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Untargeted metabolic profiling of environmental volatile compounds by Headspace-Solid Phase Micro Extraction-Gas Chromatography-Mass Spectrometry: an introduction to environmental “volatilomics”

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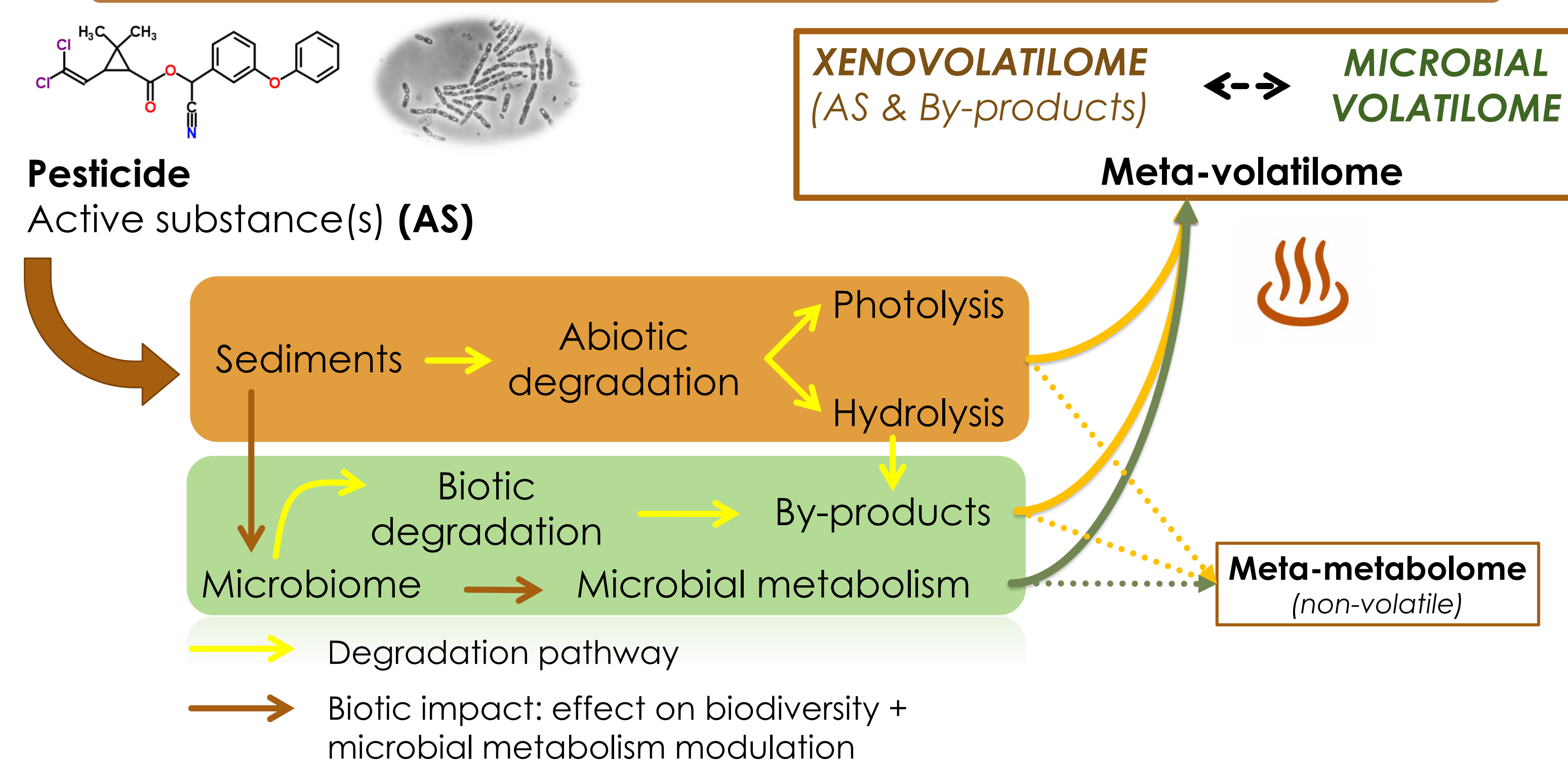
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Abstract

Pesticide use is permanently increasing for several reasons. However, these chemical compounds are threatening human health and environment. Thus, natural pesticides are recently emerging as an alternative solution. In fact, as these biopesticides are issued from nature, they are supposed less harmful versus the environment. However, the evaluation of biopesticides' environmental impact remains an actual challenge. In fact, classical methods e.g. half-life are limited, due to the complexity of biocontrol products. Thus, new omics-based methods are being developed in order to adapt new environmental evaluation protocols. In this context, Environmental Metabolic Footprinting (EMF) was recently developed using Liquid Chromatography-Mass Spectrometry (LC-MS) based metabolomics approach. Recently, a new approach was considered in order to study the volatile compounds in environmental samples. In fact, pesticide degradation can lead to volatile by-products. Moreover, volatile microbial compounds can signalize biodiversity disruptions. Thus, novel Headspace-Solid Phase Micro Extraction-Gas Chromatography-Mass Spectrometry (HS-SPME-GC-MS) based analytical method is being developed, in order to analyze the environmental “Volatilome” (xenovolatilome + microbial volatilome). This methodology shows several advantages: no laborious and complex steps for sample preparation are needed. Therefore, this method reduces time, solvents and chemical reagents consumption, which agrees with green chemistry and reduce analysis cost. Preliminary tests were performed with sediment samples treated with *Bacillus thuringiensis israelensis* (*Bti*); a complex bio-insecticide, and the α -Cypermethrin, a standard chemical insecticide.

1. Introduction to “environmental volatilomics” concept



2. Material and Methods

Matrix studied: Sediments
 Kinetics: 2 points (Day 0 and Day 8)
 Incubation in dark at 22±2 °C
 4 groups applied:

Control H ₂ O	Commercial <i>Bti</i>	Control MeOH	Pure α -Cypermethrin
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Extraction conditions:

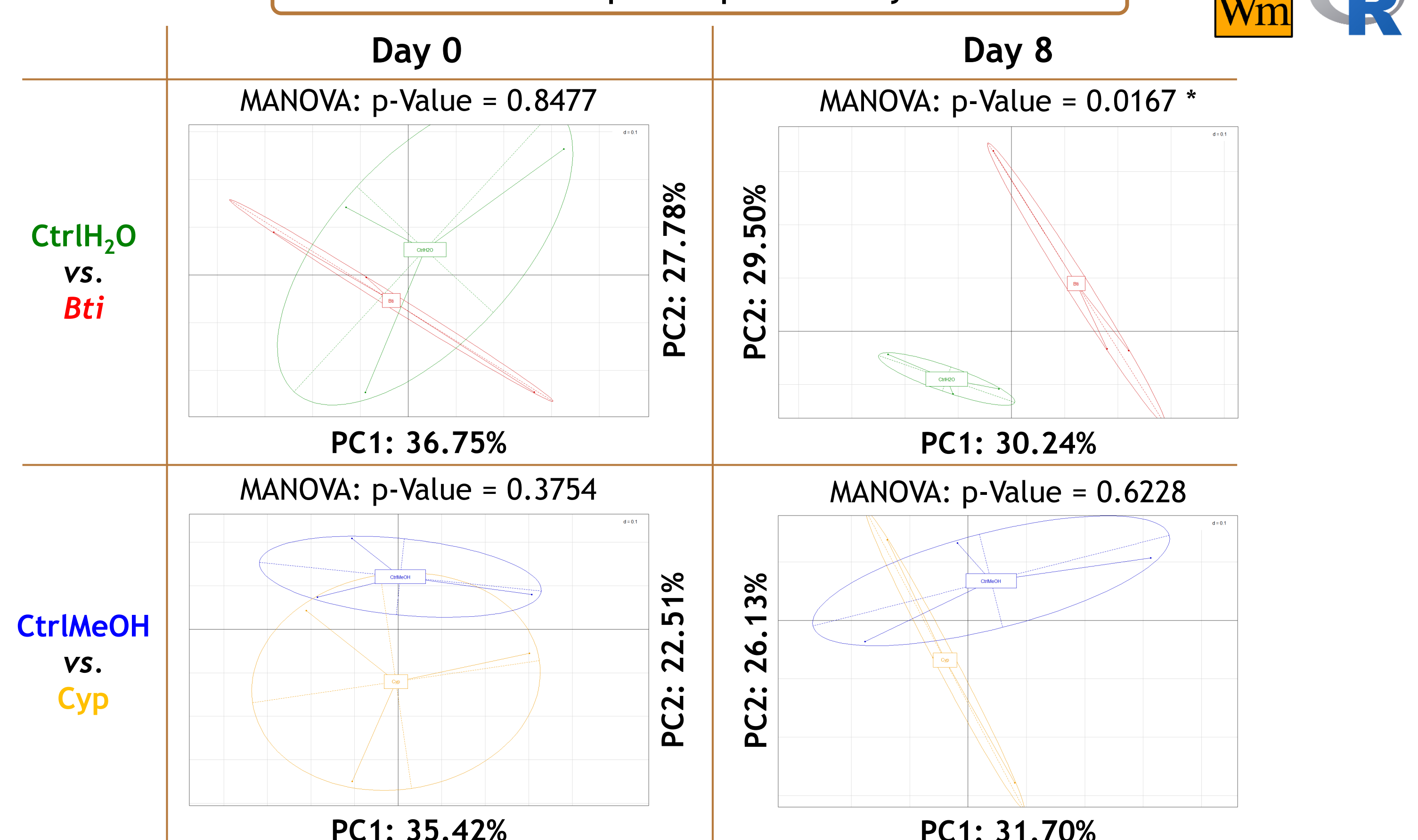
- Temperature: 45 °C
- Incubation: 10 min
- Extraction: 50 min
- Fiber type: DVb/CAR/PDMS

Analytical system & conditions:

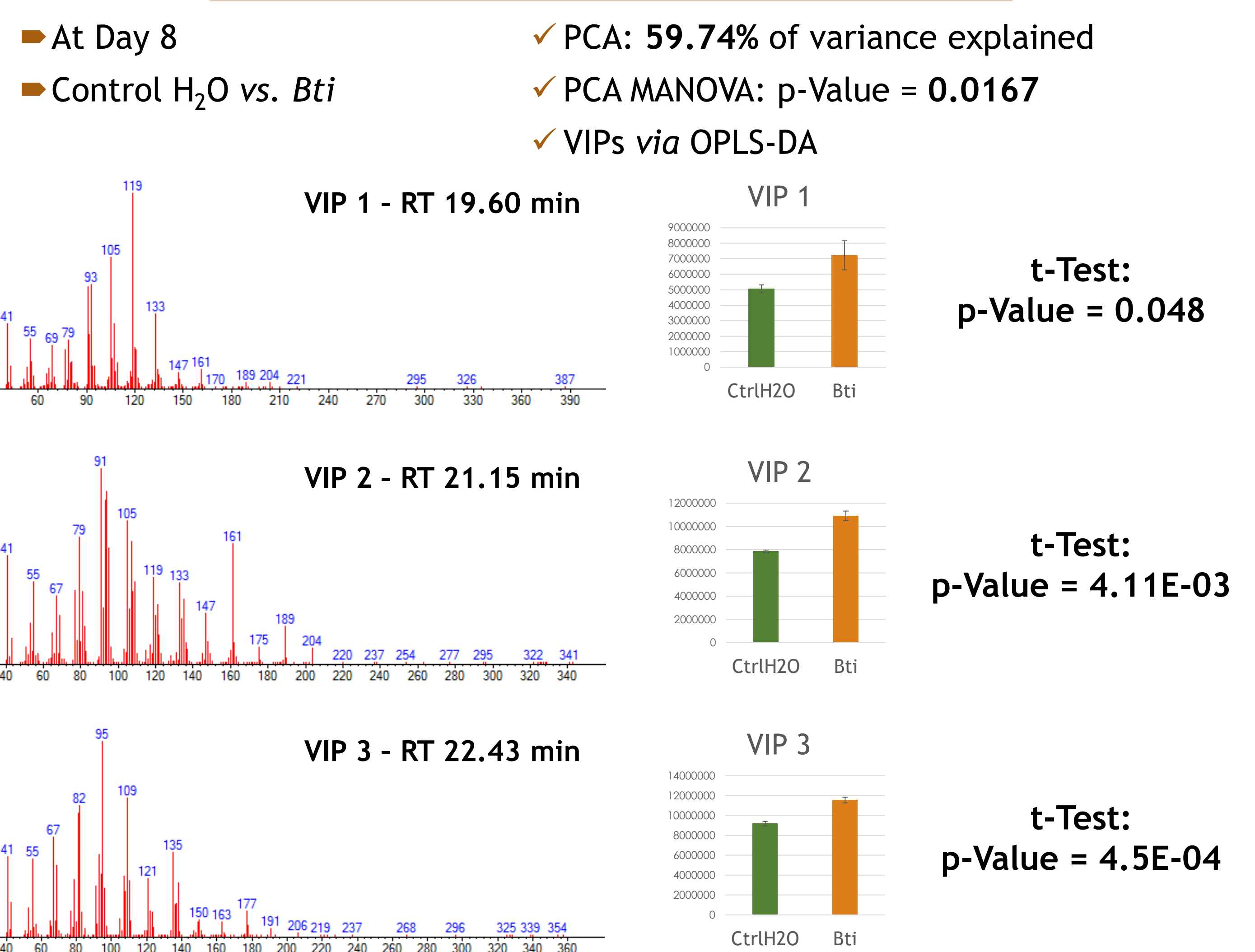
- Thermo Focus-DSQ II (GC-MS)
- Capillary column: Zebtron ZB-5MS (30 m)
- Gradient: 50-300 °C
- Scan range: 40-400 m/z

3. Results and Discussion

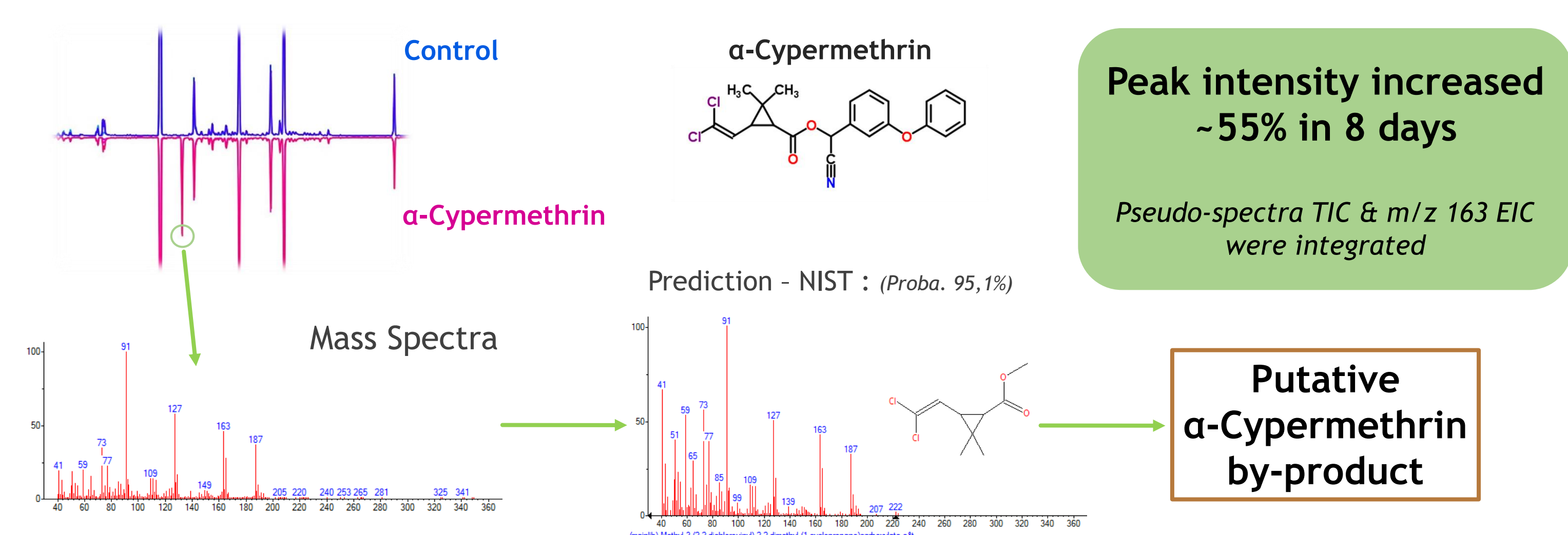
3.1. Principal Component Analysis



3.2. CtrlH₂O vs. *Bti* - Variable Importance in Projection



3.3. α -Cypermethrin metabolite - Days 0 and 8



4. Application and Perspectives

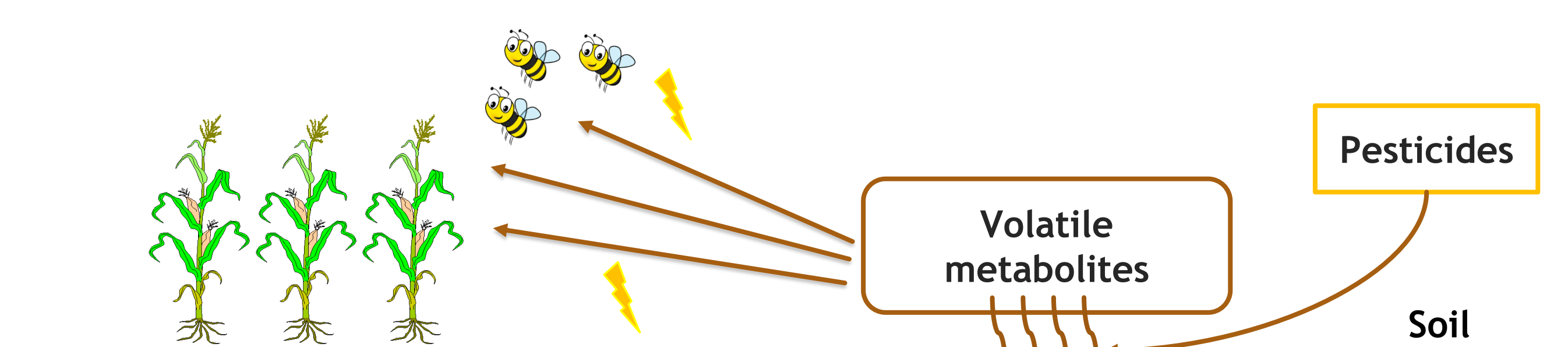
Results demonstrated sufficient sensitivity to discriminate between *Bti* treated samples and control samples

Perspectives:

- Enhancing sampling strategy
- Improving extraction & analytical conditions

Application:

- Integration in the EMF approach for resilience time determination
- Detection of potentially harmful volatile compounds



References:

- Environmental Metabolic Footprinting: A novel application to study the impact of a natural and a synthetic β -triketone herbicide in soil, Patil C., Calvayrac C., Zhou Y., Romdhane S., Salvia M. V., Cooper J. F., Dayan F., Bertrand C., *Science of The Total Environment*, 1 October 2016. <https://doi.org/10.1016/j.scitotenv.2016.05.071>
- Environmental Metabolic Footprinting (EMF) vs. half-life: a new and integrative proxy for the discrimination between control and pesticides exposed sediments in order to further characterise pesticides' environmental impact, Salvia M. V., Ben Jrad A., Raviglione D., Zhou Y., Bertrand C., *Environmental Science and Pollution Research*, 28 June 2017. <https://doi.org/10.1007/s11356-017-9600-6>

Acknowledgments

