

**Top 25 Changing Metabolites for Tomato Introgression Lines in Green Fruit
(MS Positive Mode)**

Chromosome 1

Changing Bin	Possible ID	Formula	Accurate Mass
154	3-hydroxyanthranilate	C7H7NO3	153.0426
164			
179	pyrophosphate	H4O7P2	177.9432
183	dimethoxybenzoic acid	C9H10O4	182.0579
184	normetanephine	C9H13NO3	183.0895
198	3-4-dihydroxy-L-phenylalanine	C9H11NO4	197.0688
204			
205	oxaloglutarate	C7H8O7	204.0270
224	4-methyl-5-(2-phosphoethyl)-thiazole	C6H10NO4PS	223.0068
226	4-amino-4-deoxychorismate	C10H11NO5	225.0637
242			
243	thymidine	C10H14N2O5	242.0903
256	2-amino-4-hydroxy-6-(D-erythro-1,2,3-trihydroxypropyl)-7,8-dihydropteridine	C9H13N5O4	255.0968
263	mannitol-1-phosphate	C6H15O9P	262.0454
264			
273	naringenin	C15H12O5	272.0685
290	atropine	C17H23NO3	289.1678
292			
301			
305	pentahydroxyflavanone	C15H12O7	304.0583
361	rosmarinic acid	C18H16O8	360.0845
371	sedoheptulose-1,7-bisphosphate	C7H16O13P2	370.0066
383	trans,trans-farnesyl diphosphate	C15H28O7P2	382.1310
384			
393	chenodeoxycholic acid	C24H40O4	392.2927

Chromosome 2

Changing Bin	Possible ID	Formula	Accurate Mass
103	2-oxobutanoate	C4H6O3	102.0317
123	benzoic acid	C7H6O2	122.0368
138	4-aminobenzoate	C7H7NO2	137.0477
139	salicylic acid	C7H6O3	138.0317
151	arabinose	C5H10O5	150.0528
152	guanine	C5H5N5O	151.0494
162	2-aminoadipic acid	C6H11NO4	161.0688
164			
170	1-amino-propan-2-one-3-phosphate	C3H8NO5P	169.0140
177	ascorbic acid	C6H8O6	176.0321
183	dimethoxybenzoic acid	C9H10O4	182.0579
194			
196	glucosaminic acid	C6H13NO6	195.0743
204			
205	oxaloglutarate	C7H8O7	204.0270
213			
214	4-phospho-L-aspartate	C4H8NO7P	213.0038
216	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
221	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
249	pyridoxamine phosphate	C8H13N2O5P	248.0562
250	pyridoxine-5'-phosphate	C8H12NO6P	249.0402
281	linoleic acid	C18H32O2	280.2402
362			
383	trans,trans-farnesyl diphosphate	C15H28O7P2	382.1310
544			

Chromosome 3

Changing Bin	Possible ID	Formula	Accurate Mass
107	glyceric acid	C3H6O4	106.0266
135	malic acid	C4H6O5	134.0215
153	alloxanthine	C5H4N4O2	152.0334
154	3-hydroxyanthranilate	C7H7NO3	153.0426
195	5-keto-D-gluconic acid	C6H10O7	194.0427
219			
220	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
221	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
224	4-methyl-5-(2-phosphoethyl)-thiazole	C6H10NO4PS	223.0068
225	sinapate	C11H12O5	224.0685
233			
234			
241	cystine	C6H12N2O4S2	240.0238
244	cytidine	C9H13N3O5	243.0855
249	pyridoxamine phosphate	C8H13N2O5P	248.0562
260	glucosamine-1-phosphate	C6H14NO8P	259.0457
282			
283	elaidic acid	C18H34O2	282.2559
290	atropine	C17H23NO3	289.1678
292			
327	6,7-dimethyl-8-(1-D-ribityl)lumazine	C13H18N4O6	326.1226
393	chenodeoxycholic acid	C24H40O4	392.2927
399	(24R)-24-methyl-cholest-4-en-3-one	C28H46O	398.3549
400			
401	(24R)-24-methyl-5alpha-cholestan-3-one	C28H48O	400.3705

Chromosome 4

Changing Bin	Possible ID	Formula	Accurate Mass
76	glycine	C2H5NO2	75.0320
102			
105	hydroxypyruvic acid	C3H4O4	104.0110
123	benzoic acid	C7H6O2	122.0368
143			
183	dimethoxybenzoic acid	C9H10O4	182.0579
186	3-phosphoserine	C3H8NO6P	185.0089
192			
196	glucosaminic acid	C6H13NO6	195.0743
201	erythrose-4-phosphate	C4H9O7P	200.0086
205	oxaloglutarate	C7H8O7	204.0270
208			
232			
240			
247	D3-isopentenyl-PP	C5H12O7P2	246.0058
249	pyridoxamine phosphate	C8H13N2O5P	248.0562
259	glucono-1,5-lactone-6-phosphate	C6H11O9P	258.0141
268	neuraminic acid	C9H17NO8	267.0954
290	atropine	C17H23NO3	289.1678
307	2',3'-cyclic UMP	C9H11N2O8P	306.0253
317	isorhamnetin	C16H12O7	316.0583
415	sitosterol	C29H50O	414.3862
424			
430			
586			

Chromosome 5

Changing Bin	Possible ID	Formula	Accurate Mass
94			
104	3-amino-2-methylpropanoate	C4H9NO2	103.0633
118	aspartate-4-semialdehyde	C4H7NO3	117.0426
143			
144	5-(2-hydroxyethyl)-4-methylthiazole	C6H9NOS	143.0405
153	alloxanthine	C5H4N4O2	152.0334
155	dihydroxybenzoic acid	C7H6O4	154.0266
162	2-aminoadipic acid	C6H11NO4	161.0688
179	pyrophosphate	H4O7P2	177.9432
183	dimethoxybenzoic acid	C9H10O4	182.0579
192			
195	5-keto-D-gluconic acid	C6H10O7	194.0427
198	3-4-dihydroxy-L-phenylalanine	C9H11NO4	197.0688
208			
215	2-oxo-3-hydroxy-4-phosphobutanoate	C4H7O8P	213.9879
224	4-methyl-5-(2-phosphoethyl)-thiazole	C6H10NO4PS	223.0068
225	sinapate	C11H12O5	224.0685
232			
235			
243	thymidine	C10H14N2O5	242.0903
259	glucono-1,5-lactone-6-phosphate	C6H11O9P	258.0141
281	linoleic acid	C18H32O2	280.2402
282			
325	5-enolpyruvyl-shikimate-3-phosphate	C10H13O10P	324.0246
417	6-oxocampestanol	C28H48O2	416.3654

Chromosome 6

Changing Bin	Possible ID	Formula	Accurate Mass
69			
87			
91	oxalic acid	C2H2O4	89.9953
124	nicotinic acid	C6H5NO2	123.0320
136	homocysteine	C4H9NO2S	135.0354
148	glutamic acid	C5H9NO4	147.0532
152	guanine	C5H5N5O	151.0494
153	alloxanthine	C5H4N4O2	152.0334
162	2-aminoadipic acid	C6H11NO4	161.0688
163	anabasine	C10H14N2	162.1157
170	1-amino-propan-2-one-3-phosphate	C3H8NO5P	169.0140
181	glucose and isomers	C6H12O6	180.0634
186	3-phosphoserine	C3H8NO6P	185.0089
199	syringic acid	C9H10O5	198.0528
244	cytidine	C9H13N3O5	243.0855
262			
269	inosine	C10H12N4O5	268.0808
275	phloretin	C15H14O5	274.0841
294	N-acetylmuramic acid	C11H19NO8	293.1111
384			
445			
446	tetrahydrofolic acid	C19H23N7O6	445.1710
511			
551			
619			

Chromosome 7

Changing Bin	Possible ID	Formula	Accurate Mass
104	3-amino-2-methylpropanoate	C4H9NO2	103.0633
153	alloxanthine	C5H4N4O2	152.0334
168	pyridine-2,3-dicarboxylate	C7H5NO4	167.0219
170	1-amino-propan-2-one-3-phosphate	C3H8NO5P	169.0140
192			
195	5-keto-D-gluconic acid	C6H10O7	194.0427
196	glucosaminic acid	C6H13NO6	195.0743
206	lipoamide	C8H15NOS2	205.0595
221	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
222	histidinol phosphate	C6H12N3O4P	221.0565
241	cystine	C6H12N2O4S2	240.0238
242			
273	naringenin	C15H12O5	272.0685
274	erythroidine	C16H19NO3	273.1365
276	physostigmine	C15H21N3O2	275.1634
281	linoleic acid	C18H32O2	280.2402
290	atropine	C17H23NO3	289.1678
295	cinchonine	C19H22N2O	294.1732
299			
362			
377	riboflavin	C17H20N4O6	376.1383
381			
382	sphinganine-1-phosphate	C18H40NO5P	381.2644
383	trans,trans-farnesyl diphosphate	C15H28O7P2	382.1310
409			

Chromosome 8

Changing Bin	Possible ID	Formula	Accurate Mass
60			
62	ethanolamine	C2H7NO	61.0528
75	glyoxylic acid	C2H2O3	74.0004
76	glycine	C2H5NO2	75.0320
83			
114	(S)-1-pyrroline-5-carboxylate	C5H7NO2	113.0477
203	spermine	C10H26N4	202.2157
209	sinapaldehyde	C11H12O4	208.0736
244	cytidine	C9H13N3O5	243.0855
265	abscisic acid	C15H20O4	264.1362
286	morphine	C17H19NO3	285.1365
294	N-acetylmuramic acid	C11H19NO8	293.1111
300	2-methyl-4-amino-5-hydroxymethylpyrimidine diphosphate	C6H11N3O7P2	299.0072
303	ellagic acid	C14H6O8	302.0063
310	N-acetylneuraminic acid	C11H19NO9	309.1060
315	5'-phosphoribosyl-N-formylglycinamide	C8H15N2O9P	314.0515
323	dTMP	C10H15N2O8P	322.0566
324	CMP	C9H14N3O8P	323.0518
333	GA20	C19H24O5	332.1624
335	2-(alpha-D-galactosyl)-sn-glycerol 3-phosphate	C9H19O11P	334.0665
339	1-(5'-phosphoribosyl)-5-amino-4-imidazolecarboxamide	C9H15N4O8P	338.0627
363	GA19	C20H26O6	362.1729
396			
399	(24R)-24-methyl-cholest-4-en-3-one	C28H46O	398.3549
400			

Chromosome 9

Changing Bin	Possible ID	Formula	Accurate Mass
60			
114	(S)-1-pyrroline-5-carboxylate	C5H7NO2	113.0477
137	hypoxanthine	C5H4N4O	136.0385
161	2-oxoadipate	C6H8O5	160.0372
163	anabasine	C10H14N2	162.1157
172			
223	cystathionine	C7H14N2O4S	222.0674
224	4-methyl-5-(2-phosphoethyl)-thiazole	C6H10NO4PS	223.0068
233			
234			
252	muramic acid	C9H17NO7	251.1005
275	phloretin	C15H14O5	274.0841
277	6-phosphogluconate	C6H13O10P	276.0246
292			
294	N-acetylmuramic acid	C11H19NO8	293.1111
303	ellagic acid	C14H6O8	302.0063
309	(R)-5-diphosphomevalonate	C6H14O10P2	308.0062
319	myricetin	C15H10O8	318.0376
328			
333	GA20	C19H24O5	332.1624
346	2',3'-cyclic GMP	C10H12N5O7P	345.0474
363	GA19	C20H26O6	362.1729
383	trans,trans-farnesyl diphosphate	C15H28O7P2	382.1310
394			
552			

Chromosome 10

Changing Bin	Possible ID	Formula	Accurate Mass
85			
91	oxalic acid	C2H2O4	89.9953
115	3-cyanoalanine	C4H6N2O2	114.0429
132	5-aminolevulinate	C5H9NO3	131.0582
141			
142	carbamoyl phosphate	CH4NO5P	140.9827
170	1-amino-propan-2-one-3-phosphate	C3H8NO5P	169.0140
178			
181	glucose and isomers	C6H12O6	180.0634
183	dimethoxybenzoic acid	C9H10O4	182.0579
191	oxalosuccinate	C6H6O7	190.0114
192			
208			
216	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
217	erythronate-4-phosphate	C4H9O8P	216.0035
223	cystathionine	C7H14N2O4S	222.0674
232			
236			
261	1L-myo-inositol-1-phosphate	C6H13O9P	260.0297
341	fructose-1,6-bisphosphate	C6H14O12P2	339.9960
344			
348	AMP	C10H14N5O7P	347.0631
359	pantetheine-4'-phosphate	C11H23N2O7PS	358.0964
360			
380	(R)-S-lactoylglutathione	C13H21N3O8S	379.1049

Chromosome 11

Changing Bin	Possible ID	Formula	Accurate Mass
68			
88	4-aminobutyraldehyde	C4H9NO2	87.0684
104	3-amino-2-methylpropanoate	C4H9NO2	103.0633
105	hydroxypyruvic acid	C3H4O4	104.0110
147	2-oxoglutarate	C5H6O5	146.0215
148	glutamic acid	C5H9NO4	147.0532
153	alloxanthine	C5H4N4O2	152.0334
162	2-aminoadipic acid	C6H11NO4	161.0688
183	dimethoxybenzoic acid	C9H10O4	182.0579
208			
210			
216	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
221	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
242			
249	pyridoxamine phosphate	C8H13N2O5P	248.0562
251	gamma-L-glutamyl-L-cysteine	C8H14N2O5S	250.0623
256	2-amino-4-hydroxy-6-(D-erythro-1,2,3-trihydroxypropyl)-7,8-dihydropteridine	C9H13N5O4	255.0968
261	1L-myo-inositol-1-phosphate	C6H13O9P	260.0297
281	linoleic acid	C18H32O2	280.2402
296	aminoimidazole ribotide	C8H14N3O7P	295.0569
334			
364	GMP	C10H14N5O8P	363.0580
371	sedoheptulose-1,7-bisphosphate	C7H16O13P2	370.0066
377	riboflavin	C17H20N4O6	376.1383
797			

Chromosome 12

Changing Bin	Possible ID	Formula	Accurate Mass
93	glycerol	C3H8O3	92.0473
184	normetanephrine	C9H13NO3	183.0895
186	3-phosphoserine	C3H8NO6P	185.0089
195	5-keto-D-gluconic acid	C6H10O7	194.0427
220	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
222	histidinol phosphate	C6H12N3O4P	221.0565
224	4-methyl-5-(2-phosphoethyl)-thiazole	C6H10NO4PS	223.0068
233			
234			
241	cystine	C6H12N2O4S2	240.0238
245	uridine	C9H12N2O6	244.0695
259	glucono-1,5-lactone-6-phosphate	C6H11O9P	258.0141
262			
275	phloretin	C15H14O5	274.0841
283	elaidic acid	C18H34O2	282.2559
294	N-acetylmuramic acid	C11H19NO8	293.1111
303	ellagic acid	C14H6O8	302.0063
311	ribulose-1,5-bisphosphate	C5H12O11P2	309.9855
326			
339	1-(5'-phosphoribosyl)-5-amino-4-imidazolecarboxamide	C9H15N4O8P	338.0627
351			
352			
363	GA19	C20H26O6	362.1729
386			
394			