

Development of an Optimized Ultrasound-Assisted Extraction Methods for the Recovery of Total Phenolic Compounds and Anthocyanins from Onion Bulbs

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SUPPLEMENTARY MATERIAL

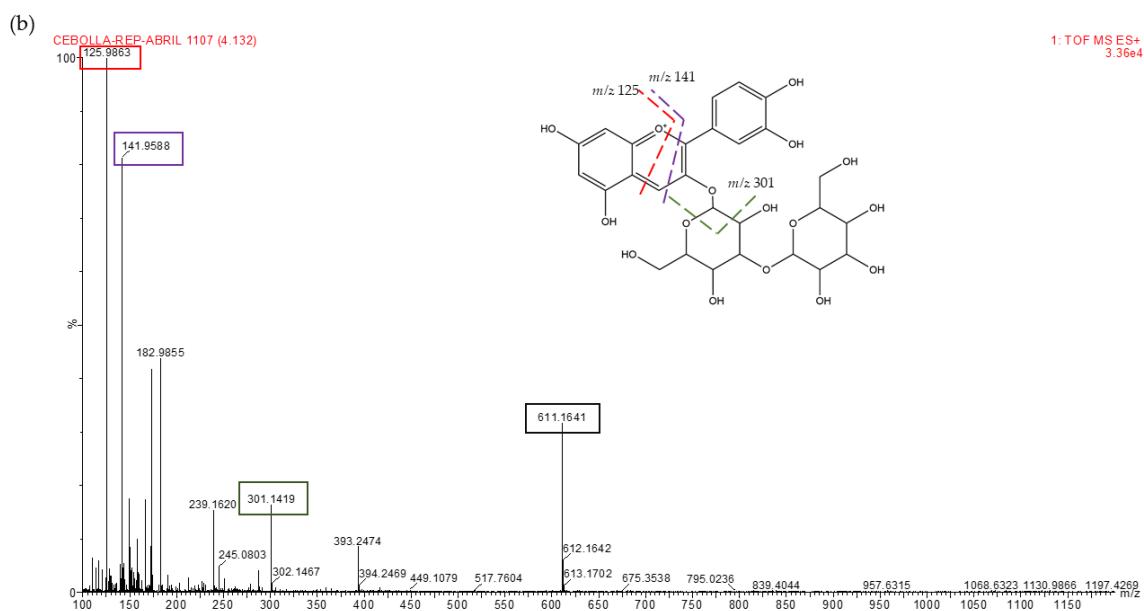
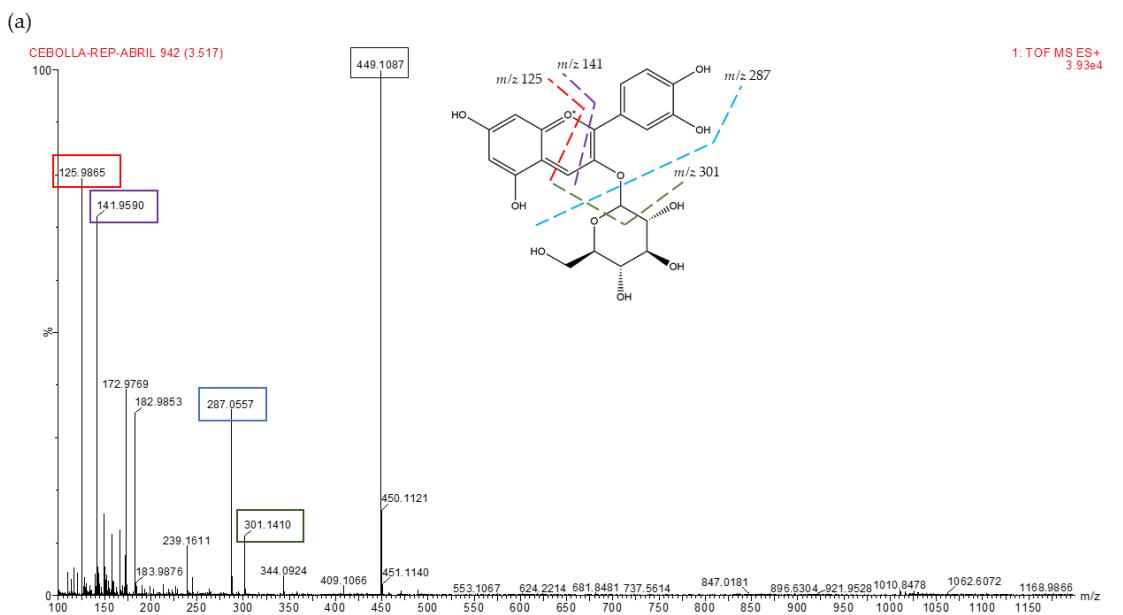
Anthocyanins present in onion		Molecular formula	R ₂	R ₃
Cyanidin 3-O-glucoside		C ₂₁ H ₂₁ O ₁₁ ⁺	H	C ₆ H ₁₁ O ₅
Cyanidin 3-O-laminaribioside		C ₂₇ H ₃₁ O ₁₆ ⁺	H	C ₁₂ H ₂₁ O ₁₀
cyanidin 3-O-(3''-malonylglucoside)		C ₂₄ H ₂₃ O ₁₄ ⁺	H	C ₉ H ₁₃ O ₈
Peonidin 3-O-glucoside		C ₂₂ H ₂₃ O ₁₁ ⁺	CH ₃	C ₆ H ₁₁ O ₅
Cyanidin 3-O-(6''-malonylglucoside)		C ₂₄ H ₂₃ O ₁₄ ⁺	H	C ₉ H ₁₃ O ₈
Cyanidin 3-O-(6''-malonyl-laminaribioside)		C ₃₀ H ₃₃ O ₁₉ ⁺	H	C ₁₅ H ₂₃ O ₁₃
Peonidin 3-O-(6''-malonylglucoside)		C ₂₅ H ₂₅ O ₁₄ ⁺	CH ₃	C ₉ H ₁₃ O ₈
-O-Glucoside -O-C ₆ H ₁₁ O ₅	-O-laminaribioside -O-C ₁₂ H ₂₁ O ₁₀	-O-3''-malonylglucoside -O-C ₉ H ₁₃ O ₈	-O-6''-malonylglucoside -O-C ₉ H ₁₃ O ₈	O-6''-malonyl-laminaribioside -O-C ₁₅ H ₂₃ O ₁₃

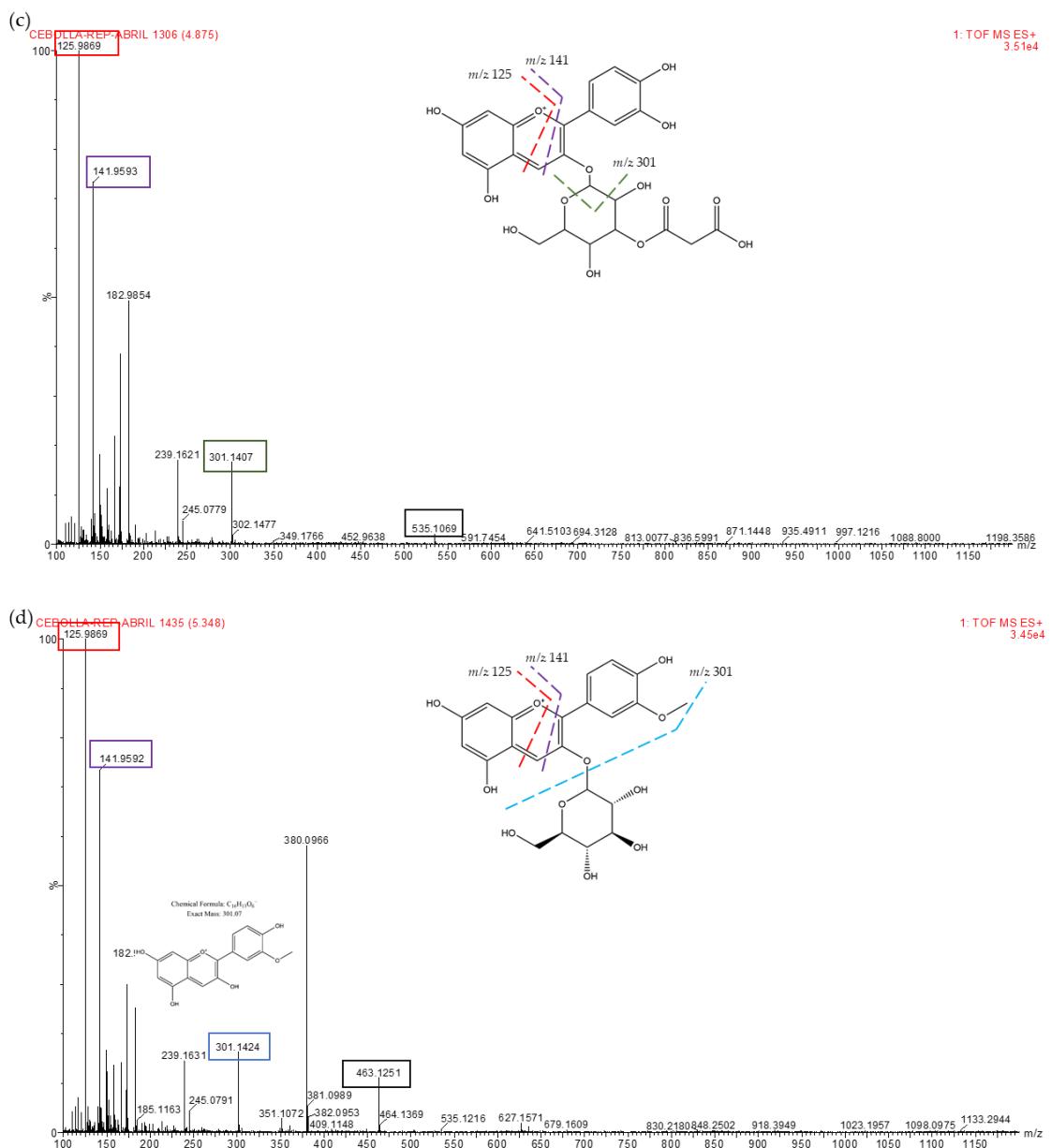
Figure S1. Information about anthocyanins identified in red onion.

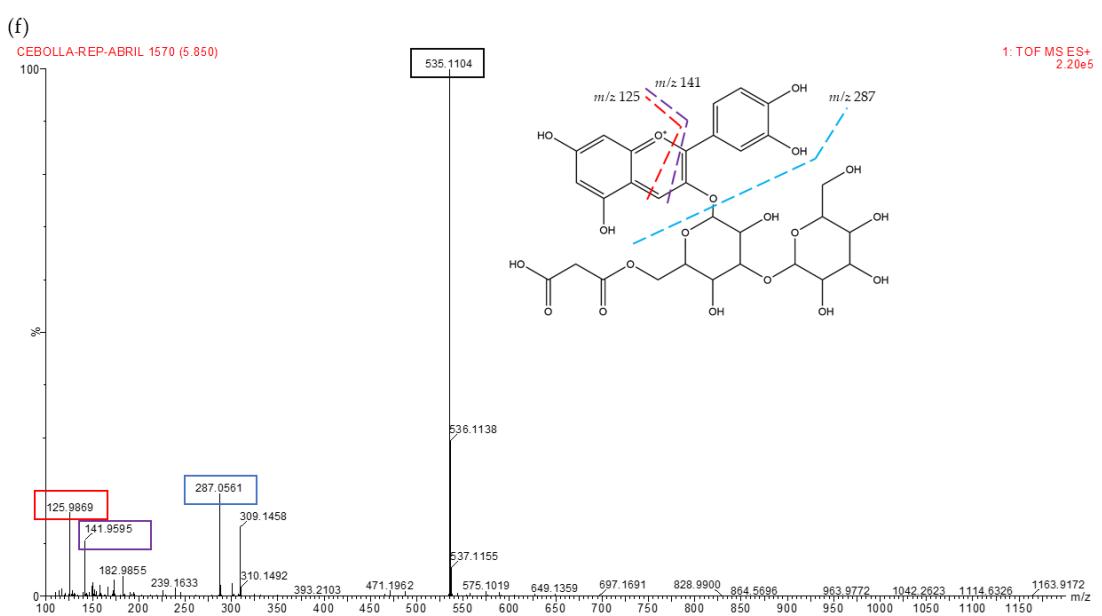
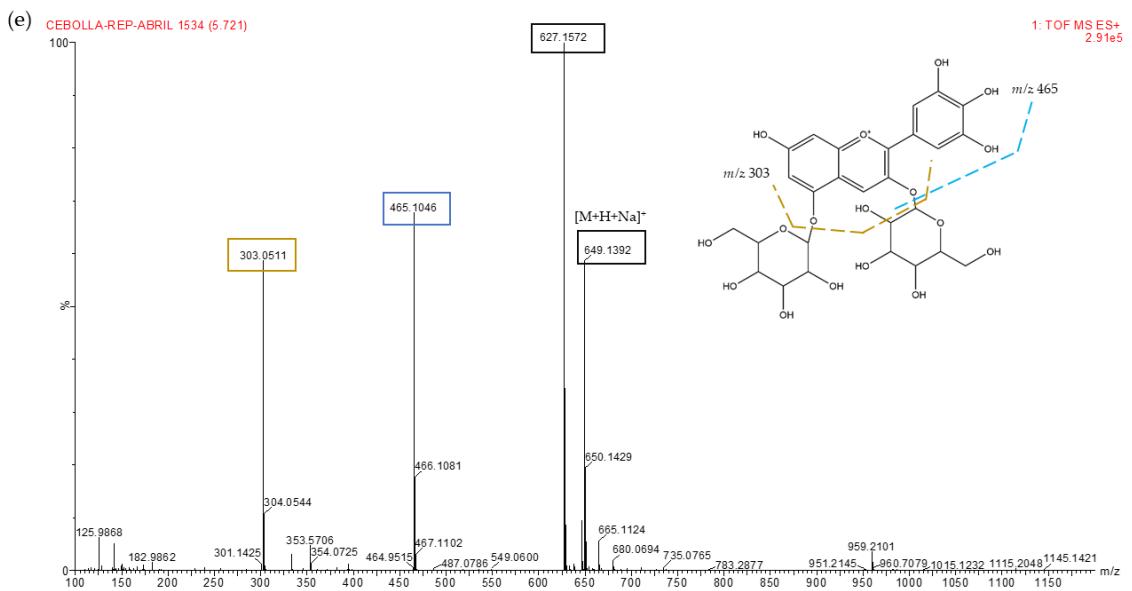
Table S1. Mass spectra information of the nine anthocyanins present in onion bulb.

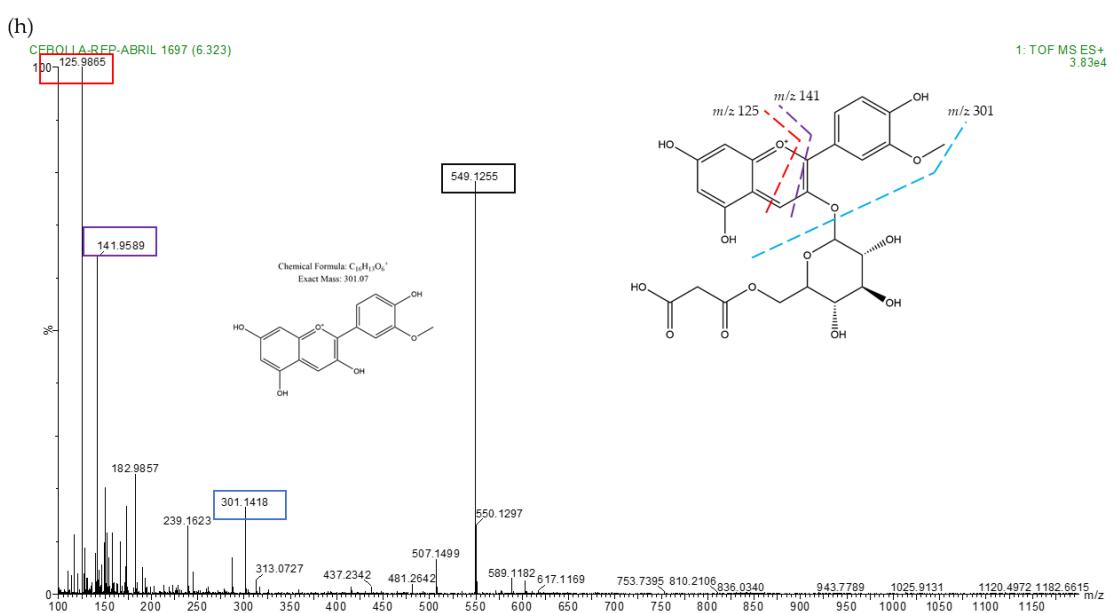
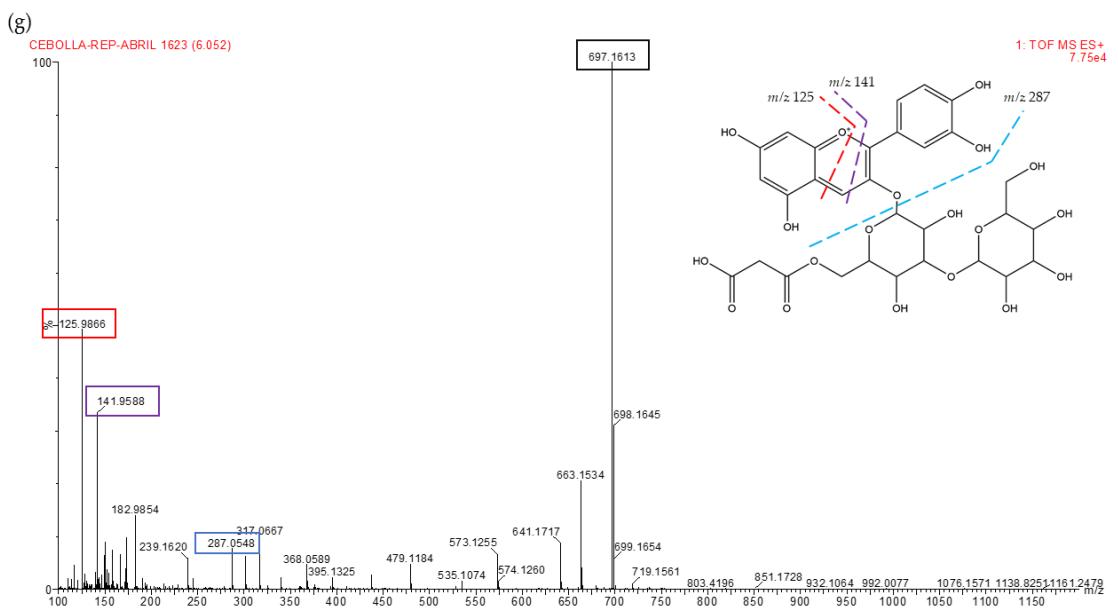
Compounds	Predicted formula	Retention time (min)	m/z*	Ion Assignment
Cyanidin 3-O-glucoside	$C_{21}H_{21}O_{11}^+$	3.517	449.1087	$[M+H]^+$
			301.1410	$[M+H-C_5H_{10}O_5]^+$
			287.0557	$[M+H-C_6H_8O_5]^+$
			141.9590	$[M+H-C_{14}H_{12}O_8]^+$
			125.9865	$[M+H-C_{15}H_{16}O_8]^+$
Cyanidin 3-O-laminaribioside	$C_{27}H_{31}O_{16}^+$	4.132	611.1641	$[M+H]^+$
			301.1410	$[M+H-C_{11}H_{18}O_{10}]^+$
			141.9590	$[M+H-C_{20}H_{22}O_{13}]^+$
cyanidin 3-O-(3"-malonylglucoside)	$C_{24}H_{23}O_{14}^+$	4.875	125.9865	$[M+H-C_{21}H_{26}O_{13}]^+$
			535.1069	$[M+H]^+$
			301.1410	$[M+H-C_8H_{10}O_8]^+$
			141.9590	$[M+H-C_{17}H_{14}O_{11}]^+$
Peonidin 3-O-glucoside	$C_{22}H_{23}O_{11}^+$	5.348	125.9865	$[M+H-C_{18}H_{18}O_8]^+$
			463.1251	$[M+H]^+$
			301.1424	$[M+H-C_6H_{10}O_5]^+$
			141.9590	$[M+H-C_{15}H_{14}O_8]^+$
Delphinidin 3,5-O-diglucoside	$C_{27}H_{31}O_{17}^+$	5.721	125.9865	$[M+H-C_{16}H_{18}O_8]^+$
			649.1392	$[M+H+Na]^+$
			627.1572	$[M+H]^+$
			465.1046	$[M+H-C_6H_{10}O_5]^+$
Cyanidin 3-O-(6"-malonylglucoside)	$C_{24}H_{23}O_{14}^+$	5.850	303.0511	$[M+H-C_{12}H_{20}O_{10}]^+$
			535.1104	$[M+H]^+$
			287.0561	$[M+H-C_9H_{12}O_8]^+$
			141.9590	$[M+H-C_{17}H_{14}O_{11}]^+$
Cyanidin- 3-O-(6"-malonyl-laminaribioside)	$C_{30}H_{33}O_{19}^+$	6.052	125.9865	$[M+H-C_8H_{18}O_8]^+$
			697.1613	$[M+H]^+$
			287.0561	$[M+H-C_{15}H_{22}O_{13}]^+$
			141.9590	$[M+H-C_{23}H_{24}O_{16}]^+$
Peonidin 3-O-malonylglucoside	$C_{25}H_{25}O_{14}^+$	6.323	125.9865	$[M+H-C_{24}H_{28}O_{16}]^+$
			549.1255	$[M+H]^+$
			301.1418	$[M+H-C_9H_{12}O_8]^+$
			141.9590	$[M+H-C_{18}H_{16}O_{11}]^+$
Delphinidin 3-O-glucoside	$C_{21}H_{21}O_{12}^+$	6.536	125.9865	$[M+H-C_{19}H_{20}O_{11}]^+$
			487.0863	$[M+H+Na]^+$
			465.1055	$[M+H]^+$
			303.0508	$[M+H-C_6H_{10}O_5]^+$
			141.9587	$[M+H-C_{14}H_{12}O_9]^+$
			125.9865	$[M+H-C_{15}H_{16}O_9]^+$

* The fragments identified have been selected based on their greater abundance or greater selectivity (larger m/z).









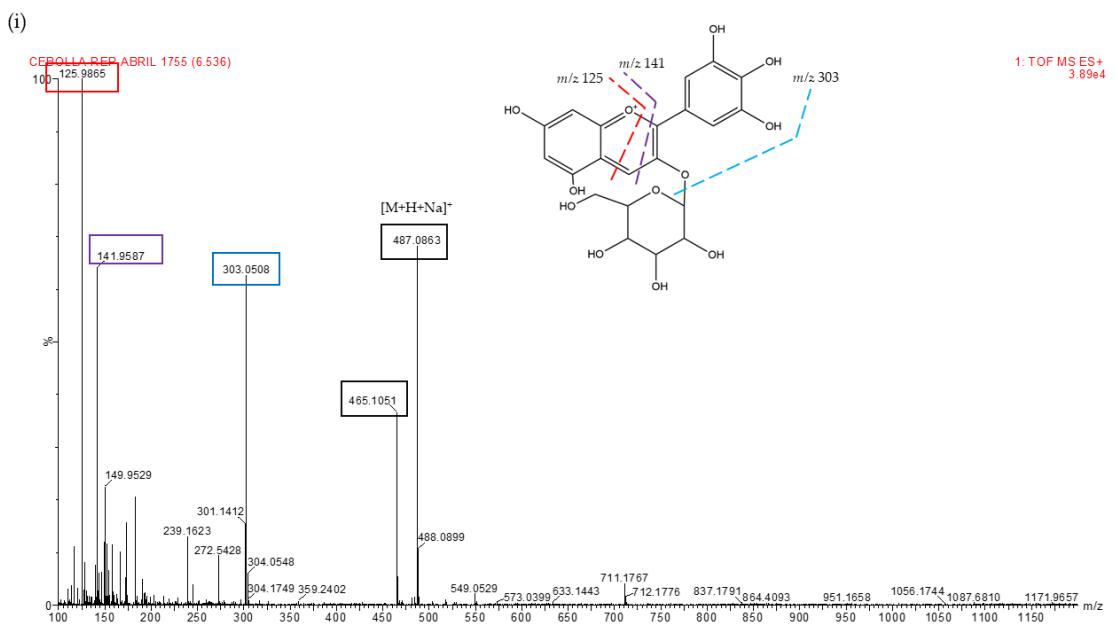


Figure S2. MS spectra and structure of the nine anthocyanins identified in onion bulb: (a) cyanidin 3-O-glucoside; (b) cyanidin 3-O-laminaribioside; (c) cyanidin 3-O-(3''-malonylglucoside); (d) peonidin 3-O-glucoside; (e) delphinidin 3,5-O-diglucoside; (f) cyanidin 3-O-(6''-malonylglucoside); (g) cyanidin 3-O-(6''-malonyl-laminaribioside); (h) peonidin 3-O-malonylglucoside; (i) delphinidin 3-O-glucoside. The molecular ion has been framed in black and the fragments in different colors.