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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

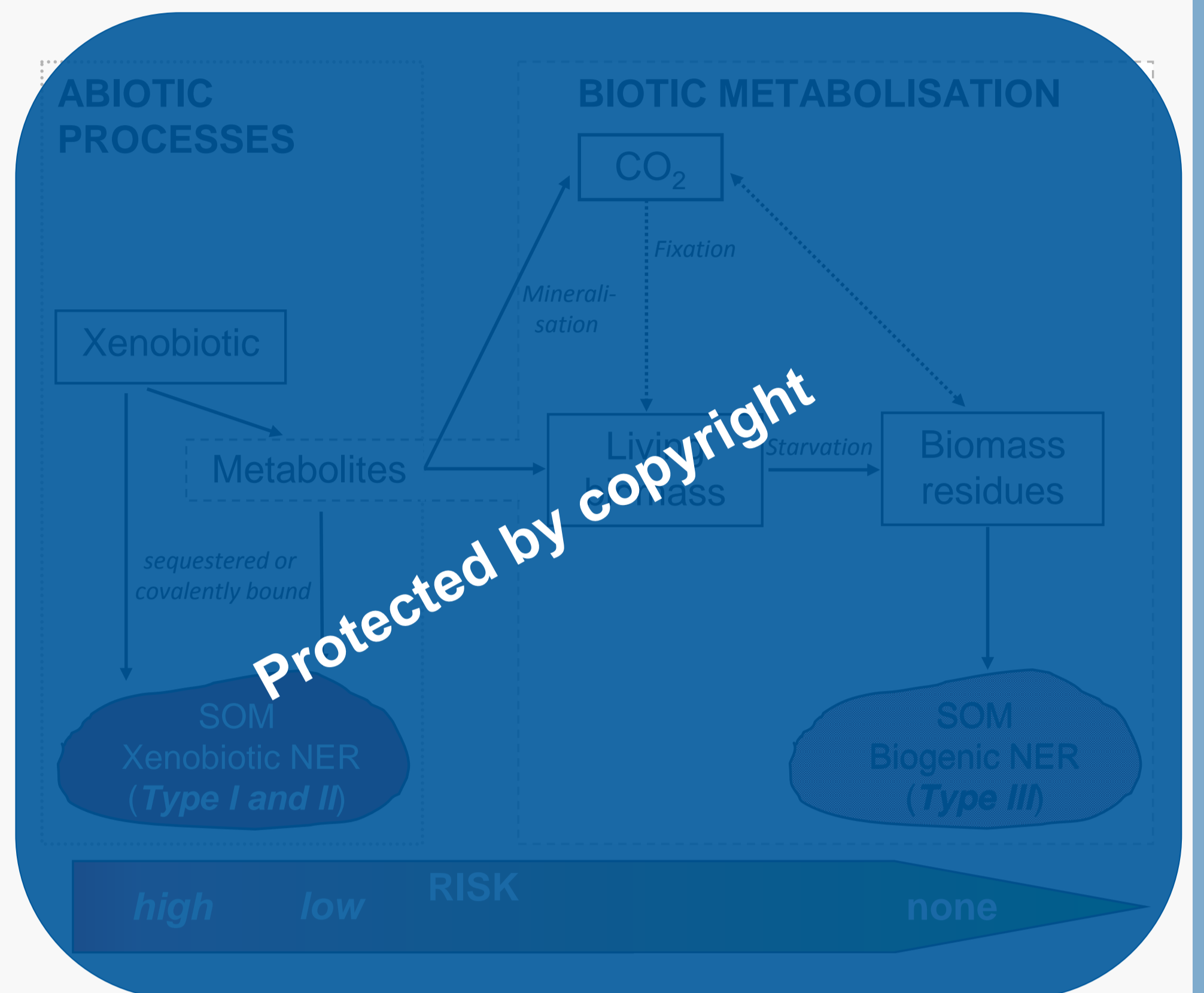
- Significant amounts** of NER formed under which **environmental conditions?**
- Do formed NER have **potential for environmental harm?**

PESTICIDES IN SOIL AND SEDIMENTS

Not publicly yet

Nowak KM et al., in preparation.

NER FORMATION



Kästner M, Nowak KM, Miltner A, Trapp S, Schäffer A 2014. Classification of Nonextractable Residue (NER) formation of xenobiotics in soil – a synthesis. Crit. Rev. ES&T. 44: 2107-2171.

CEFIC-LRI ECO-24

PROJECT TIMELINE

- Started **April 2014**
- Duration: **30 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) Low level quantum chemistry

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** characterization

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**

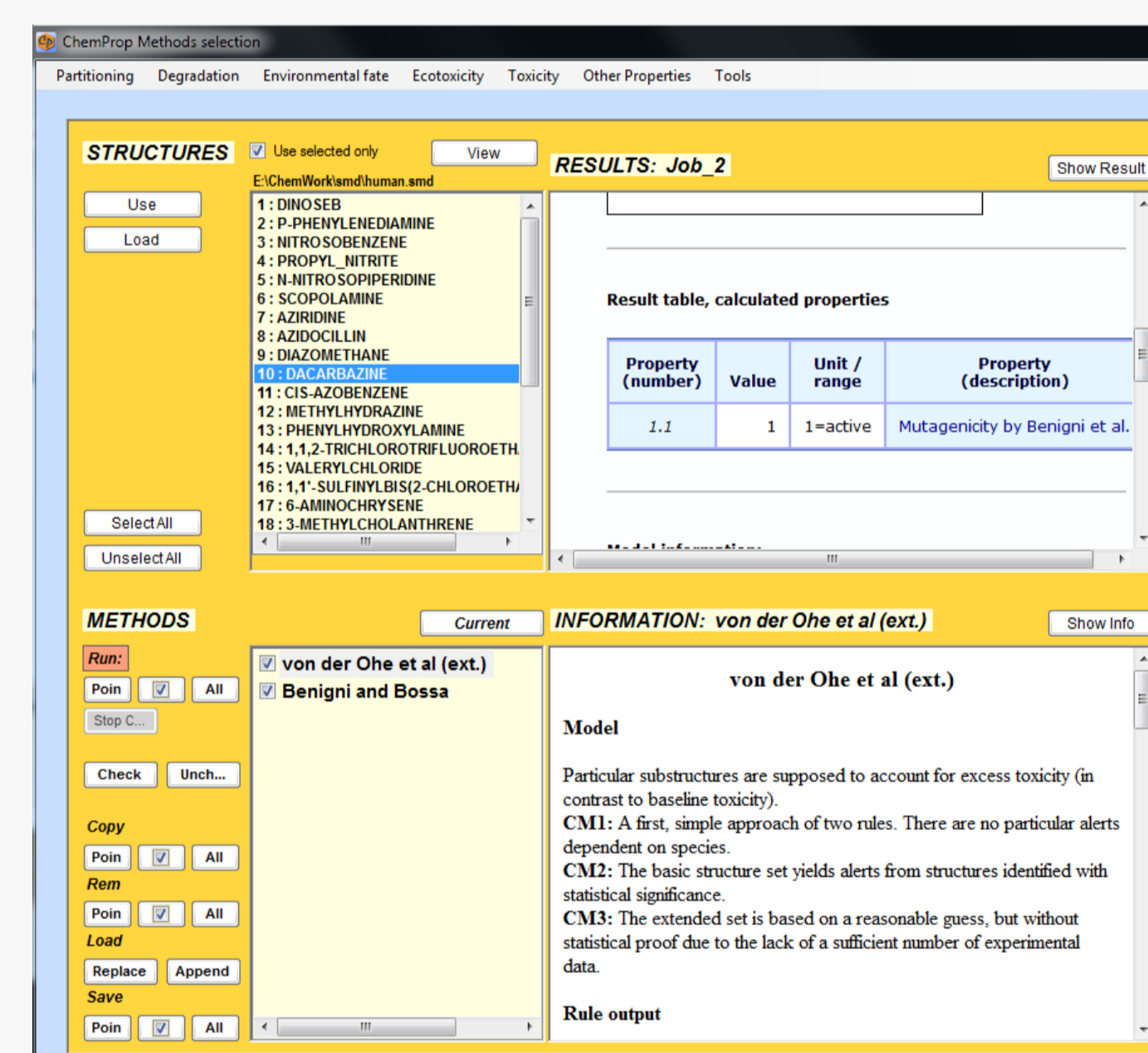
MODELING

- Structural alerts**
- Alternative models:**
 - Property thresholds from **LSER, low level quantum chemistry**
- Consensus: Weight of Evidence**

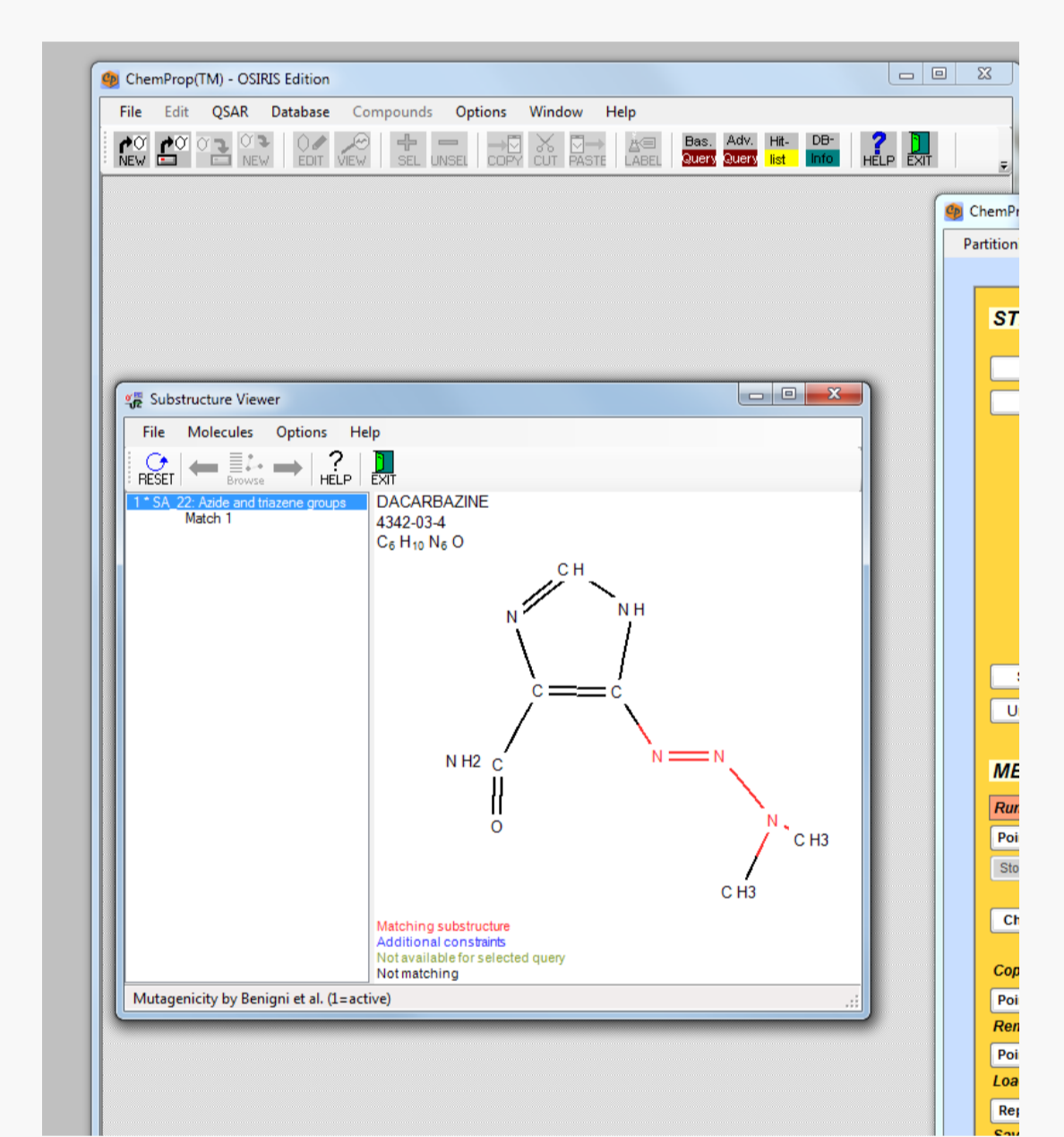
READ MORE

<http://cefic-lri.org/projects/lri-eco24-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/>

COMPUTER IMPLEMENTATION: CHEMPROP



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



CHEMPROP

- Publicly available for free** based on license
- Details:** <http://www.ufz.de/ecochem/chemprop>

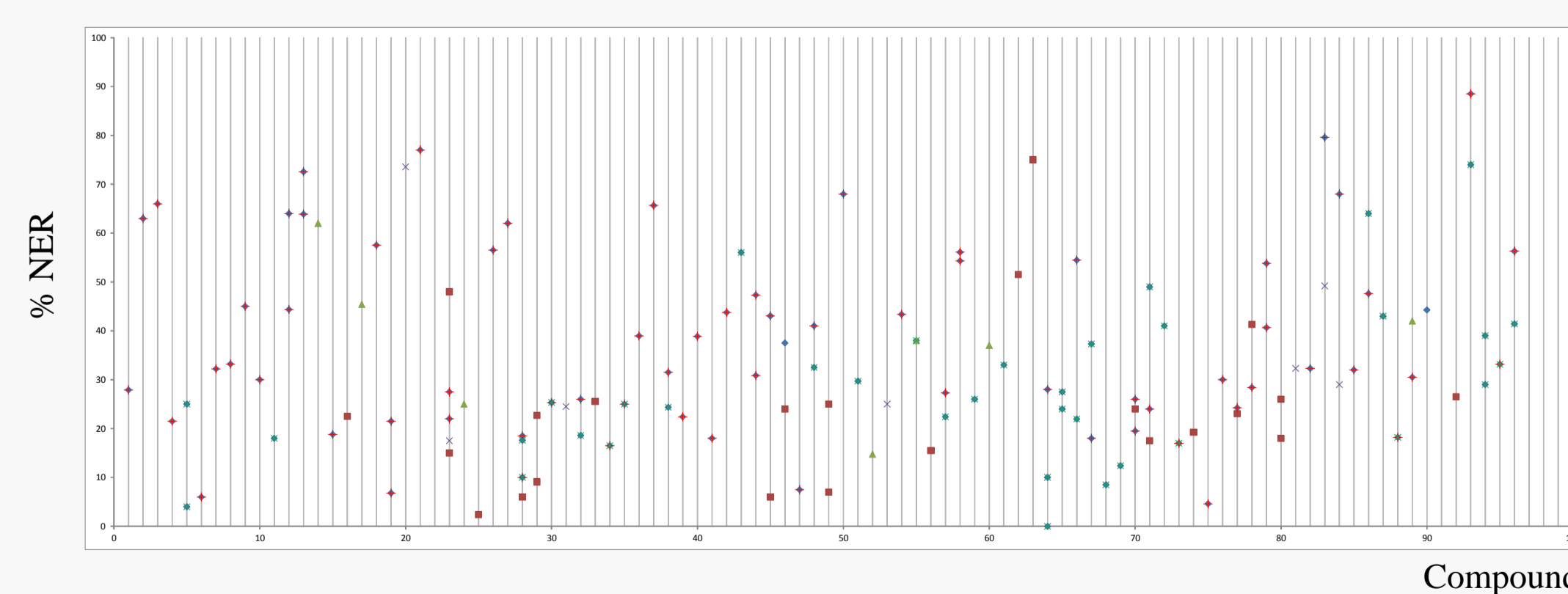
PROGRESS SO FAR (EXCERPTS)

KNOWLEDGE BASE

- Extensive **scientific literature** search performed
- Surprisingly (disappointingly) **few data** available, mainly comprised in one single review paper: 138 values for 95 compounds only
- Additional data source: **Public dossiers of EFSA** (European Food Safety Authority) 342 values for 218 compounds
- Merged **total data set:** 480 values for 295 compounds



DATA VARIABILITY

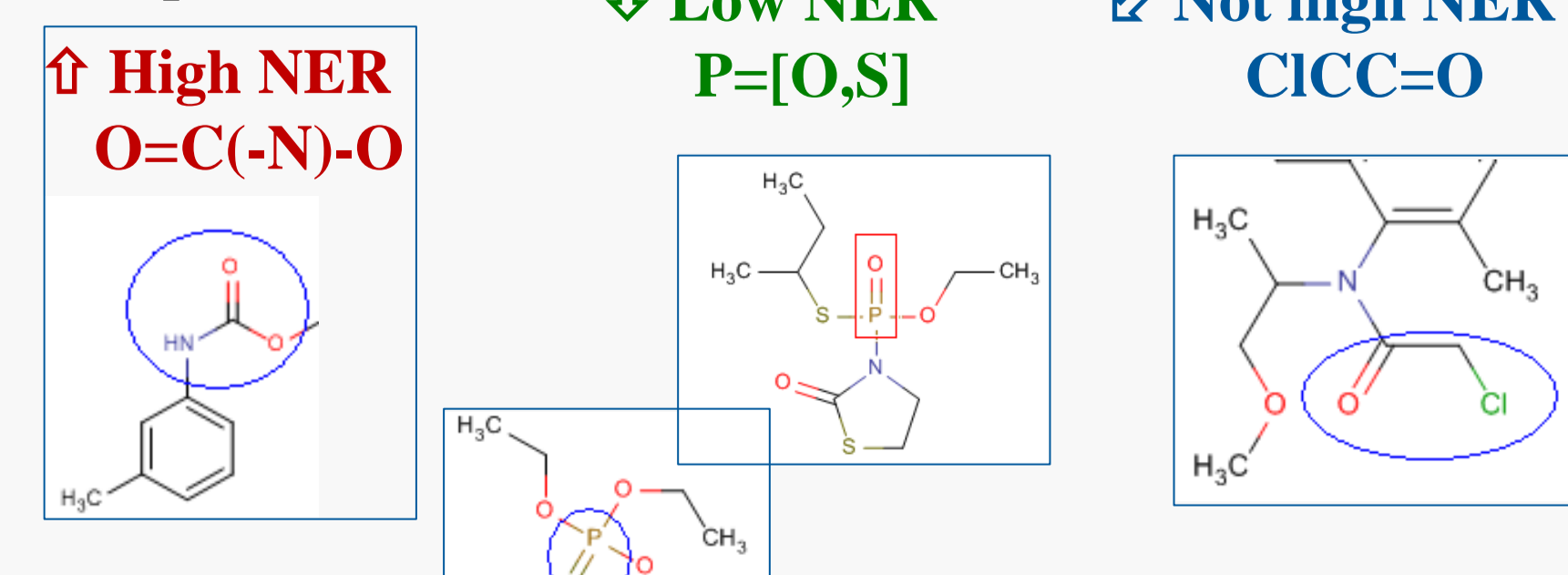


- Frequently **large variability** (scatter) even for **single chemicals**
- Additional **complication: C labelling** position

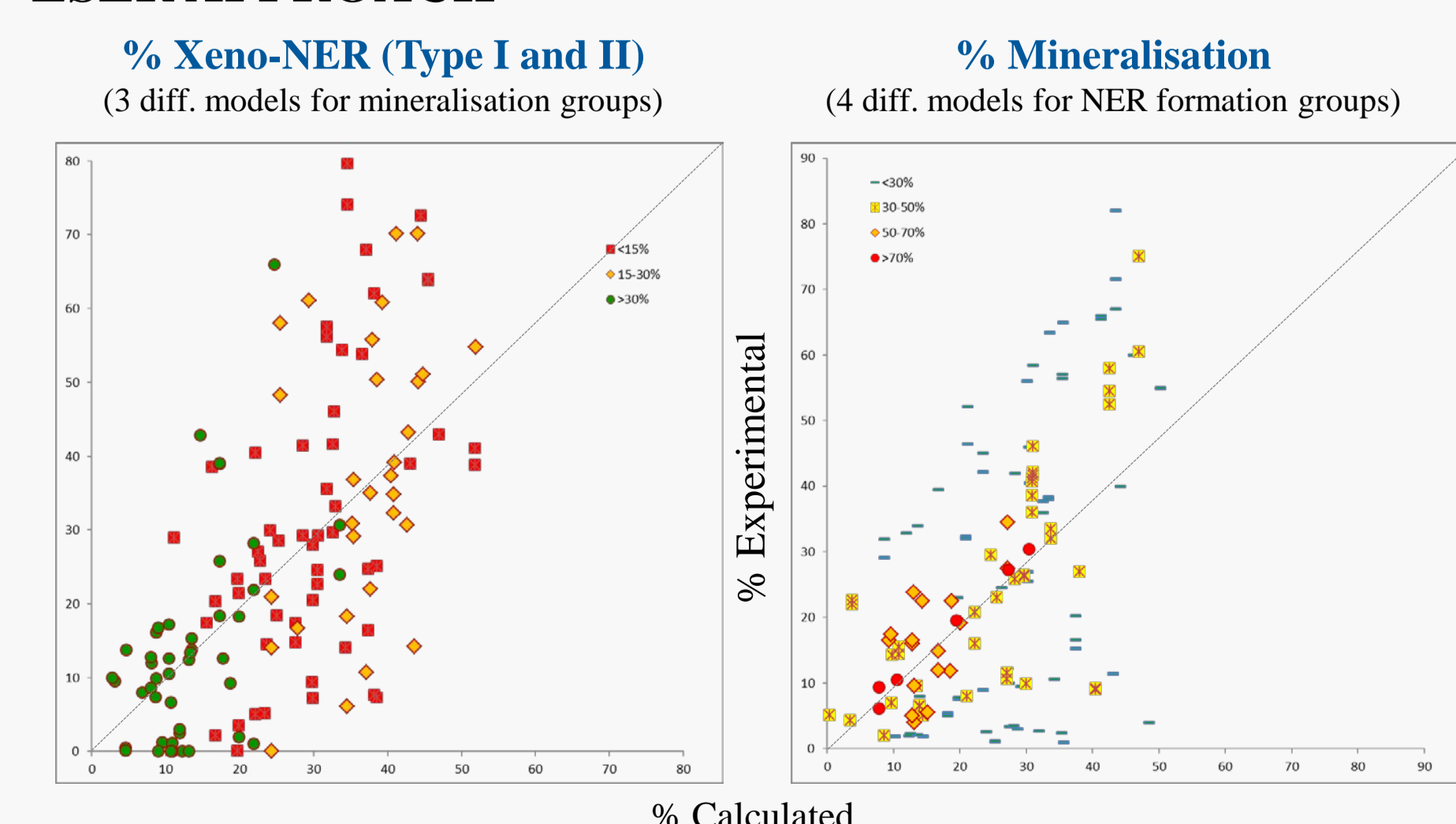
STRUCTURAL ALERTS

- Due to limited but heterogeneous data, only few alerts for **general NER formation potential**

Examples:



LSER APPROACH



ACKNOWLEDGMENT

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