From soil to structure: electron diffraction reveals crystalline compounds in roots' exudates and their environment

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Root exudates are substances that are released by the roots of plants into their environment. These compounds influence the composition of the microbial communities surrounding the plant roots and affect various biological processes in the rhizosphere. Plant roots release a wide range of substances, including inorganic ions, amino acids, amides, sugars, aliphatic and aromatic acids, volatile aromatic compounds as well as vitamins, peptides, proteins, enzymes, plant hormones, biological nitrification inhibitors, etc [1]. Root exudates play a crucial role in mediating interactions between plant roots and inorganic compounds in the soil. These interactions influence the availability of nutrients, mineral weathering and the mobility of various elements [2].

Since various compounds are released from the roots to the soil, comprehensive studies using different analytical techniques are required to accurately investigate the interactions between plants and the surrounding environment, both for basic research and for applications to increase plant resilience and improve stress tolerance. The most commonly used methods for analysing root exudates include either liquid chromatography (LC) or gas chromatography (GC) coupled with mass spectrometry (MS) and nuclear magnetic resonance (NMR) [3].

In our current work, we decided to use a different analytical technique to study the composition of root exudates, namely 3D electron diffraction (3D ED). This technique is revolutionary in its ability to analyse individual compounds from nano- to microscopic crystals has been the subject of intense progress over the last decades [4]. Compared to the other methods used for metabolomic studies mentioned above, 3D ED is not as automated, but the amount of material required for analysis is incomparably smaller, and the sensitivity of our method is very high. Only one drop of a root exudate extract (about 1 µL of the extract) was sufficient for 3D ED experiments, so that we could try to find as many different compounds as possible during the analysis - we performed a so-called untargeted analysis. The initial attempt reveal several different inorganic structures from a single drop. Currently, we are working on better differentiation by separating targets with various types of solvents.

[1] P. Dundek, L. Holík, T. Rohlík, L. Hromádko, V. Vranová, K. Rejšek, P. Formánek, *Acta Univ. Agric. Silvic. Mendelianae Brun.* **2011**, *59*, 241–246.

[2] W. Ma, S. Tang, Z. Dengzeng, D. Zhang, T. Zhang, X. Ma, *Front. Microbiol.* **2022**, *13*, 1–19.

[3] M. A. Salem, J. Y. Wang, S. Al-Babili, *Front. Plant Sci.* **2022**, *13*, 1–9.

[4] M. Gemmi, E. Mugnaioli, T. E. Gorelik, U. Kolb, L. Palatinus, P. Boullay, S. Hovmöller, J. P. Abrahams, *ACS Cent. Sci.* **2019**, *5*, 1315–1329.

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