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Environmental risk assessment of poorly soluble substances:

Improved tools for assessing biodegradation, (de)sorption, and modeling (project RABIT)

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Introduction

Chemicals with an extremely **low aqueous solubility** in the range of a few $\mu\text{g/L}$ are used in a broad range of applications, ranging from consumer products to industrial applications. High production volumes and consumer application (e.g., cosmetics) may promote the potential release of substantial amounts into wastewater and the aquatic environment. Additionally, these chemicals need to be considered as potential **PBT-candidates** due to their intrinsic properties.

Investigations on environmental fate and effects of poorly soluble substances are urgently needed, but by no means straightforward. Their **high hydrophobicity** results in **extensive sorption** to solids (soils, sediments, and organisms), and thus standard tests are often not suitable, since the biodegradation rates are often limited due to their slow desorption. In addition, analytical quantification of their typically low dissolved concentrations is challenging.

Project

As sorbed substances are usually not directly bioavailable, biodegradation is strongly dependent on (fast and slow) desorption of the substances into the water phase.

However, hydrophobic chemicals sorb significantly to the solid organic and mineral matter.

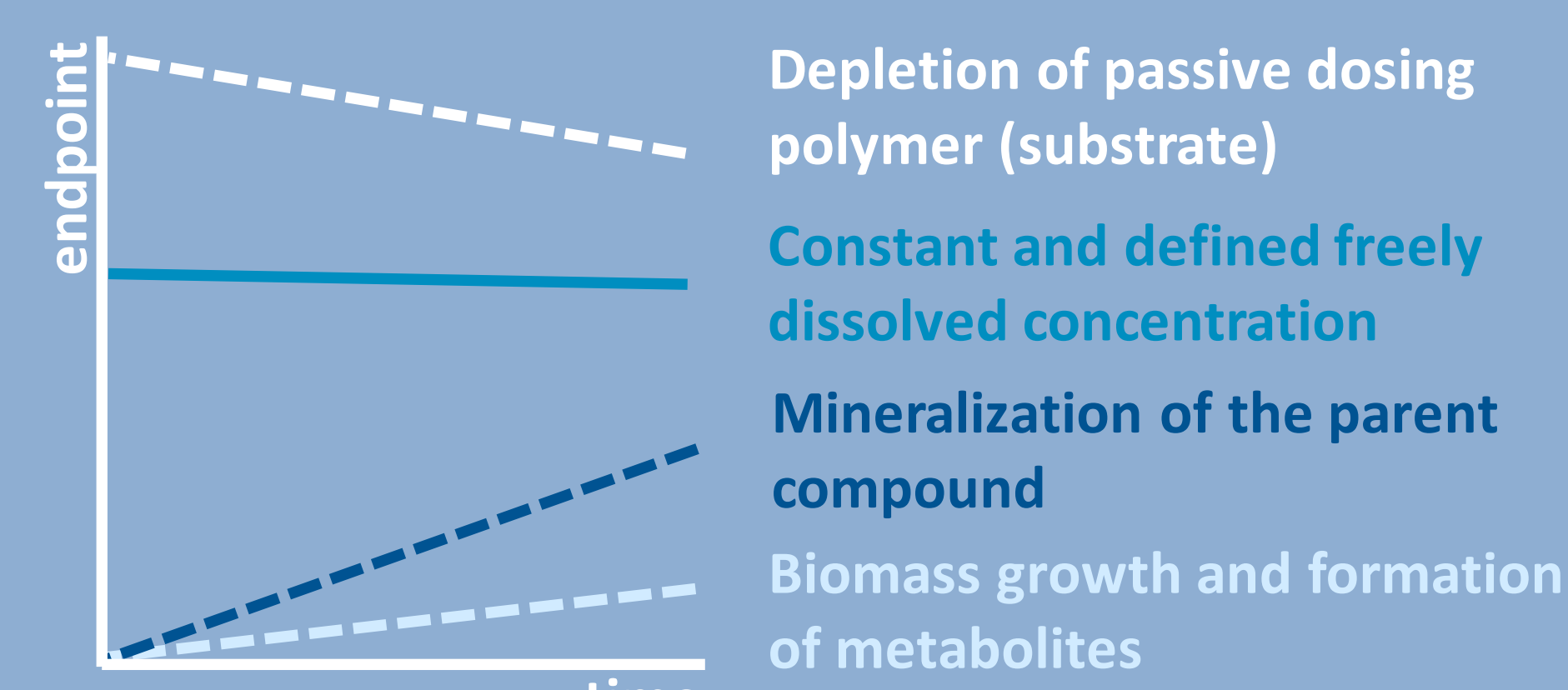
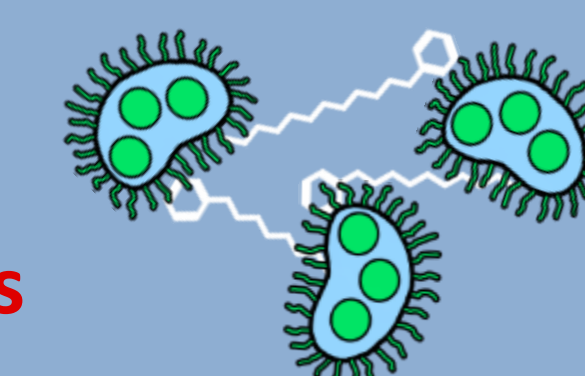
When desorption is slow, this can result in a biodegradation rate that is reduced due to limited bioavailability rather than its inherent biodegradability.

More reliable assessment of the biodegradation behavior thus requires the development of new experimental setups that can adequately decouple desorption effects from the actual biodegradation process.

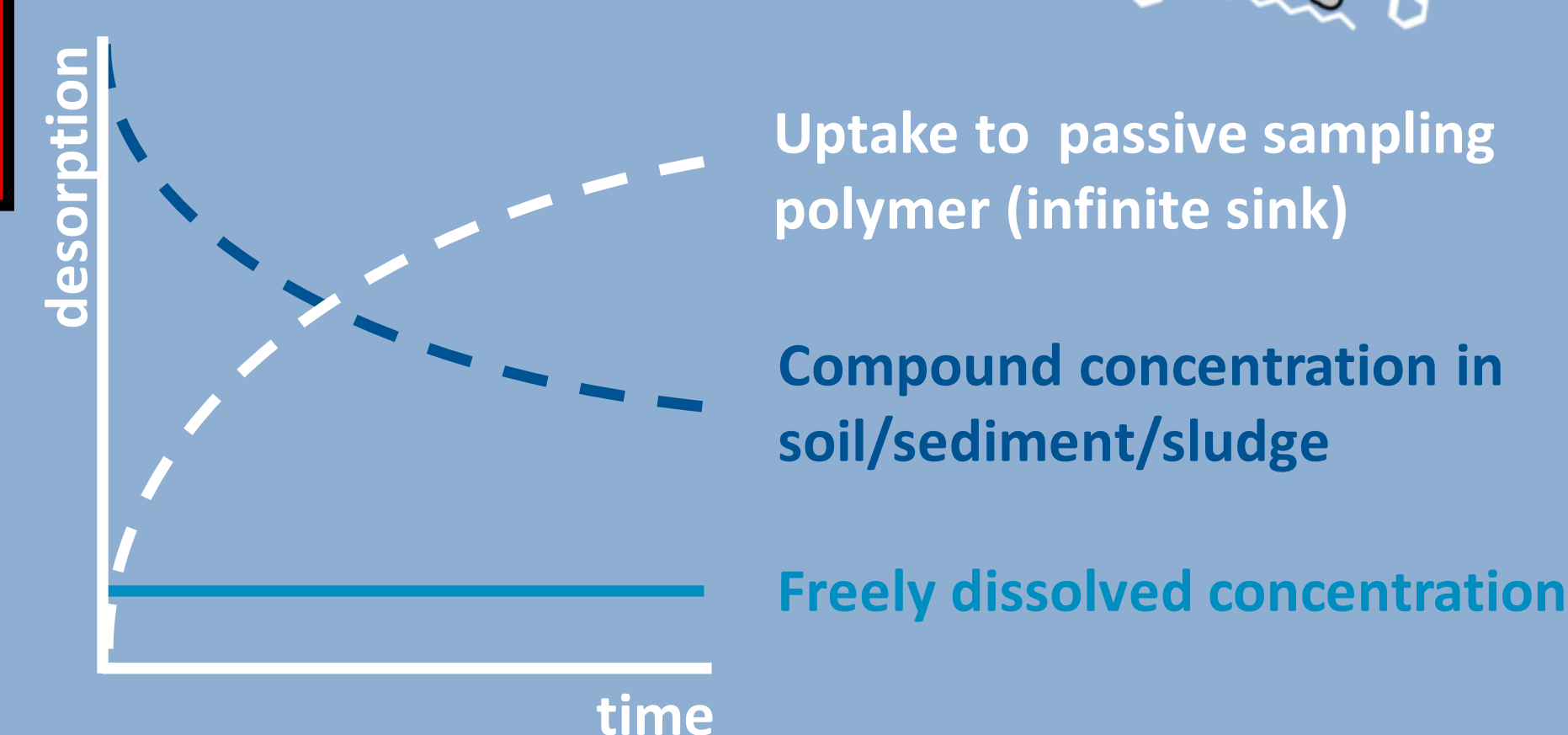
RABIT - Risk Assessment on Biodegradation and desorption: Improved Tools (CEFIC LRI-ECO32)

In 2016 a joint project of the RWTH Aachen University and the Technical University of Denmark was established, funded by the European Chemical Industry Council (CEFIC) with three main objectives:

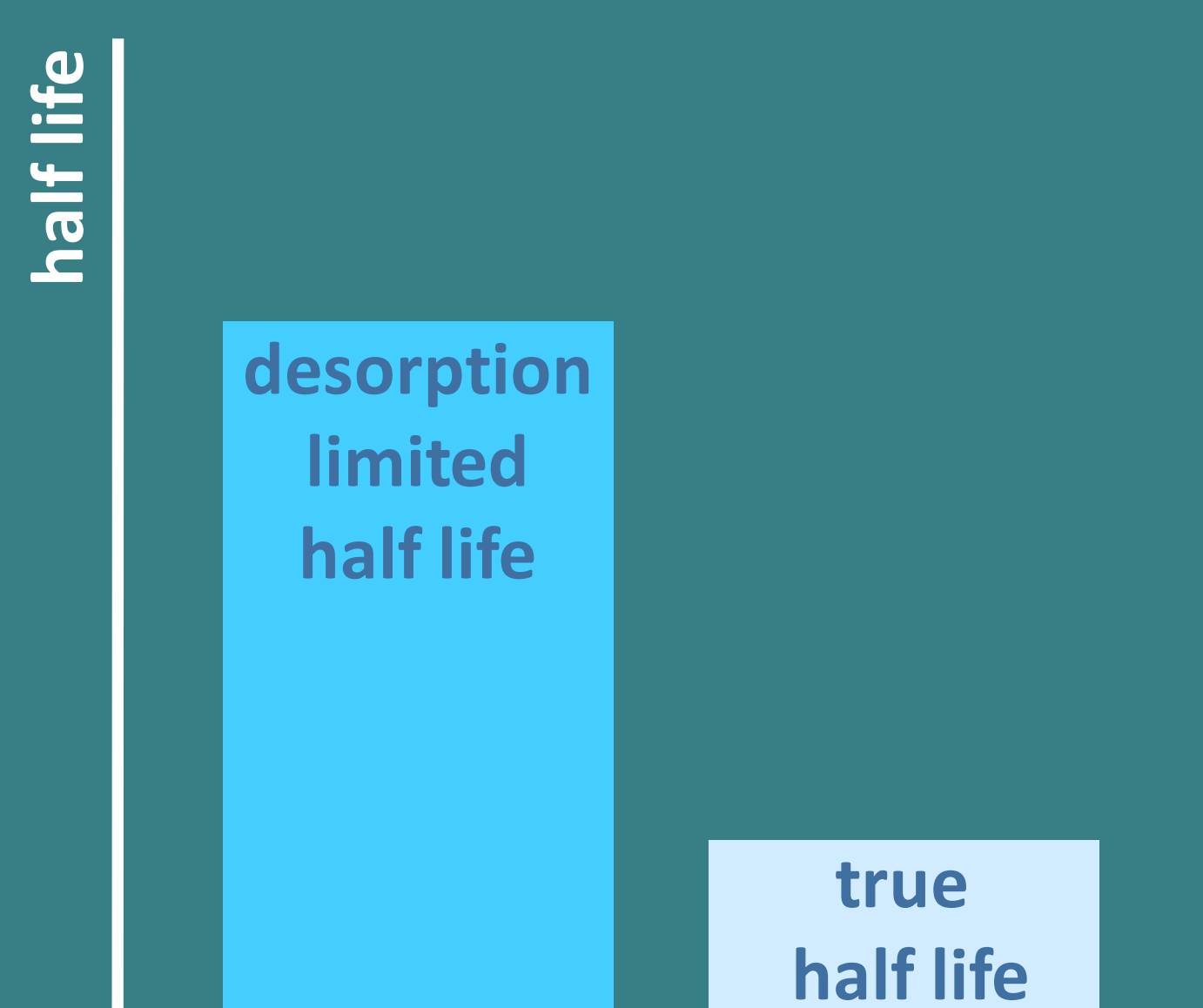
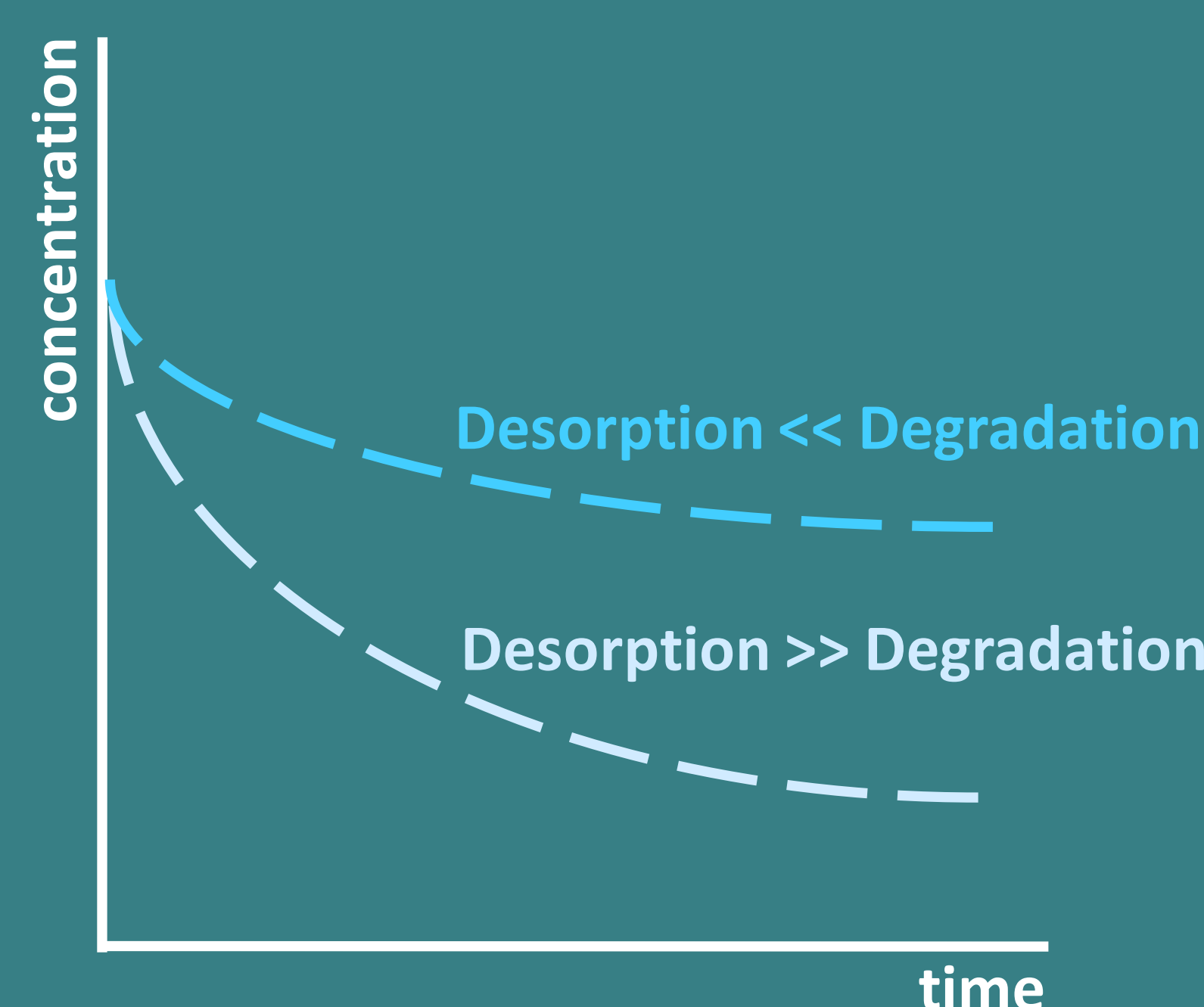
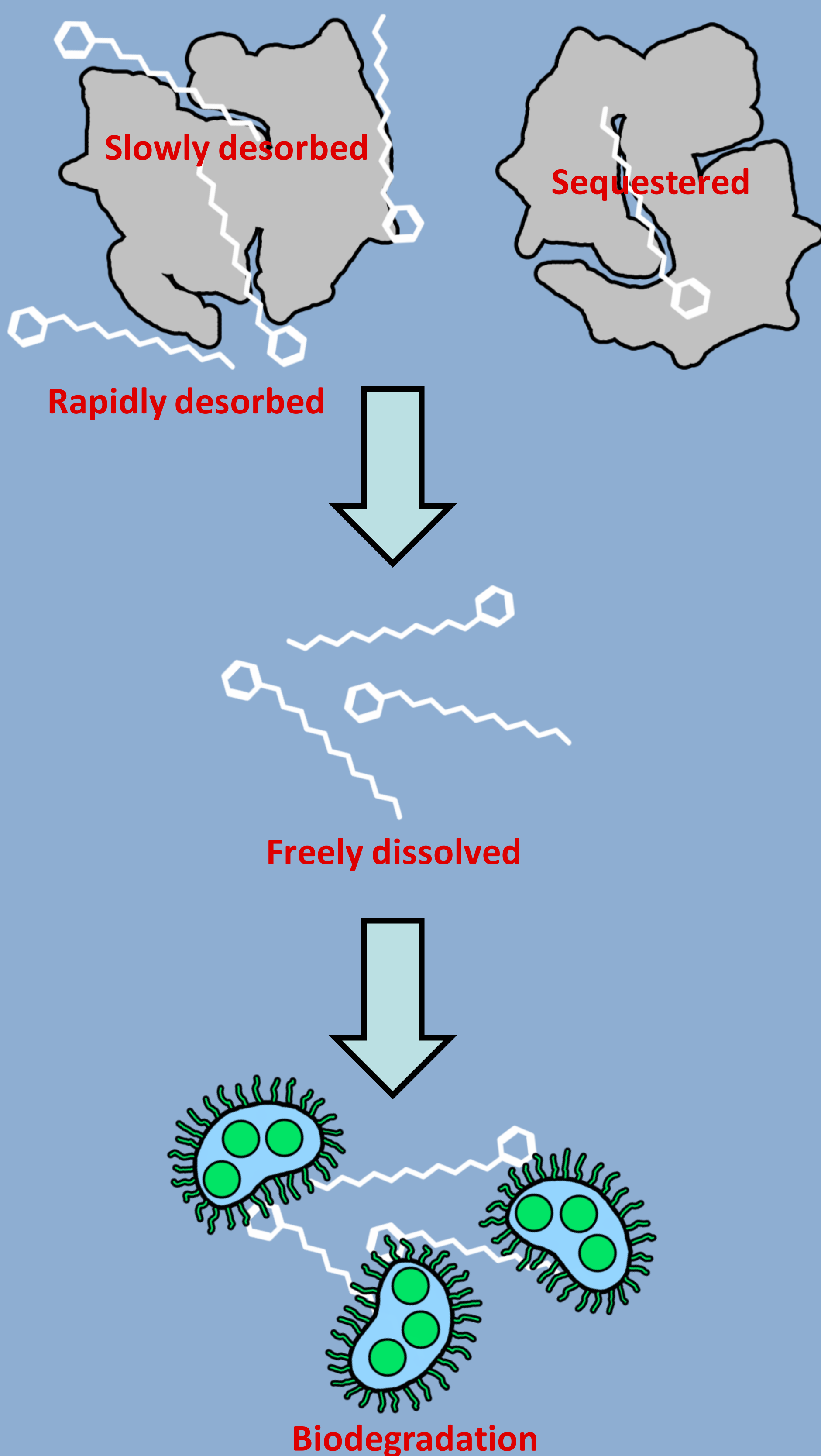
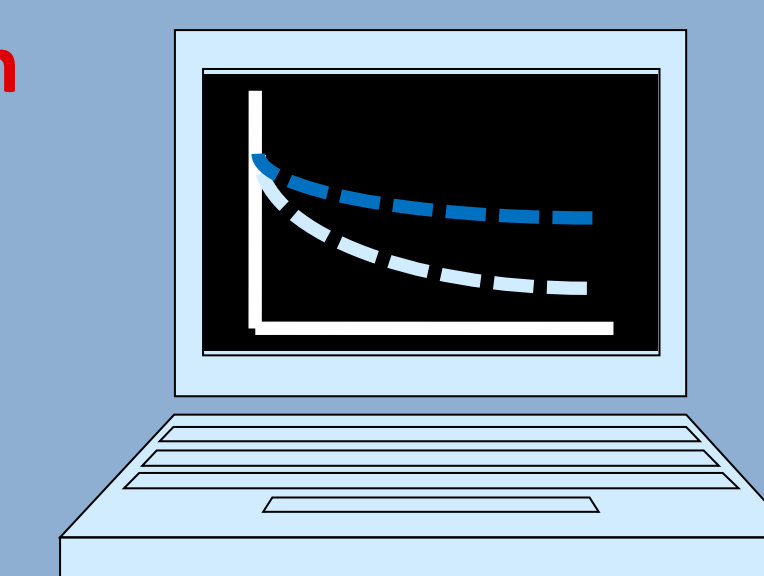
(1) Measurement of aqueous phase biodegradation without desorption effects



(2) Measurement of abiotic desorption over time



(3) Combination of both in a unified model

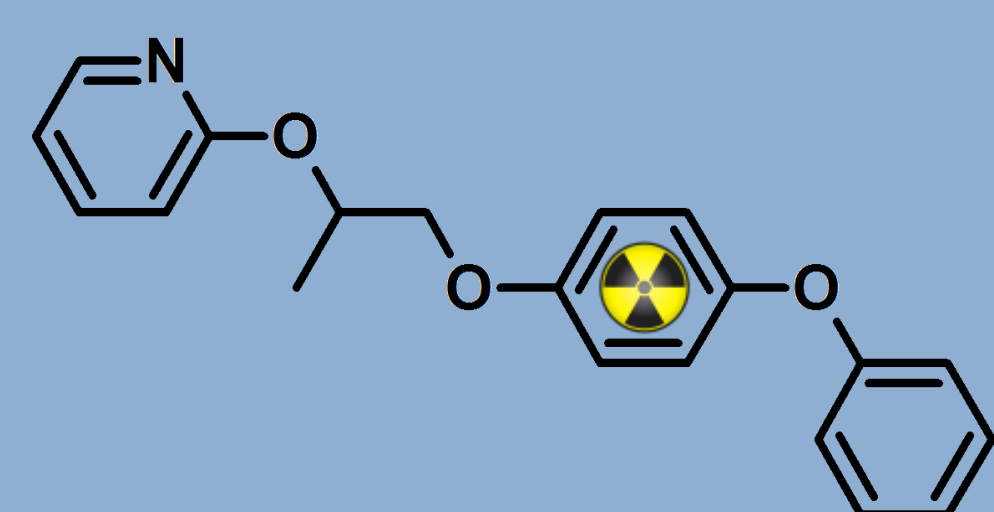


Methods

Model substances (labeled + unlabeled):

Pyriproxyfen ($\log K_{ow} = 5.55$)

Dodecylbenzene ($\log K_{ow} = 8.65$)



Standard analytical instrumentation:

LC-MS-MS (Pyriproxyfen)
GC-MS (Dodecylbenzene)

LoD $\approx 8 \mu\text{g/L}$
LoD $\approx 2 \mu\text{g/L}$

Radio analytical instrumentation:

Liquid scintillation counting
Radio HPLC
TLC