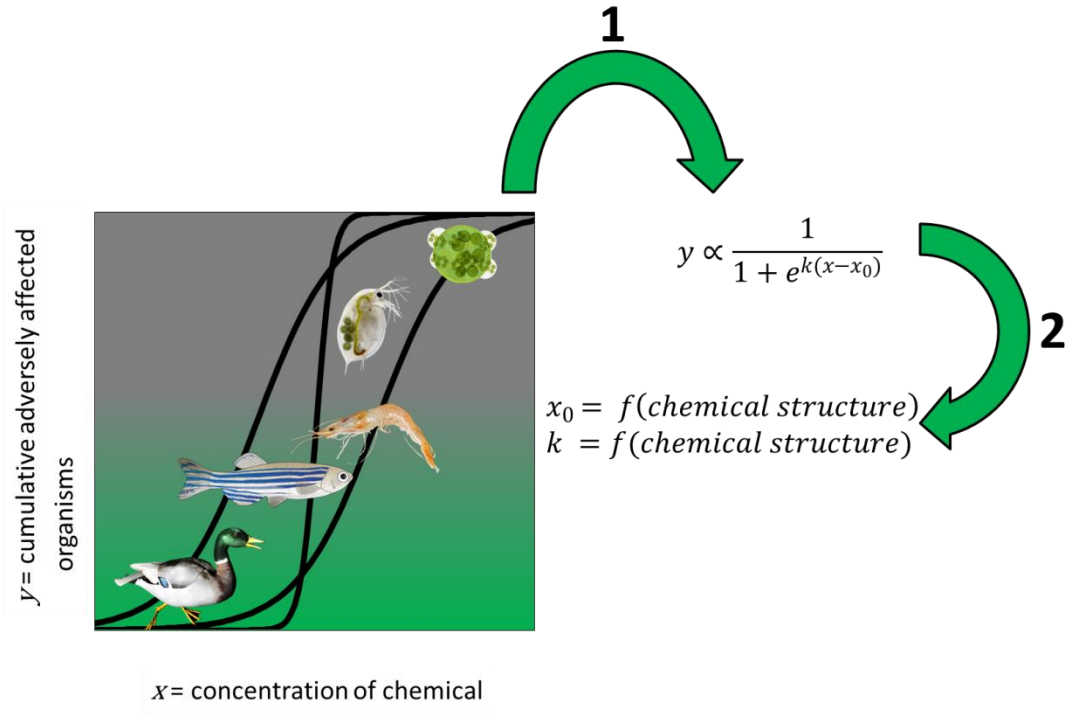
Project title: Screening 'green' substances via species sensitivity distributions
Level: Master (6 months); Bachelor (3 months)
Start: Anytime
Project form: Desk-based research, data analysis, modelling
Supervision: Leo Posthuma | Renske Hoondert | Tom Nolte | Jan Hendriks
Mail addresses: L.Posthuma@science.ru.nl | r.hoondert@science.ru.nl

Setting:
Chemical substances that 'fit' within biological, ecological and nutrient cycles must be degradable, renewable and non-toxic. Currently, 1.000.000+ chemical substances are on the market, with an additional 10.000+ registered each year. This poses a huge challenge for companies and regulatory authorities to develop methods to 'screen' substance libraries and detect 'green' alternatives.

Description of the project:
During this internship you will use ecosystem species-sensitivity distributions (SSDs, Figure 1) to detect potential 'green' alternative substances: you **1)** determine the ecosystem SSD-parameters 'mean' (x_0) and 'variation' (k), and **2)** relate the SSD-parameters for 10.000+ substances to chemical structure:



The result will enable us to accurately estimate the behavior of a chemical substance in an ecosystem as a whole. This reduces the need for cost-inefficient organism-specific assessment, and enable efficient detection of 'green' alternatives.

Literature: Hoondert, Renske, et al. "QSAR-based estimation of SSD parameters–an exploratory investigation." *Environmental toxicology and chemistry* (2019).