GLUCOSINALTE PROFILING BY PRECURSOR ION SCANNING

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Glucosinolates (β-thioglucoside-N-hydroxysulfates) are secondary plant metabolites identified in many plants of the order Brassicales. Few garden crops and vegetables like e.g. broccoli, cauliflower, brussel sprouts, raddish and Chinese cabbage contain nutritional relevant amounts of glucosinolates in their dry weight. We present an LC-UV-MS/MS method for the detection and quantification of glucosinolates from seeds and edible parts of these plants. The product ion spectra of glucosinolates have in common the occurrence of four characteristic fragment ions with m/z values of 97, 96, 80 and 75. We utilize this fragmentation pattern for parallel quadruplicate precursor ion scanning in negative mode. This scan type indicates directly the mass of negatively charged molecular ions which give rise to formation of these characteristic fragment ions. Since a glucosinolate is only considered as detected if all four fragment ions share the same precursor mass this MS experiment is highly specific for glucosinolates. Compared to other scan modes like e.g. selected reaction monitoring experiments the precursor ion scan is not only more specific but also unbiased. It has the capability to detect unknown glucosinolates which would fail to be detected in an MRM experiment if the preset transitions do not match. We applied the method successfully to screen seeds, plant extracts and also processed foods like broccoli soup for glucosinolates. In cases where reference standards were available a quantitative determination by UV-detection at 227 nm was also possible.