Title Characterization of a new anthocyanin in black raspberries (*Rubus occidentalis*) by liquid

chromatography electrospray ionization tandem mass spectrometry

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Abstract

Anthocyanin composition of black raspberry (*Rubus occidentalis*) was studied using high-performance liquid chromatography coupled to photodiode array (PDA) detection and electrospray ionization mass spectrometry (LC-ESI/MS) and tandem mass spectrometry (MS/MS). Pelargonidin 3-rutinoside was isolated and identified in black raspberries using HPLC, UV–Vis spectroscopy, MS, and NMR spectroscopy. No pelargonidin derivative had been previously found in *Rubus occidentalis*. In addition, the presence and identities of four previously reported anthocyanins (cyanidin 3-glucoside, cyanidin 3-sambubioside, cyanidin 3-rutinoside and cyanidin 3-xylosylrutinoside) were confirmed by HPLC/MS and MS/MS analyses.