

# SUMMER SCHOOL (CNRS / SETAC)

## PREDITOX ECOTOXICOLOGY AND PREDICTIVE MODELLING

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[HTTPS://SITES.GOOGLE.COM/VIEW/PREDITOX2017/HOME](https://sites.google.com/view/preditox2017/home)

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### Pre-registration



<https://lc.cx/ovNt>

European guidelines for risk assessment of chemicals have recently been modified (REACH, directives for pesticides and biocides) in particular to improve their ecological realism while limiting the use of laboratory animal testing. In addition, the OECD undertook a revision of guidance documents for laboratory bioassays in order to strengthen the relevance of data analysis methods (e.g., OECD guideline 243, July 2016).

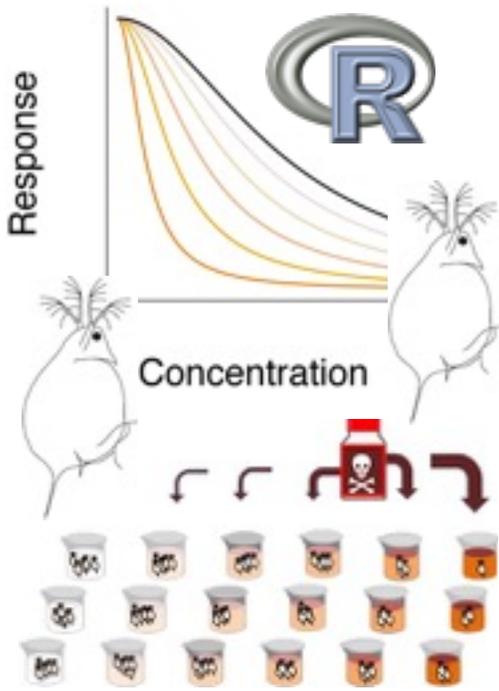
These new official texts all recommend the use of appropriate mathematical and statistical modelling tools, for cognitive and predictive purposes. They promote the optimisation of data analysis (e.g., interpolation between the

concentrations tested in bioassays) and the use of modelling as a basis for predicting effects under different environmental conditions (e.g., extrapolation between different scenarios and different exposure times, extrapolation from the individual to the population level, or extrapolation from one species to another).

This school aims at helping ecotoxicologists to improve their skills in modelling and statistical inference for, among other things, a better analysis of their bioassay experimental data.

### All details at

<https://sites.google.com/view/preditox2017/home>



# Topics

## Introduction to R software

R is a language and environment for statistical computing and graphics (<http://cran.r-project.org/>). It provides a wide variety of statistical and graphical techniques. It is highly extensible through a great number of packages dedicated to specific topics. R is available as a free software under the terms of the Free Software Foundation's GNU General Public License in source code form. It compiles and runs on a wide variety of platforms (Linux, Windows and MacOS). Participants will be introduced to R programming and to basic statistics in R, especially to the use of linear models in R.

## Dose-response modelling

For some years now, there has been a large consensus that ECx has many advantages over NOEC and should be considered as an appropriate way of analysis as far as data are sufficient and properly fitted with suitable concentration- response models. Nevertheless, the choice of the appropriate model is not straightforward: both the deterministic and the stochastic parts must be appropriately chosen in accordance with the nature of the experimental data (quantal data for survival, continuous data for growth or count data for reproduction). Participants will be introduced to up-to-date methods, especially generalized non-linear models and TK-TD models, for improving their modelling of different types of dose-response data.

## Distribution fitting

Fitting distributions to data is a very common task in statistics and is particularly useful in ecotoxicology to fit species sensitivity distributions. Fitting distributions consists in choosing a probability distribution modelling the random variable, as well as finding parameter estimates for that distribution. This requires judgment and expertise and generally goes through an iterative process of distribution selection, parameter estimation and quality of fit assessment. Participants will be introduced step-by-step to fit distributions using the R package fitdistrplus, which provides R users a set of functions dedicated to help the overall process and enables to include censored data. Participants will also be introduced to the use of hierarchical models to describe inter-species variabilities.

## Bayesian inference

In the last decade, Bayesian inference has showed its usefulness in ecotoxicology as a relevant alternative to classical frequentist methods (maximum-likelihood algorithms, least squares regression...). In particular, Bayesian inference reveals convenient when estimating parameters of models, simultaneously fitted to different types of data. Within the Bayesian framework, parameter estimation requires three steps: (i) a model is built, defining the logical and stochastic links between parameters and variables; (ii) prior distributions over all parameters are specified. These distributions reflect the state of knowledge available before analysing the data set; (iii) posterior distributions over all parameters are computed using Bayes' theorem, which combines prior distributions and observed data. Posterior distributions contain updated beliefs about model parameters; they can be used as the new state of knowledge for future calculations. Bayesian inference is very flexible and makes the use of generalized non-linear models and hierarchical models very easy. Participants will be trained step-by-step to the use of Bayesian inference using the JAGS software (<http://mcmc-jags.sourceforge.net/>).

## Programme

Based on the use of the R software and some associated packages, the following topics will be tackled:

- **Getting started with R:**  
Basic programming, graphics, some basic statistical analyses
- **Dose-response modelling:**  
Generalized non linear models, frequentist versus Bayesian inference
- **Toxicokinetics – toxicodynamics (TKTD) modelling:**  
Introduction to advanced dose-response modelling including time dependency
- **Species Sensitivity Distribution (SSD):**  
Fit of probability distributions, censored data, introduction to hierarchical modelling

## Registration fees

- 1000 € (full academia)
- 1500 € (full business and government)
- 700 € (students)
- 850 € (SETAC members from academia)
- 1250 € (SETAC members from business and government)