

S1 Table. List of the compounds identified by Metaboanalyst software and were found significantly up-regulated in transgenic fruits of lines 6 and 7.

35 compounds have been tentatively identified by comparison to either a database or publication, 11 of which are flavonoids. Where the table lists KEGG as a source, MZmine software was used to compare the peak list to the database for identification purposes before the peak list was uploaded to Metaboanalyst, which was used for statistical analysis after MZmine completed processing the raw data. Not all compounds are in the KEGG database, but KEGG IDs are listed for those that were found.

m/z	RT (min)	KEGG ID	Tentative Identification	Source	Group
119.1066	28.6	C00601	Phenylacetylaldehyde	KEGG	aldehydes
128.1572	9.6	C01879	Pyroglutamic Acid	Gómez-Romero, Segura-Carretero, & Fernández-Gutiérrez, 2010	amino acids and derivatives
130.3659	10.7	C00123	Fructosyl leucine (-hexose)	Gómez-Romero, Segura-Carretero, & Fernández-Gutiérrez, 2010	amino acids and derivatives
151.1071	28.6	C07271	Limonene Oxide	Gómez-Romero, Segura-Carretero, & Fernández-Gutiérrez, 2010	terpenoids
170.8274	28.5				
267.2984	10.4	C02572	Feruloylquinic Acid	Gómez-Romero, Segura-Carretero, & Fernández-Gutiérrez, 2010	hydroxycinnamic acids
271.5263	28.6	C00509	Naringenin	Gómez-Romero, Segura-Carretero, & Fernández-Gutiérrez, 2010	flavonoids
278.8388	28.6	C01964	Tos-Ph-CH ₂ Cl	KEGG	sulfonic acid derivative
278.8401	28.5				
278.8969	28.6				
290.5020	6.8		Fructosyl Glutamate (-H ₂ O)	Gómez-Romero, Segura-Carretero, & Fernández-Gutiérrez, 2010	amino acids and derivatives
292.7480	28.6		Fructosyl leucine	Gómez-Romero, Segura-Carretero, & Fernández-Gutiérrez, 2010	amino acids and derivatives
310.8639	28.6				

310.880328.6					
311.005128.6			Hydroperoxy-octadecanedioic acid	Gómez-Romero, Segura-Carretero, & Fernández-Gutiérrez, 2010	fatty acids
320.853928.5					
320.897628.7					
320.980628.8	C00364		Thymidine 5'-phosphate	KEGG	nucleotides
324.855928.6	C14967		1-[2-Bromo-1-(4-chlorophenyl)ethenyl]-2-chlorobenzene	KEGG	diarylmethane
324.914028.6					
324.941728.6					
365.547516.8					
365.687116.9					
367.256510.5	C03309		Strictosidine aglycone	KEGG	alkaloids
368.679828.5					
435.041025.4	C01604		Phlorizin	KEGG	flavonoids
440.150425.3	C00504		Folate	KEGG	vitamins
451.173922.3	C07349		3'-Demethylstaurosporine	KEGG	alkaloids
452.75874.3			Torvanol A	KNAPSAck	hydrogen sulfate salt
455.021522.3	C00061		Riboflavin-5-phosphate	KEGG	coenzymes
456.199522.3	C00143		5,10-Methylenetetrahydrofolate	KEGG	coenzymes
456.394522.2					
456.43785.3					
456.778122.3					
457.09175.3	C01847		Reduced Flavin Mononucleotide	KEGG	coenzymes

464.89314.2				
464.92684.2				
499.482923.3				
499.803522.7				
499.918725.4				
500.086125.4				
500.199423.0				
500.19965.2				
500.222223.5				
500.325923.1				
500.425725.4				
500.668425.4				
500.783225.4				
501.71313.6				
514.61473.8				
554.836928.6				
554.848428.5				
558.617320.1				
564.771328.6				
565.777728.6				
566.512623.7				
566.728623.6				
567.110723.7				

593.199026.3	C03870	Isoorientin 2"-O-rhamnoside	KEGG	flavonoids
594.868328.5	C15641	XCT790	KEGG	cinnamamides
594.876419.6				
594.885419.7				
594.908319.7				
594.925428.4		Kaempferol 3-O-Rutinoside	KomicMarket	flavonoids
595.808921.3	C00509	Naringenin dihexose	Gómez-Romero, Segura-Carretero, & Fernández-Gutiérrez, 2010	flavonoids
597.008822.8				
597.204523.4	C00774	Phloretin Dihexoside	Gómez-Romero, Segura-Carretero, & Fernández-Gutiérrez, 2010	flavonoids
597.701522.5				
605.95485.0	C00043	UDP-N-acetyl-alpha-D-glucosamine	KEGG	nucleotides
606.983911.6				
609.641921.2		Rutin hexoside (-hexose)	Gómez-Romero, Segura-Carretero, & Fernández-Gutiérrez, 2010	flavonoids
609.717221.3		Kaempferol 3,7-dihexoside	Gómez-Romero, Segura-Carretero, & Fernández-Gutiérrez, 2010	flavonoids
610.546921.2				
610.907726.1				
611.457121.1				
611.480321.1				
611.991526.1				
612.328821.1				

614.314022.0					
614.348122.1					
614.83164.8					
622.893028.5					
622.933728.6					
622.940128.6					
624.889820.2					
624.909420.2					
626.921023.3					
626.990523.4					
630.897519.5					
630.920419.5					
630.950119.4					
630.971020.5	C19971	UDP-2,4-bis(acetamido)-2,4,6-trideoxy-beta-L-altropyranose	KEGG		nucleotides
635.126128.3					
635.159228.3	C04360	1-O,2-O,6-O-Trigalloyl-beta-D-glucose	KEGG		tannins
635.233428.2					
637.776524.6					
637.927624.8	C12632	Luteolin 7-O-beta-D-diglucuronide	KEGG		flavonoids
638.583124.9					
638.693724.8					
639.189223.5	C10084	Isorhamnetin 3-sophoroside	Gómez-Romero, Segura-Carretero, & Fernández-Gutiérrez, 2010		flavonoids

646.934521.1				
647.023521.1				
652.893715.0				
652.897015.1				
653.000222.1		Cilistol p	KNAPSAck	steroid glycoside
653.036522.1				
653.529427.5	C05811	3-Octoprenylcatechol	KEGG	flavonoids
655.138725.4				
655.184225.3	C10466	Hellicoside	KEGG	hydroxycinnamic acids
660.847520.6				
680.822724.7				
680.880924.9				
682.906124.5				
754.874321.4				
755.823221.4				
758.862621.0				
758.874221.0				