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Metabolite profiling analysis and quantification of phenolic compounds between the yellow- and black-seeded rapeseed by HPLC-MS

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Brassica napus L. is the most important oil crop with high amounts of secondary metabolite profiling in seed, which are important to improve rapeseed quality. The aim of the present study was to characterize the phenolic acids, flavonoids, and other antioxidant properties of seeds collected from different yellow and black rapeseed. Therefore, a high-performance liquid chromatography (HPLC) and liquid chromatography–mass spectrometry (LC-MS) method was developed for the identification of the secondary metabolite profiling. A total of 227 metabolic features could be detected in the *B. napus* seeds, including 29 phenolic acids, 37 flavonoids, 24 glucosinolates, 65 Fatty Acyls and lipids, and 72 other polar compounds. The phenolic acids were identified, with the most abundant being sinapic acid and derivatives, including sinapic acid, 1-O-beta-D-Glucopyranosyl sinapate, 1,2-disinapoylglucoside, and disinapoylgentiobiose. The flavonoids, the kaempferols, isorhamnetins, quercetins, epicatechin and their derivatives were also widely detected, but the epicatechin and their derivatives were most abundant. However, 47 phenolic acids and flavonoids revealed significantly differences between yellow and black-seeded *B. napus*, with the different accumulation pattern in during the seed maturation. Among them, the sinapic acid, epicatechin and their derivatives might be the main different phenolic acids and flavonoids, which displayed the significantly lower levels in the yellow than in the black. In addition, 3-Butenyl GSL, 4-Pentenyl GSL, R-2-hydroxy-3-butenyl glucosinolate, 4-Hydroxyindol-3-ylmethyl GSL, and 4-Methoxy-3-indolylmethyl glucosinolate are the most abundant of glucosinolates in *B. napus* seeds. These outcomes not only enrich our knowledge of secondary metabolite profiling in rapeseed, as well as provide a guide for well understanding of yellow-seeded *B. napus* utilization in rapeseed breeding for better seed quality.