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ACCEPTED MANUSCRIPT

Glycerolipid Profiling of Yellow Sarson Seeds using Ultra High Performance Liquid Chromatography Coupled to Triple Time-of-Flight Mass Spectrometry

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Abstract

Yellow sarson (Brassica rapa ssp. trillocularis) is an important rapeseed-mustard species of Brassica rapa due to its high seed oil content. Glycerolipids and fatty acid composition affect seed germination and determine the quality of seed oil. To date, no information is available on the composition of individual glycerolipids in this species. Therefore, in this study the glycerolipid profiling of yellow sarson seeds was performed using ultra high performance liquid chromatography coupled to triple timeof-flight mass spectrometry (UPLC-Triple-TOF-MS). A fast and efficient chromatographic separation of glycerolipids was accomplished based on an UPLCTM BEH C₈ column within 22 min. In ESI positive ion mode, TOF-MS scan-information dependent acquisition-product ion scan was carried out to acquire both high resolution MS and MS/MS information from one injection. According to MS/MS spectra, predominant fragmentation patterns of glycerolipids were elucidated in detail. Based on retention time, accurate mass, isotopic distribution, and fragmentation patterns, the composition of 144 glycerolipids and fatty acids were finally identified in yellow sarson seeds, including 77 triacylglycerols, 32 diacylglycerols, 18 sulfoquinovosyl-diacylglycerols, 5 monogalactosyl-diacylglycerols, and 12 digalactosyl-diacylglycerols. Of them, the most abundant glycerolipids in yellow sarson seeds were triacylglycerols, the major storage form of seed oil in plants. In addition, diacylglycerols were found as a minor component of glycerolipids. The lowest amounts of glycerolipids detected in seeds were glycosylacylglycerols. The results revealed the composition and relative content of glycerolipids in yellow sarson seeds, which will provide a more comprehensive assessment of the quality of seed oil and also help to select functional cultivars with higher beneficial glycerolipids. This profiling method has the advantages

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