <3 but >2 or water solubility >50 mg/L but <1 g/L (yellow)
- **Data sources**
  - Predominantly automatically retrievable data from
  - Public dossiers on the ECHA website
  - Scientific literature
  - QSARs

**Present approach**
- **Criteria**
  - P: An environmental half-life >40 d in freshwater (red)
  - M: log Koc <3.5 or water solubility >50 mg/L (red)
  - log Koc <5 but >3.5 and water solubility >0.15 mg/L but <50 mg/L (yellow)
- **Data sources**
  - Same as for Kalberlah approach

### Results and Discussion

#### Assessment results of the individual approaches

**Persistence**
- Relatively large differences between the results of the different assessment approaches (Fig. 1, see also Fig. 3)
- Main reasons for the differences: Use of different test results - Interpretation of degradation test results with respect to the criterion (half-life in freshwater)
  - Use of experimental vs. QSAR data

**Mobility**
- Good comparability of results between PROMOTE and Present approaches (Fig. 2)
- Main difference: yellow in Kalberlah vs. red in the other approaches
  - Based on different interpretation (red or yellow) of QSAR data for ionic and ionizable compounds outside the application domain

### Comparison of assessment results

**Fig. 3.** Comparison of the results of P and M for all approaches

- Only 32 chemicals were assessed P red by all approaches (Fig. 3) vs. up to 105 chemicals in the individual approaches (Fig. 1). For P green these numbers are 6/42, for M red 56/141 (Fig. 2) and for M green 3/8
- For both P and M there were chemicals that were assessed with red in one approach and green in another (results not shown)

**Fig. 4.** Chemicals assessed red for both P and M

### Conclusions

- Assessment of intrinsic substance properties depends on the evaluation approach, criteria and data sources. This is more pronounced for P than for M.
- Experimental data should preferably be used in chemical assessments. For QSARs the application domain is important to consider (e.g. for ionic chemicals).
- Large data gaps exist for experimental property data as well as test results. The REACH registration process should be sharpened to help close the data gaps.
- All approaches deliver valuable results in terms of identifying chemicals for scientific scrutiny.
- In order to use assessment approaches in the regulatory context, a well-defined, harmonized and validated approach is necessary.