

# Computer based prediction of the formation of Non-Extractable Residues (NER) of xenobiotics and their metabolites in soils and sediments with regard to their environmental hazard

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## 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

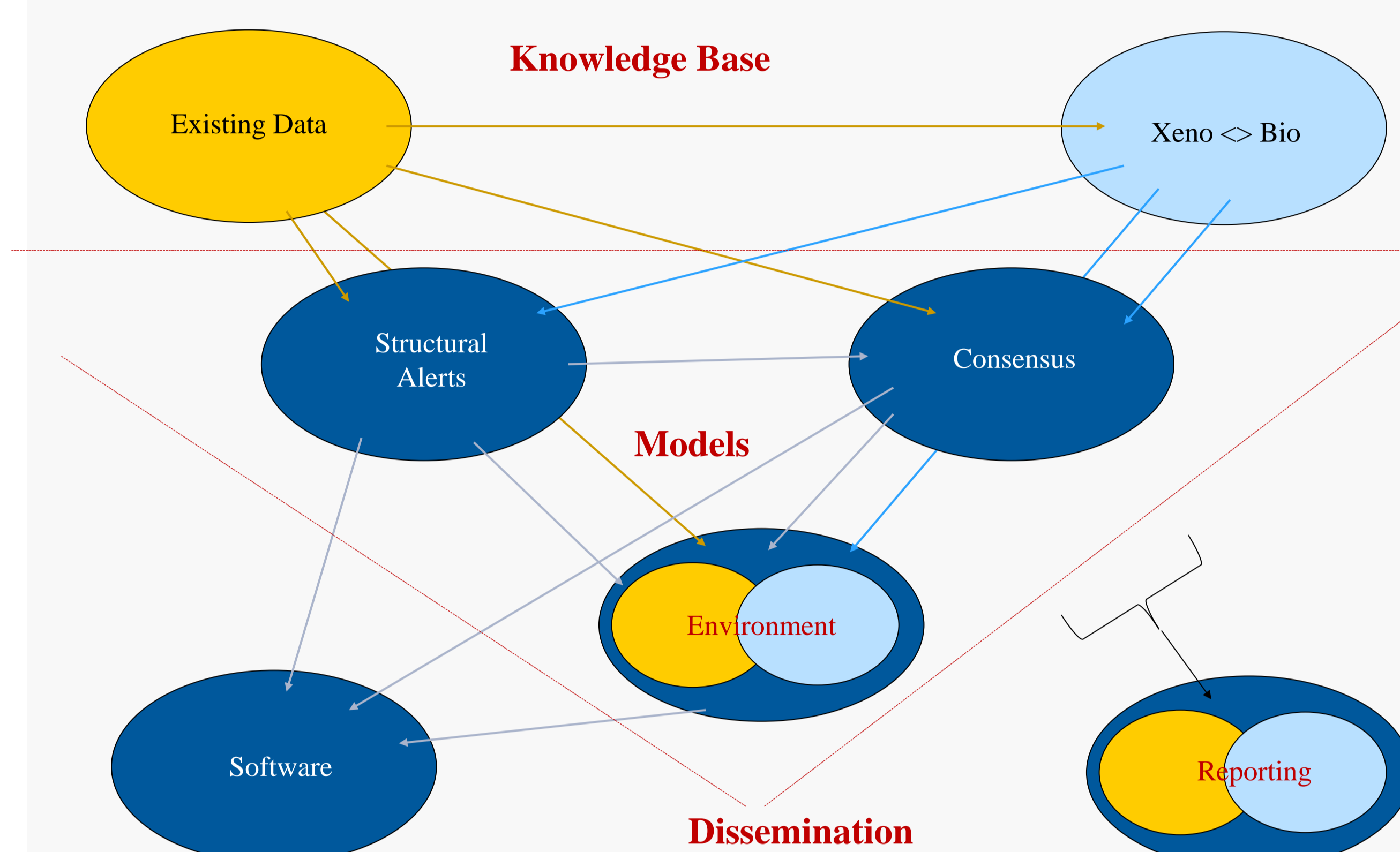
### ENVIRONMENTAL RELEVANCE

- 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?**

## 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**

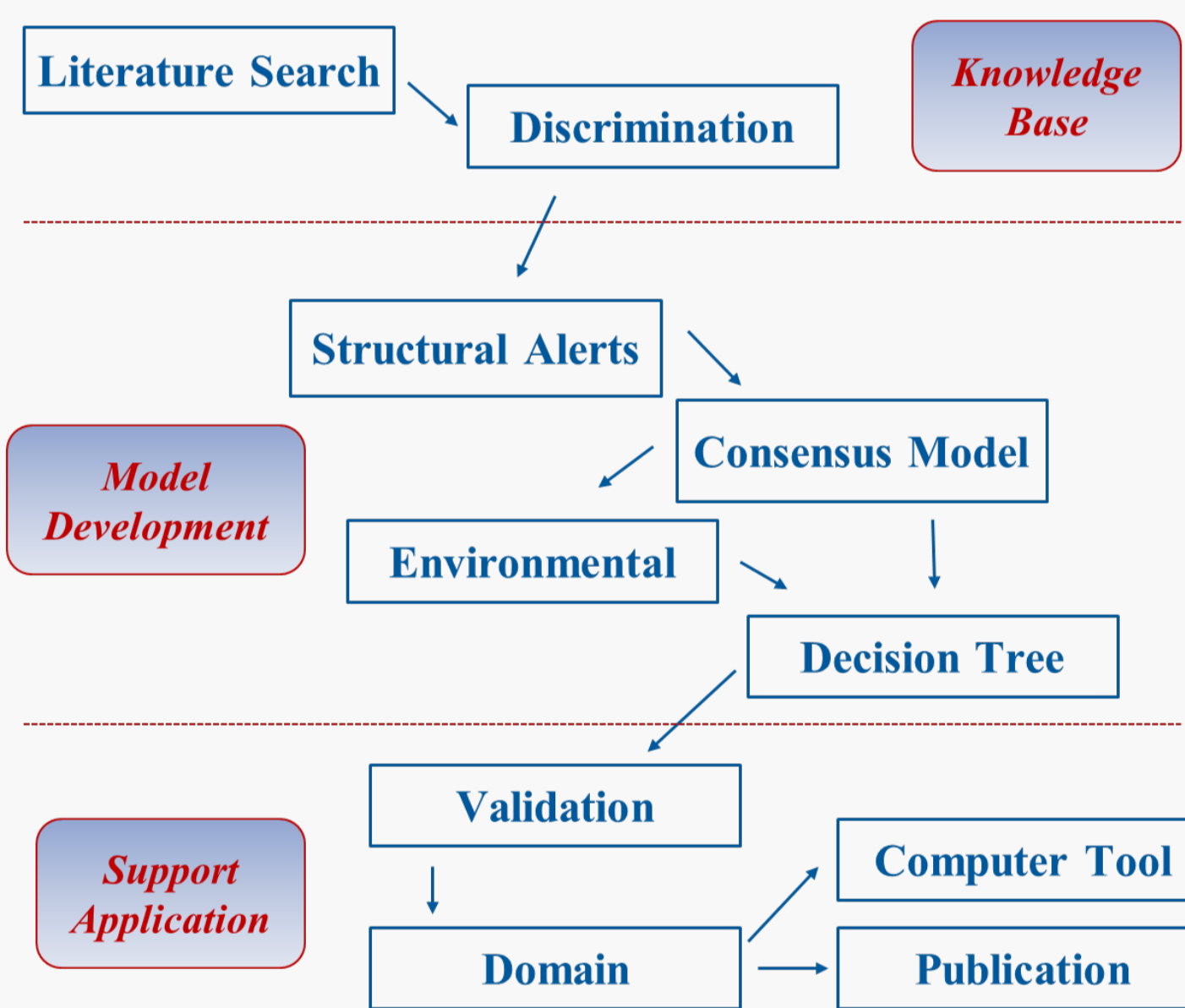
### AIM: COMPUTERISED TOOL TO DISTINGUISH

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

### MODEL RELIABILITY

- Consensus** with complementary approaches  $\Rightarrow$  **Decision tree**
- Applicability domain** characterisation

## WORK FLOW



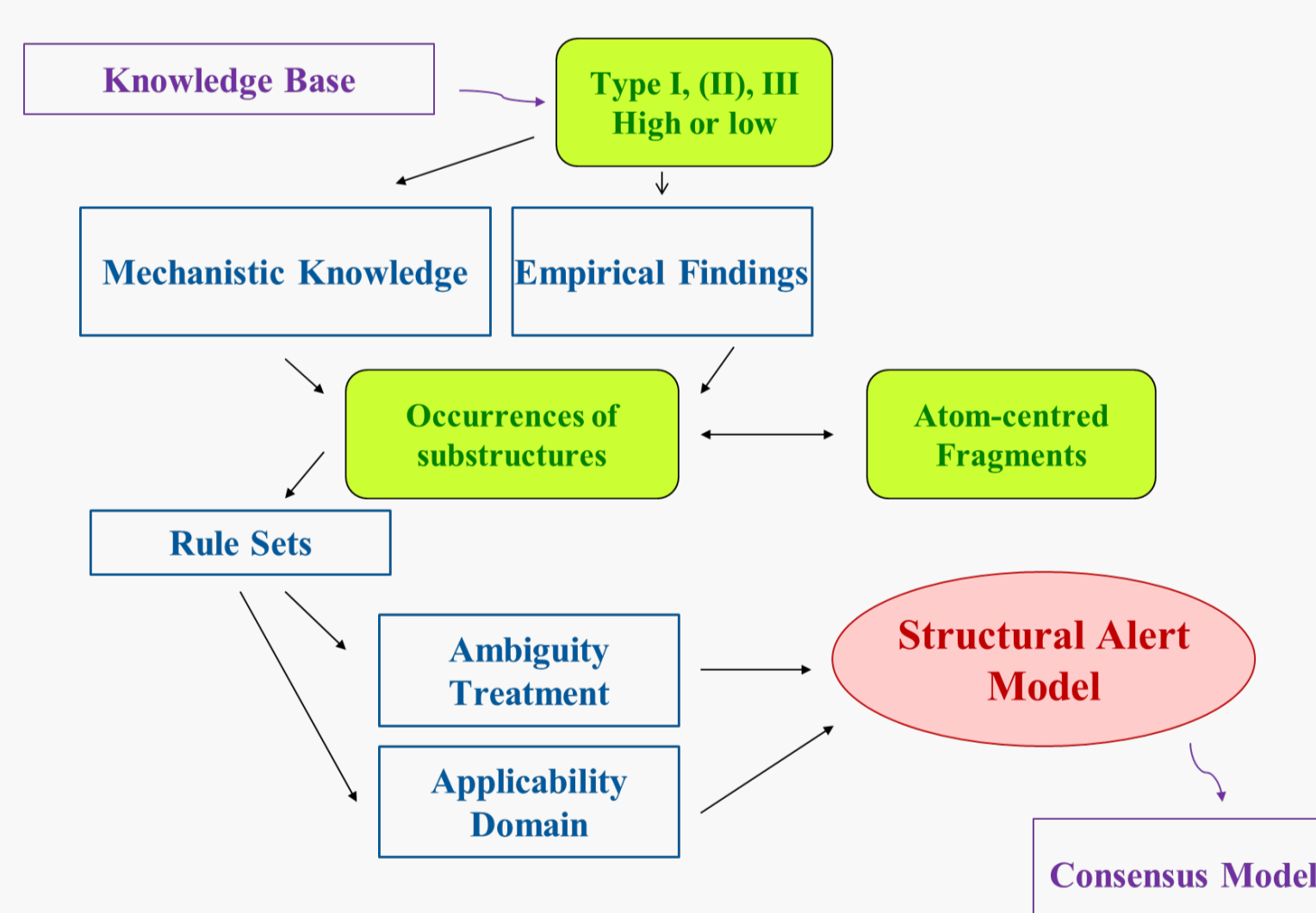
### KNOWLEDGE BASE

#### 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**



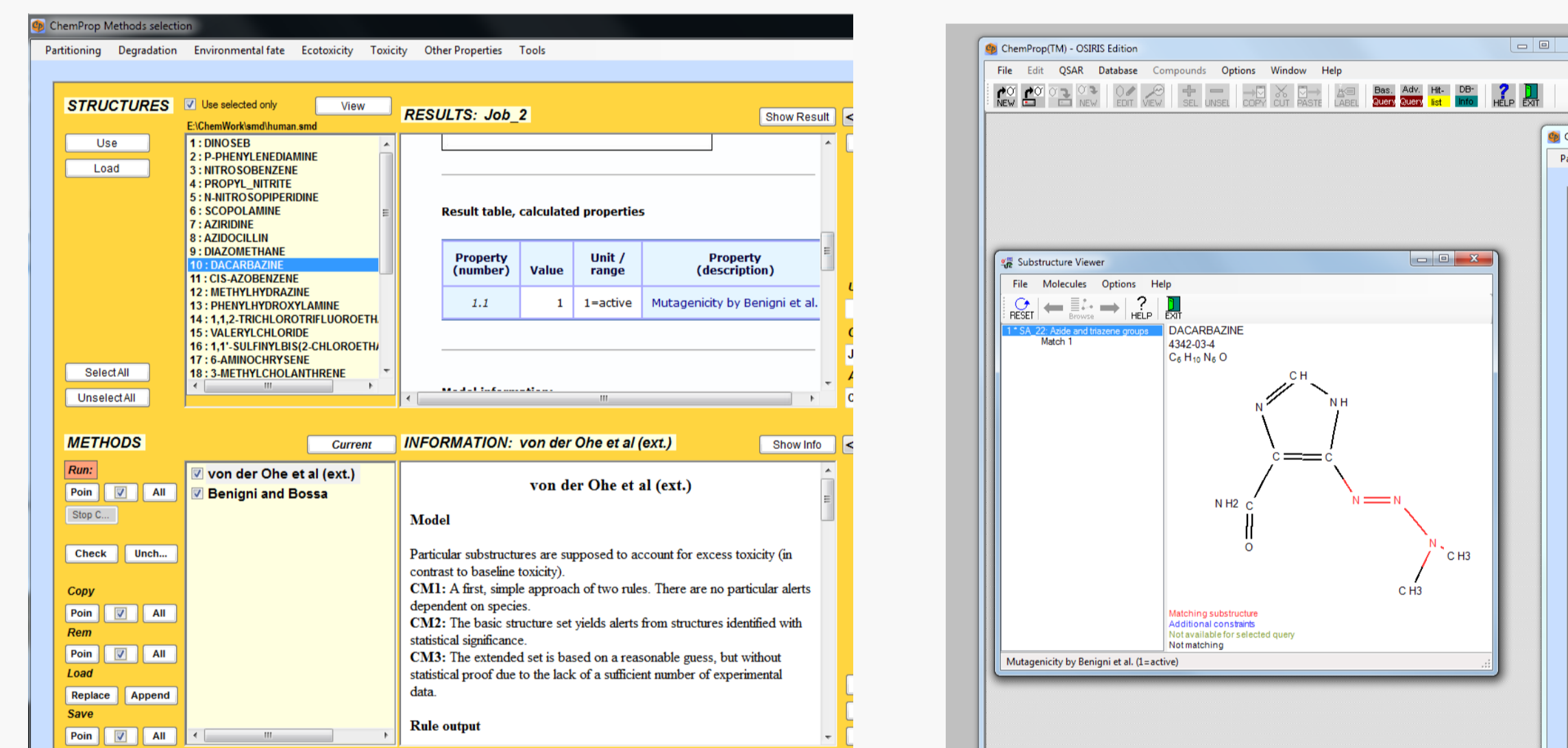
### MODELING

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

### ENVIRONMENTAL CONDITIONS

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

## COMPUTER IMPLEMENTATION: CHEMPROP

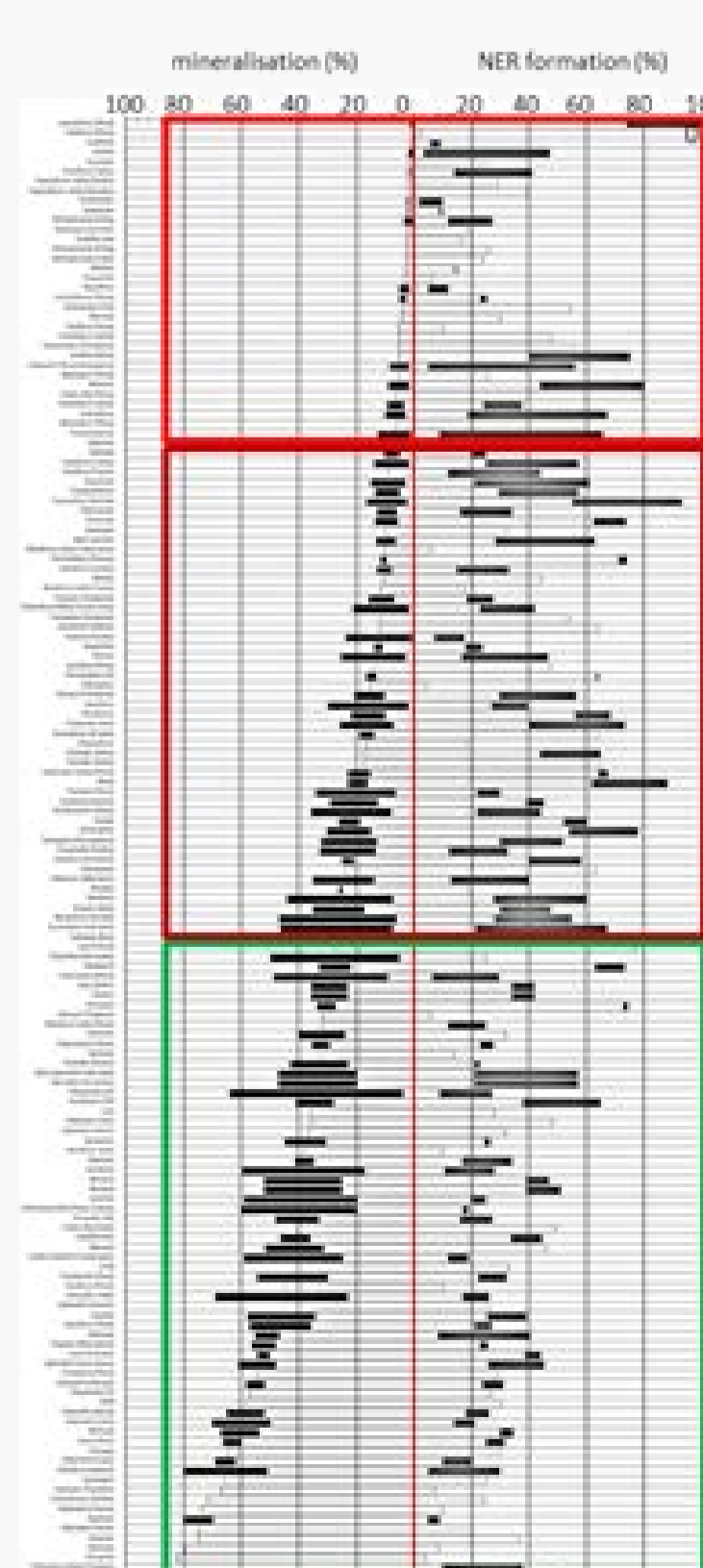


- Automated property and descriptor estimation**
- Reasonable default for environmental conditions**
- Database for chemical structures and project data**
- Model reliability**
- Documentation**

### CHEMPROP

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

## PROGRESS SO FAR (6 MONTHS)



### KNOWLEDGE BASE

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

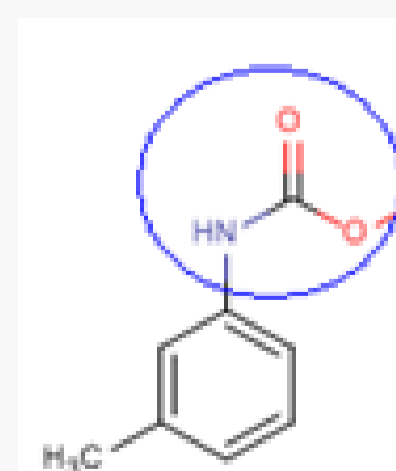
Preliminary classification of pesticides according to mineralisation and NER formation based on data from Barriuso E, Benoit P, Dubus I 2008. Formation of pesticide nonextractable (bound) residues in soil: Magnitude, controlling factors and reversibility. *Environ. Sci. Technol.* **42**: 1845–1854.

### MODELING

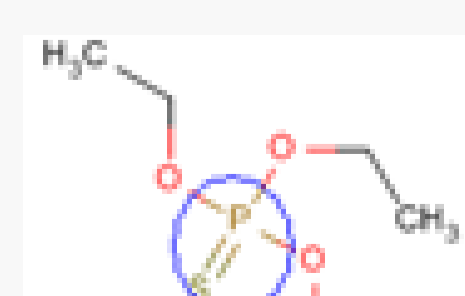
- First step: Structural alerts for general NER formation potential**
- Preliminary model: 10 confirmed alerts**
  - 8 for low potential,**
  - 2 for high potential**

#### 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

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