

Ralph Kühne,¹ Anja Miltner,² Karolina Nowak,³ Matthias Kästner,² Andreas Schäffer,³
Qingzhu Jia,^{1,4} Gerrit Schüürmann^{1,5}

Contact:
ralph.kuehne@ufz.de

¹ UFZ Department of Ecological Chemistry, Helmholtz Centre for Environmental Research, Leipzig, Germany

² UFZ Department of Environmental Biotechnology, Helmholtz Centre for Environmental Research, Leipzig, Germany

³ Institute for Environmental Research, RWTH Aachen University, Germany

⁴ Tianjin University of Science and Technology, Tianjin, China

⁵ Technical University Bergakademie Freiberg, Freiberg, Germany

INTRODUCTION

BACKGROUND

- Many **different mechanisms** for NER formation
- 3 main **types of interaction**
 - Sorption
 - Binding
 - Sequestration
- In addition, xenobiotics may be degraded and transformed to **microbial biomass**, which can be **stabilized in soil (biogenic NER)**
- Dependence on **chemical structure**
- Only **rudimentary predictions** feasible

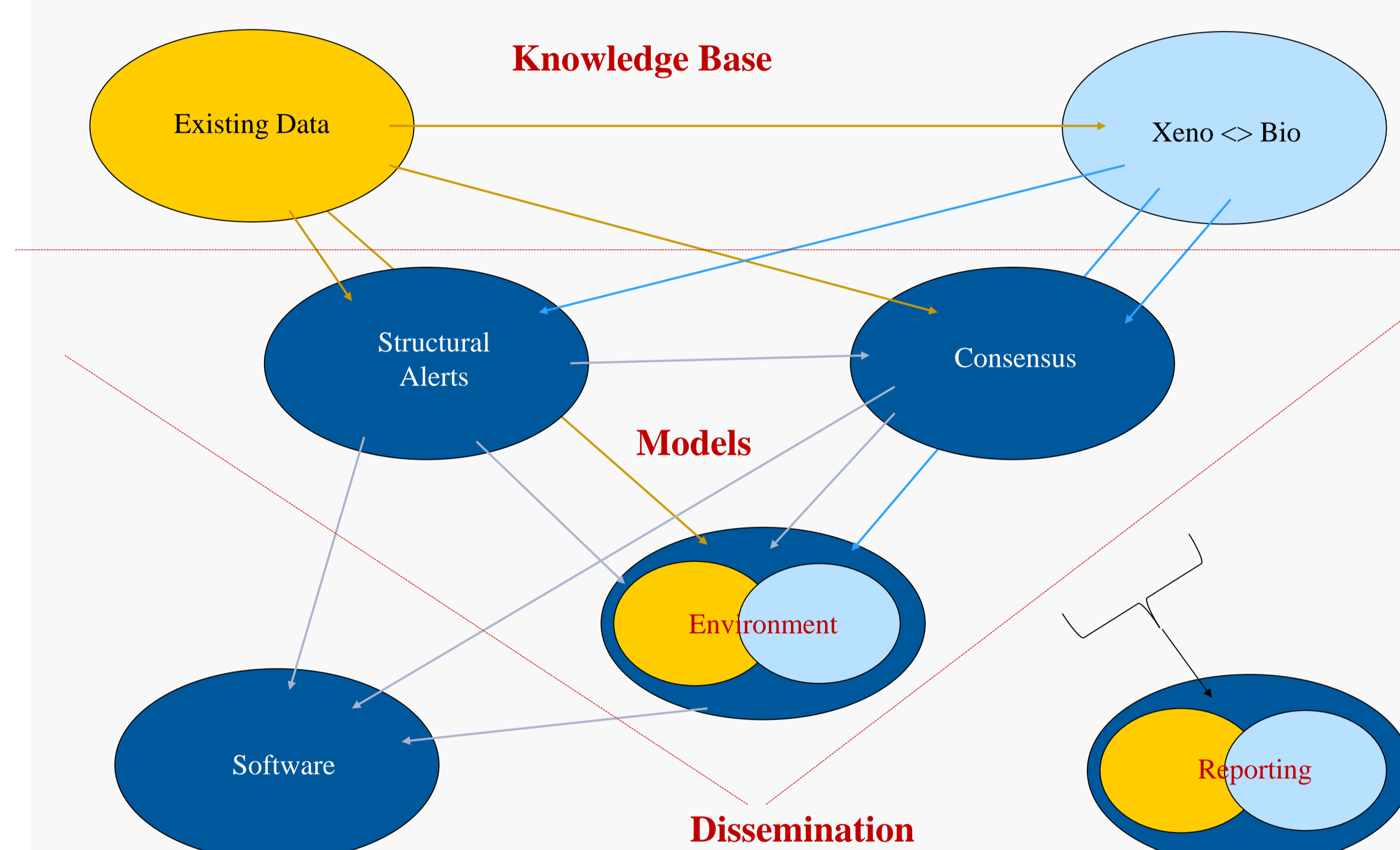
ENVIRONMENTAL RELEVANCE

- Sorbed/entrapped** xenobiotic NER (I) cause harm
- Bonded** xenobiotic (II) and biogenic (III) do **not**

QUESTIONS TO BE ANSWERED

- Significant amounts** of NER formed under which **environmental conditions?**
- Do formed NER have **potential for environmental harm?**

CEFIC-LRI ECO-24: PROJECT OUTLINE



TIMELINE

- Started **April 2014**
- Duration: **24 months**

OBJECTIVES

- Develop rules to identify **structural alerts** for NER formation
- Consider also **biogenic NER**
- If suitable, **key parameters** to be modelled quantitatively e.g. by **Abraham (LSER)** **Neural network**

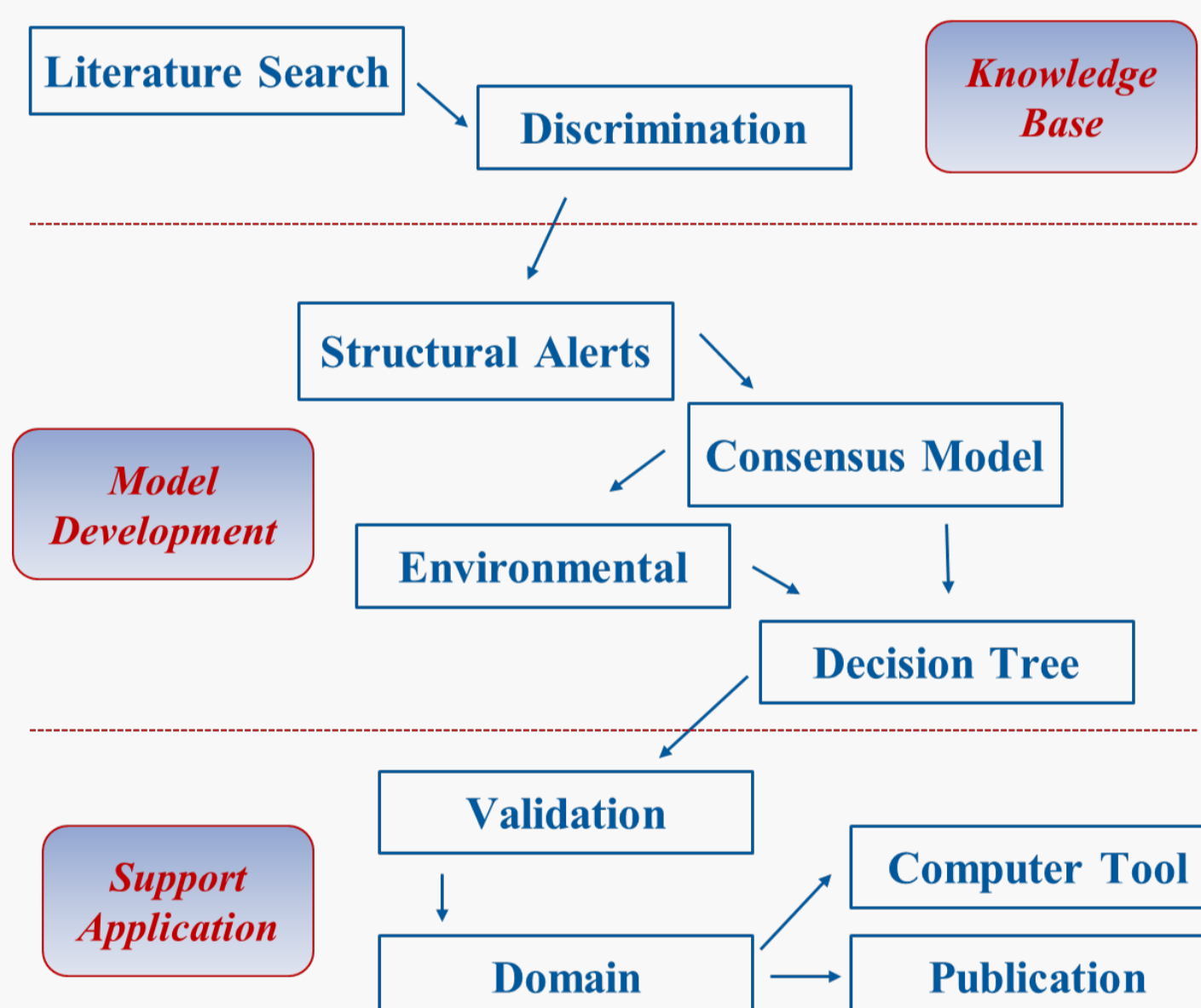
AIM: COMPUTERISED TOOL TO DISTINGUISH

- Intrinsic structural alerts** for NER I and III
- Environmental conditions** triggering NER formation

MODEL RELIABILITY

- Consensus** with complementary approaches ⇒ **Decision tree**
- Applicability domain** characterisation

WORK FLOW



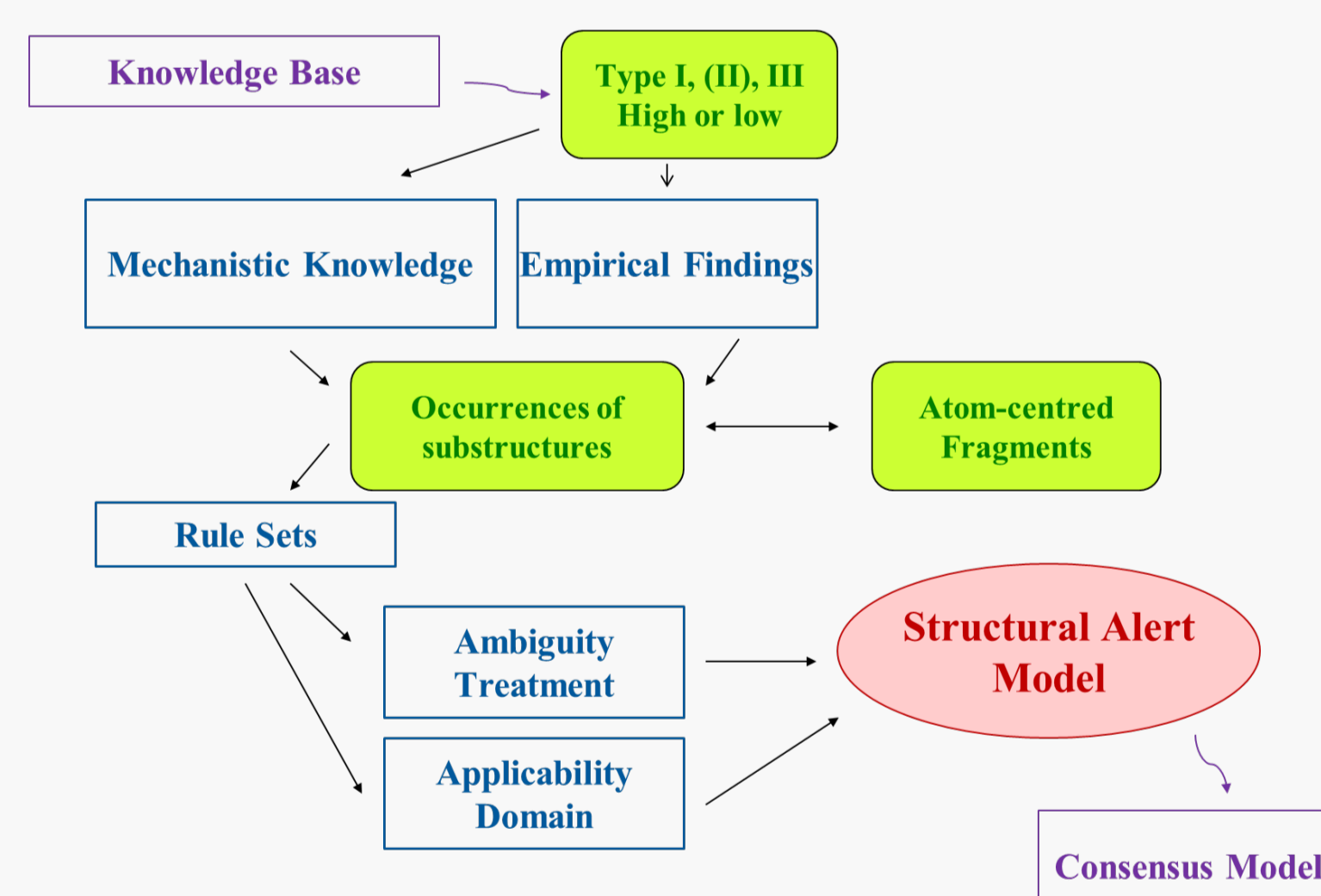
KNOWLEDGE BASE

Literature Search

- Chemical structures and properties**
- Kinetic data**
- Soil data**

NER Discrimination

- Correlation of Type I to amounts mineralized and Type III**
- Structures with highly limited intrinsic and environmental biodegradation potential**
- Link principal biotic turnover reactions to environmental conditions**



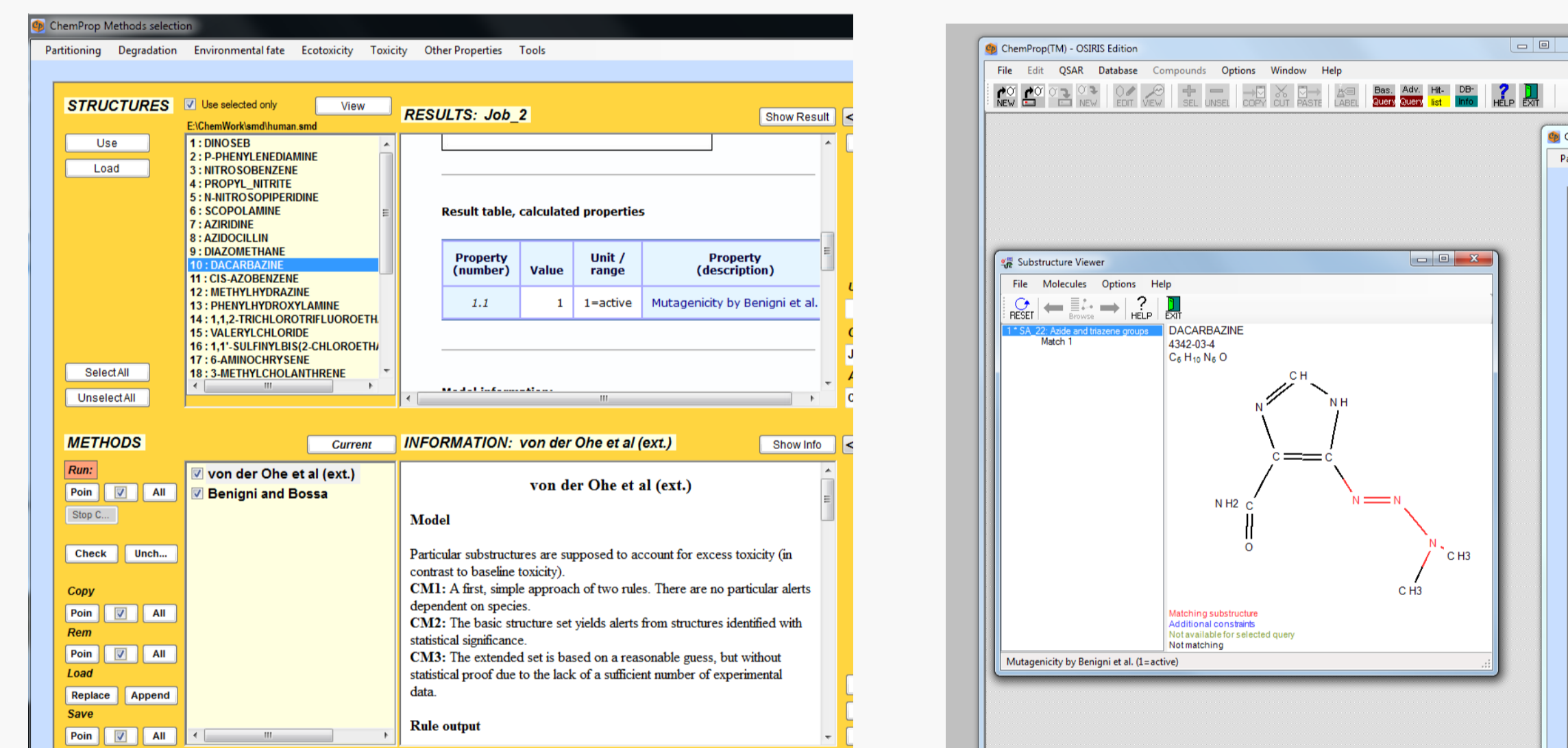
MODELING

- Structural alerts**
- Alternative models:**
 - Property thresholds, worst case by **LSER, Read-across**
- Consensus: Decision tree**

ENVIRONMENTAL CONDITIONS

- Formation potential ≠ formation
- Model with environmental conditions:**
 - Identify **relevant properties**, relate **structural alerts**

COMPUTER IMPLEMENTATION: CHEMPROP

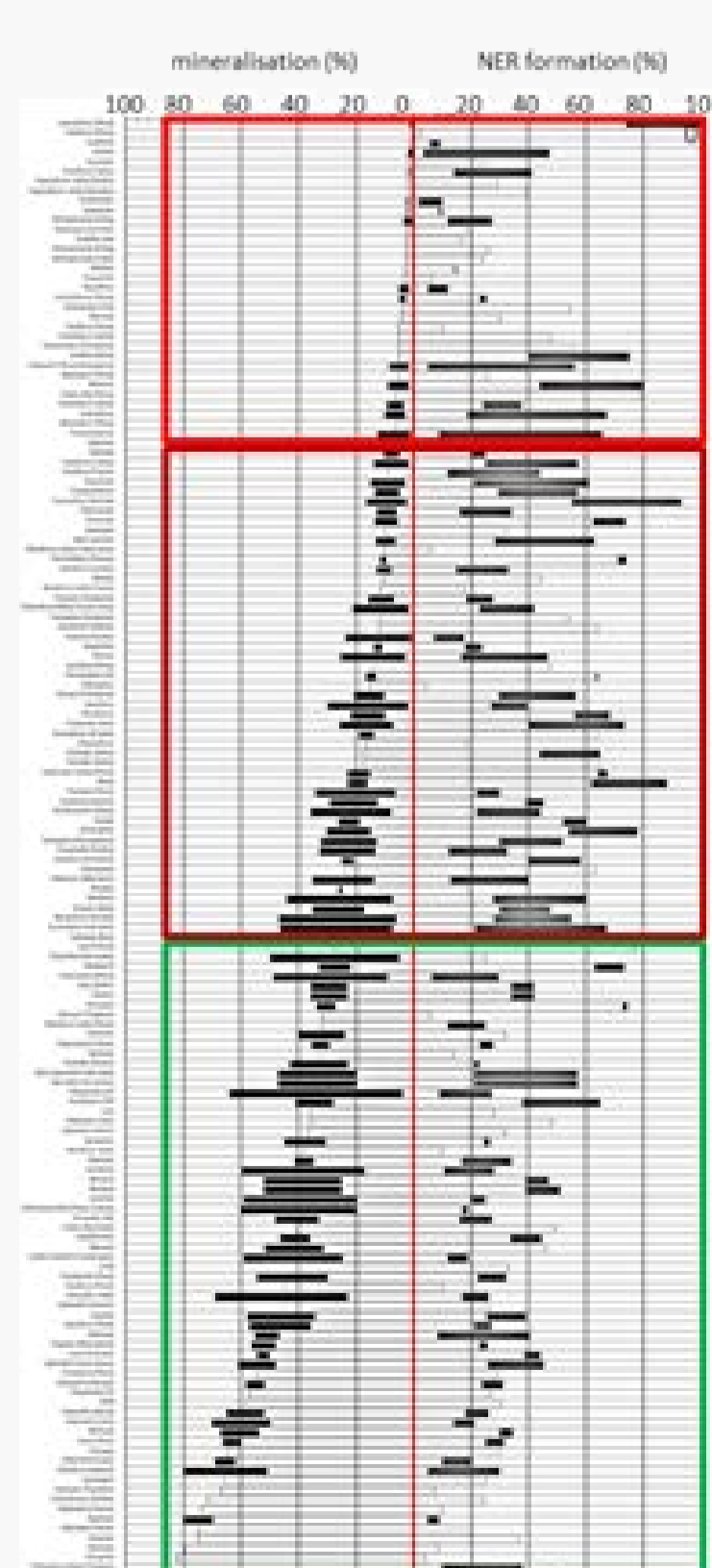


- Automated property and descriptor estimation**
- Reasonable default for environmental conditions**
- Database for chemical structures and project data**
- Model reliability**
- Documentation**

CHEMPROP

- Publically available for free** based on license
- Details:**
 - <http://www.ufz.de/index.php?de=6738>

PROGRESS SO FAR



KNOWLEDGE BASE

- Extensive literature search performed**
- Parameters** for further work identified
- NER amount linked to extent of mineralisation** ⇒ **3 groups identified**

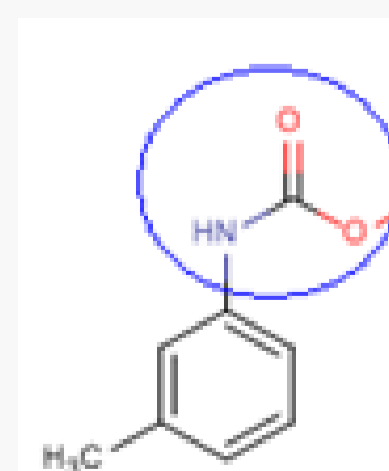
Preliminary classification of pesticides according to mineralisation and NER formation based on data from Barriuso E, Benoit P, Dubus I 2008. Formation of pesticide nonextractable (bound) residues in soil: Magnitude, controlling factors and reversibility. *Environ. Sci. Technol.* **42**: 1845–1854.

MODELING

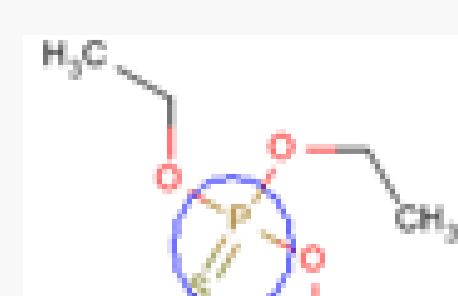
- First step: Structural alerts for general NER formation potential**
- Preliminary model: 10 confirmed alerts**
 - 8 for **low potential**,
 - 2 for **high potential**

Examples:

High potential:



Low potential:



PROJECT TEAM

UFZ Department of Ecological Chemistry

- Principal investigator, project management
- Model development and implementation

UFZ Department of Environmental Biotechnology, & Institute for Environmental Research, RWTH Aachen University

- Knowledge base

ACKNOWLEDGMENT

This project is funded by the CEFIC-LRI (ECO24).



The research stay of Prof. Dr. Qingzhu Jia was sponsored by the Tianjin University of Science and Technology, China.

