ARISTO PROJECT NEWSLETTER

Issue 4 – November 2023

ARISTO

Academia Network for RevIsing and Advancing the Assessment of the Soil Microbial TOxicity of Pesticides.

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EDITORIAL

Prof. Dr. Kathrin Fenner – ARISTO Project

Modeling methods for pesticide evaluation

Chemical modeling has emerged as a valuable tool for predicting the fate and toxicity of various substances, notably pesticides, and has gained some regulatory acceptance, especially in the field of industrial chemicals. However, opinions on these models vary, with some proponents seeing them as the ultimate solution for managing the chemicals' assessment challenge, while others approach them with skepticism, perceiving them as mysterious "black boxes" that generate numbers of uncertain reliability (1).

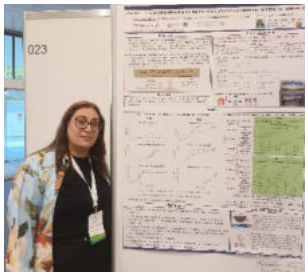
The utility of modeling becomes particularly evident when experimental investigations become difficult and resource-intensive. Take, for instance, transformation products (TPs) of pesticides, which significantly increase the assessment challenge, with approximately 4-5 TPs per parent pesticide recorded in regulatory dossiers, and some TPs likely still unnoticed. Noticeably, pesticide TPs often exhibit lower toxicity than their parent compounds for classical aquatic toxicity endpoints, but we must question whether this trend holds true for toxicity to soil microorganisms.

Two types of models are distinguished: data-driven, often referred to as machine learning (ML) or artificial intelligence (AI), and mechanistic, grounded in a deeper understanding of the underlying processes. Predicting the fate and toxicity of chemicals poses challenges on both fronts. Data, though relatively abundant for pesticides compared to other compounds, is still considered "scarce" in the context of data science applications, making purely data-driven models less feasible. Mechanistic understanding can provide valuable insights for certain processes, like partitioning, but falls short when dealing with complex interactions with living organisms, such as is the case for microbial degradation or toxicity. The crux of the challenge is finding a balance between incorporating our partial understanding of underlying mechanisms and making sense of existing data (2).

Model development in the ARISTO project illustrates two cases where we tried to enhance the learning capabilities of models by various strategies: (i) the prediction of transformation products (TPs) and (ii) the prediction of toxicity to soil microorganisms (AOMs) caused by pesticide TPs. For predicting TPs, a hybrid approach blends mechanistic understanding, represented by reaction rules, with a data-driven machine learning model. This combination is shown to yield superior results compared to relying solely on one approach (3). The prediction of toxicity involves a different "trick," leveraging the correlation between toxicity and the hydrophobicity of chemicals. By employing transfer learning, we try to develop models that are pretrained with the hydrophobicity of compounds and fine-tunned on AOM toxicity data. With the chemistry knowledge gained from pretraining on hydrophobicity, the toxicity model demonstrated a smoother training behavior and higher accuracy. These innovative approaches demonstrate how chemical modeling can be a powerful tool for understanding and managing the complexities of pesticide fate and toxicity.

1. Kostal et al (2020). Going all in: a strategic investment in in silico toxicology. *Chemical research in toxicology*, *33*(4), 880-888.
2. Satoh et al (2023). Can AI help improve water quality? Towards the prediction of degradation of micropollutants in wastewater. *Chimia*, *77*(1/2), 48-48.
3. Zhang et al (2023). enviRule: An End-to-end System for Automatic Extraction of Reaction Patterns from Environmental Contaminant Biotransformation Pathways. *Bioinformatics*, btad407.

UPDATES FROM THE FELLOWS



Eleftheria Bachtsevani

ESR1. In vitro assessment of the toxicity of pesticides on AOM

Ecole Centrale de Lyon – Dr. Graeme Nicol

NCIMB Ltd – Dr. Carol Phillips

Eleftheria is in the last year of her Ph.D. She is working on the comparison of pesticide toxicity on AOM and commercially available toxicity kit MARA (NCIMB, Aberdeen, Scotland). Also, in cooperation with the University of Vienna, the toxicity mechanisms of pesticides with the highest impact on the most sensitive of AOM are investigated.

Marjan Roshanfekrrad

ESR2. In vitro assessment of the toxicity of pesticides on AMF

Universite Catholique de Louvain – Prof. Stephane Declerck

INOQ – Dr. Carolin Schneider

Marjan has recently finished her experimental set up in INOQ company in Germany and has just harvested the trial two weeks ago. She is now occupied with different following analysis.

Laura Johanna Müller

ESR3. Studying the toxicity of pesticides on AOM, and other nitrifiers, in soil

Swedish University of Agricultural Sciences – Prof. Sara Hallin

SAYENS – Dr Abdelwahad Echairi

Laura and her industrial partner SAYENS have finished the field trial that was running in Bretenière, France, over the summer and sampled the last time point in October. The analysis will give insights in the effect of pesticides on the ammonia oxidising bacteria and archaea in the rhizosphere and roots under field conditions. Marta E. Pérez-Villanueva (ESR6) joined the first harvest and provided much needed help during her secondment!

Anna Manukyan

ESR4. Assessing the toxicity of pesticides on natural soil and plant assemblages of AMF

University of Thessaly – Dr. Kalliope Papadopoulou

INOQ – Dr. Caroline Schneider

Anna has successfully completed her field experiment at INOQ. Her research focused on assessing the impact of pesticides on the native soil communities of arbuscular mycorrhizal fungi, as well as the commercial inoculum containing *Rhizophagus irregularis*, in combination with the natural microbial community. She presented her microcosm experiment on a poster at the FEMS2023 Conference held in Hamburg, Germany, and she is also scheduled to share her work at MIKROBIOKOSMOS 2023 in Larissa, Greece. Furthermore, she is actively planning an experiment for her upcoming three-month secondment at Bayer in Germany, which is planned to start in January 2024.

Cara Meyer

ESR5. Studying the toxicity of pesticides on soil microbial networks

INRAE – Dr. Laurent Philippot

SYNGENTA – Dr. Claudio Screpanti

Cara has completed three microcosm experiments and has submitted her first article for publication. This article describes her first experiment and is entitled "Soil microbial community fragmentation reveals indirect effects of fungicide exposure mediated by biotic interactions between microorganisms".

Marta E. Pérez-Villanueva

ESR6. Pesticides toxicity at the soil food-web level: Defining effects on microbial predator-prey systems

UFZ – Leipzig – Prof. Antonis Chatzinotas

HYDREKA – Dr. Cedric Malandain

Marta is working on the analysis of the results for two different papers on the effects of predation in community composition and the top-down effect of pesticides on soil microbial communities in the framework of a food-web. In the last period, she completed her secondment at Sayens in Dijon, France, where she collaborated with Laura Müller (ESR3) and her field experiment. Additionally, she presented results of her research in a poster at the Conference BAGECO 2023 in Copenhagen, Denmark, and will also be present at the EcotoxicomicYR_23 webinar with an oral presentation.

Camilla Drocco

ESR7. Assessment of the toxicity of pesticide mixtures on soil microorganisms

INRAE – Dr. Fabrice Martin-Laurent

ECT Oecotoxicologie – Dr. Jorg Roembke

Camilla have completed her secondment at Syngenta, now she is back at INRAE in Dijon to finalize some lab work. She is currently analyzing the data from her experiments

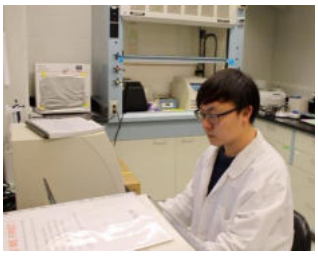
Alexandre Pedrinho

ESR8. Assessing the toxicity of bio-pesticides on soil microorganisms

University of Thessaly – Prof. Dimitrios Karpouzas

Metabolic Insights Ltd – Dr. G. Wittenberg

Alexandre has completed his experiment at Metabolic Insights in Israel. In this study, he assessed the impacts of selected synthetic and bio- pesticides on microorganisms in the rhizosphere of cucumber plants, both in the presence and absence of a target pathogen (Rhizoctonia). Currently, he is getting training on the use of bioinformatic tools and analyzing the amplicon sequencing data derived from his previous experiments.



Kunyang Zhang

ESR9. Development of tools for in silico prioritization of pesticide TPs for soil microbial ecotoxicity testing

EAWAG – Dr. Kathrin Fenner

ENVIPATH – Tim Lorshbach

Kunyang published his first work reading automatic rule generation on the Journal of Bioinformatics. This manuscript is entitled “enviRule: An End-to-end System for Automatic Extraction of Reaction Patterns from Environmental Contaminant Biotransformation Pathways”.

UPCOMING EVENTS

ARISTO Webinars
27.10.2023
24.11.2023
26.01.2024

Mikrobiokosmos Conference
Special ARISTO Session
Larissa, Greece
30.11.2023

ARISTO School Visits
Larissa, Greece
29.11.2023

ARISTO Open Day
Larissa, Greece
30.11.2023

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