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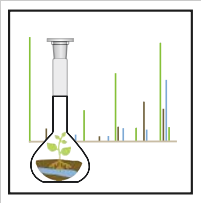

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An Innovative Approach for Analyzing Phytotoxins as Micropollutants in the Environment

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Phytotoxins (PTs) are bioactive compounds originating from plants. Typically, they are small molecules (<1000 Da) acting as secondary metabolites to support plant growth and development. When released into the environment, PTs are recognized as a new category of environmental micropollutants and can lead to adverse effects when the exposure levels exceed the tolerance thresholds for humans and animals.[1] To date, only a small number of PTs have been investigated in terrestrial and aquatic environments. Consequently, our understanding of their environmental occurrence, transport, fate, and eco-toxicological risk remains limited.

Detecting and monitoring PTs in terrestrial and aquatic environments is challenging. This is due to their structural diversity, spatial variability influenced by *e.g.* vegetation and land use, and fluctuating loads tied to seasonal and climatic factors. The lack of reference standards and informational databases further complicates their qualitative and quantitative analysis.

To tackle the challenge, we suggest *Source Supported Suspect Screening* (4S), a liquid chromatography-mass spectrometry based analytical strategy in combination with knowledge on plant secondary metabolites to detect and identify specific source-related chemicals. The 4S approach enables fingerprinting analysis of PTs along their temporal and spatial trajectories, from plant origin to environmental occurrence and fate in soil and water. Demonstrated in a five-month crop field experiment in Switzerland with blue lupin (*Lupinus angustifolius* L) (Fig. 1), the 4S approach successfully enabled the detection of 41 flavonoids and 12 alkaloids in agricultural soil, drainage water or surface water, linking them to the lupin plant (Fig. 2).[2] The study also revealed that the occurrence and abundance of PTs in terrestrial soil and aquatic environments can be influenced by both the stage of plant growth and weather conditions. The successful application of the 4S approach in the lupin field study suggests a great potential for using source-supported strategies in investigations of PTs in aquatic and terrestrial environments.

The 4S approach can be an efficient and reliable strategy for analyzing PTs in plant, soil and water, elucidating their occurrence from downstream environments back to the plant's origin.

Fig. 1. Photo of the lupin plant. Lupins are a popular European legume crop. The seeds are rich in protein content, making them a promising substitute for soybeans. However, the plant produces alkaloids and flavonoids which can become toxic when exceeding certain thresholds. © Agroscope, Gabriela Brändle

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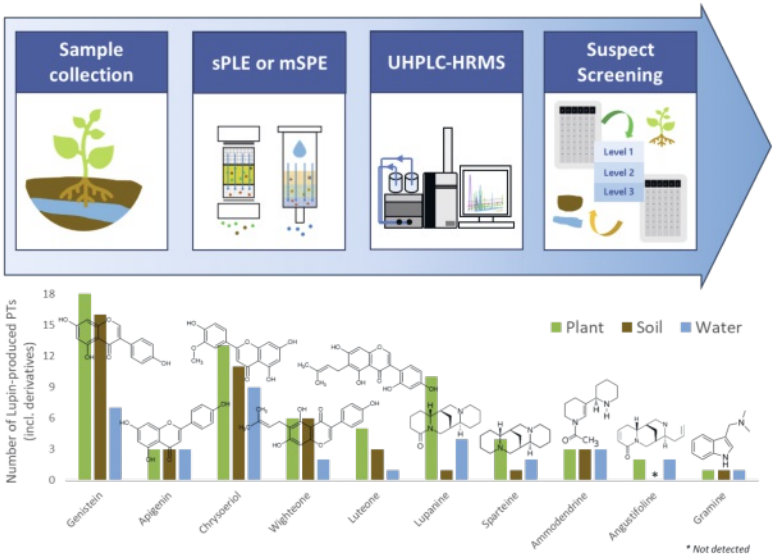

Fig. 2. Illustration of using 4S strategy to identify lupin-produced phytotoxins (PTs; flavonoids and alkaloids) in the downstream terrestrial and aquatic environments. sPLE, selective pressurized liquid extraction; mSPE, multi-layer solid phase extraction; UHPLC, ultrahigh-performance liquid chromatography; HRMS, high resolution mass spectrometry.

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