European Laboratory for enhanced automatic metabolite annotation (ELution)

Initiative: Kurswechsel – Forschungsneuland zwischen den Lebenswissenschaften und Natur- oder Technikwissenschaften

Ausschreibung: Planning Grants

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Laufzeit: 1 Jahre

Projekt-Website: Not applicable

Laboratory instruments can now detect signals from thousands of metabolites in biological samples. With these data, goals that were beyond reach, such as identifying food intake biomarkers or compounds formed in the gut microbiota, become reachable. But major obstacles remain. Currently no more than 20% of the overall metabolites can be identified through spectral analysis of their fragments, and this is really the main bottleneck for innovation. ELution's main goal is to implement a new multidisciplinary concept to enhance annotation of metabolites by (a) integrating existing metabolomics platforms for more accurate combined annotation, and (b) supplementing mass spectral databases with synthetic mass spectra from quantum chemistry-based simulation methods. This highly improved annotation of metabolites will allow to create new possibilities in data analysis and knowledge discovery. By combining multidisciplinary expertise in one lab, the applicants propose a synergy with the potential of a large impact in nutrition, and human health in general.

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