Bio-transformation of Xenobiotics

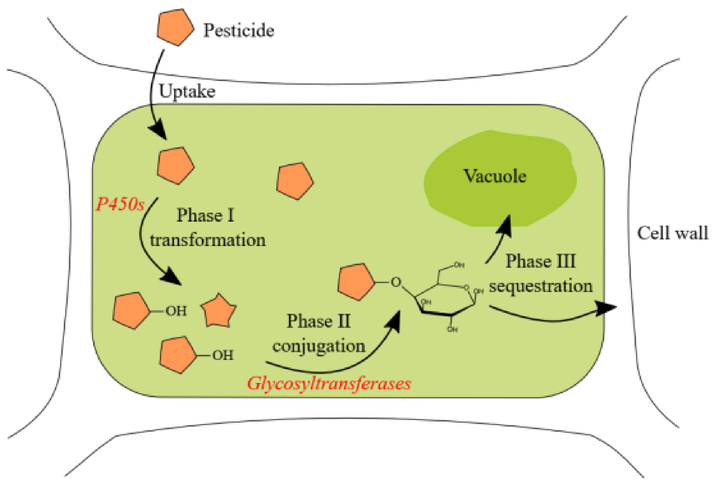


Figure 1. Example of xenobiotic biotransformation processes in plants involving a three-phase process, known as the "green liver model".

What is being measured: The degradation products and metabolites of man-made chemicals, also referred to as xenobiotics, are screened for and identified in various biological and environmental sample matrices using a mass spectrometry-based targeted and non-targeted metabolomics approach. Following the intake of xenobiotics perceived to be harmful to a biological system, the organism responds through a three-phase detoxification process. Phase-I chemical reactions transform the parent molecules through oxidation, reduction, or hydrolysis. Phase-II reactions involve conjugation of phase-I products to glucopyranosides and/or glutathione. In phase-III, less toxic phase-II metabolites are sequestered into vacuoles or cell walls. Understanding the metabolic pathways of xenobiotics in microbes, plants, and animals is critical for comprehensively addressing their impacts on various ecosystems.

How it is done: Tissue extracts are analyzed using ultra-high performance liquid chromatography coupled with an ultra-high resolution mass spectrometer. The acquired data are subsequently processed using custom designed workflows for spectra alignment, compound detection, grouping, and identification of potential degradant products and metabolites.

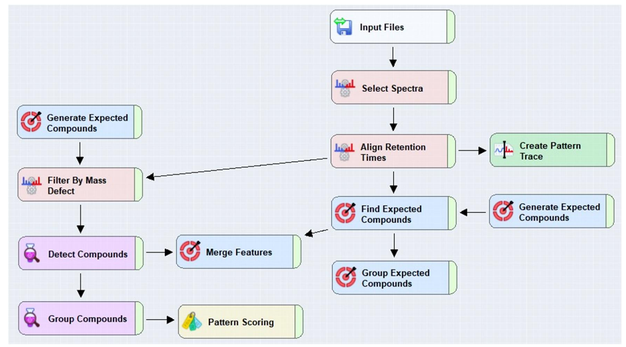


Figure 2. Data analysis workflow employed for the identification of unknown metabolites or degradation products of xenobiotic chemicals.

RESULTS

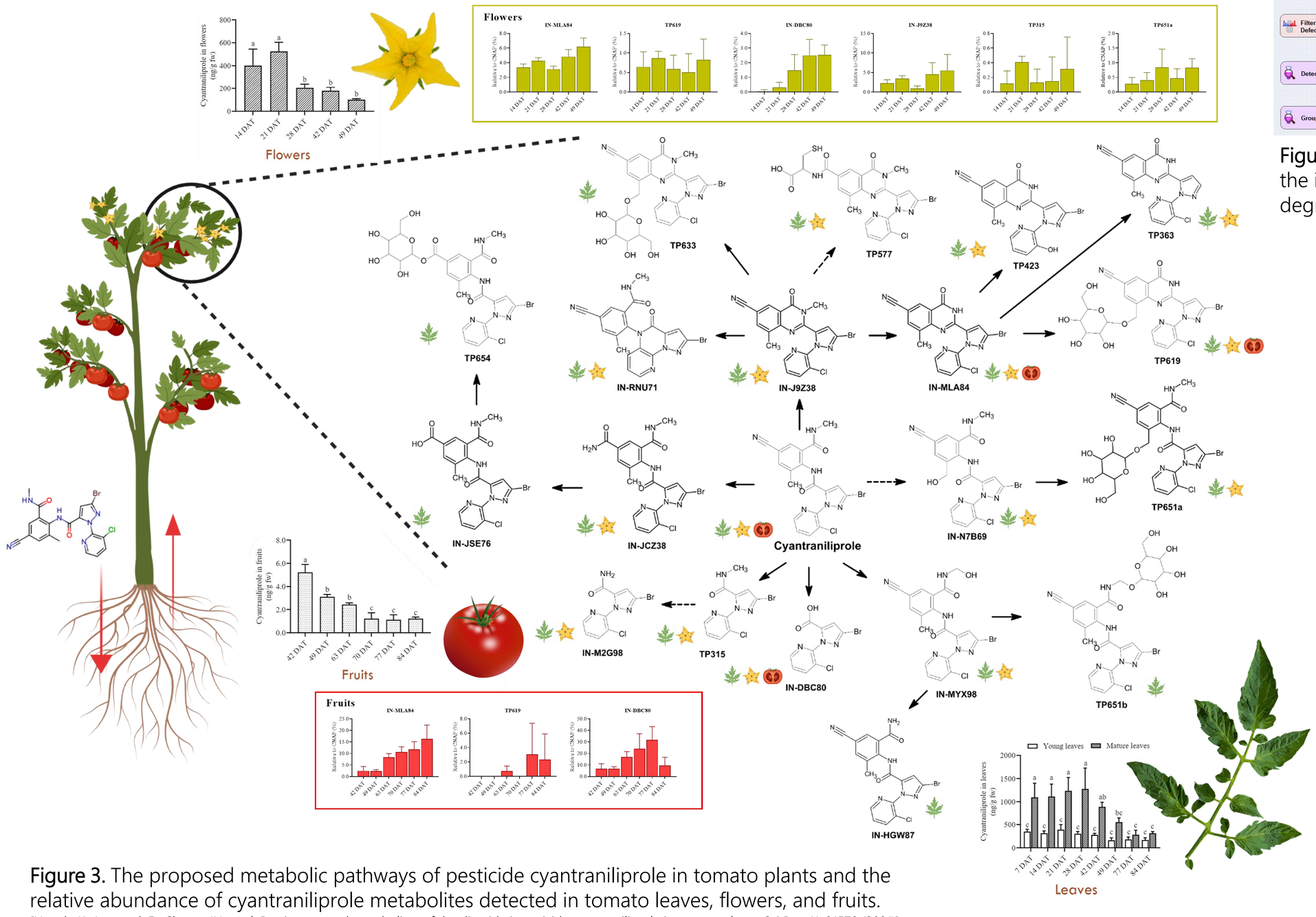


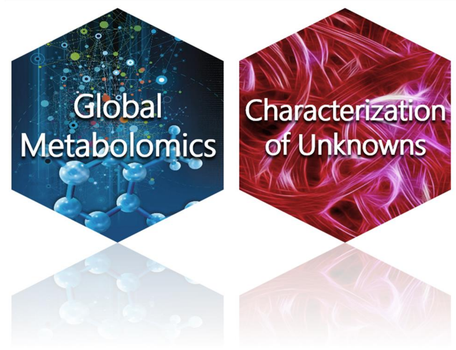
Figure 3. The proposed metabolic pathways of pesticide cyantraniliprole in tomato plants and the relative abundance of cyantraniliprole metabolites detected in tomato leaves, flowers, and fruits.
[Huynh, K., Leonard, E., Chong, JH. et al. Persistence and metabolism of the diamide insecticide cyantraniliprole in tomato plants. Sci Rep 11, 21570 (2021)]

INSTRUMENTATION

Thermo Orbitrap Fusion™ Tribrid™ Mass Spectrometer

- Combines quadrupole, ion trap and Orbitrap mass analysis in Tribrid architecture
- Ultrahigh resolution up to 500,000 FWHM
- Sub ppm mass accuracy
- Multiple dissociation techniques—CID, HCD, ETD
- ID-X capability for small molecule identification
- Coupled to HESI and nano-ESI interfaces
- UltiMate 3000 RS UHPLC & UltiMate 3000 RSLCnano

Primary applications



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