

Changing Metabolites for Tomato Introgression Lines (Negative Mode)

Chromosome 1

Changing Bin	Possible ID	Formula	Accurate Mass
99			
107			
108			
113	3-cyanoalanine	C4H6N2O2	114.0429
117	succinic acid	C4H6O4	118.0266
143	4-guanidino-butanamide	C5H12N4O	144.1011
149	arabinose	C5H10O5	150.0528
150	guanine	C5H5N5O	151.0494
152	3-hydroxyanthranilate	C7H7NO3	153.0426
159	2-oxoadipate	C6H8O5	160.0372
161	anabasine	C10H14N2	162.1157
163	coumaric acid	C9H8O3	164.0473
179	glucose and isomers	C6H12O6	180.0634
180	tyrosine	C9H11NO3	181.0739
181	dimethoxybenzoic acid	C9H10O4	182.0579
182	normetanephine	C9H13NO3	183.0895
185	2-phosphoglyceric acid	C3H7O7P	185.9929
205	homocitrate	C7H10O7	206.0427
221	cystathionine	C7H14N2O4S	222.0674
222	4-methyl-5-(2-phosphoethyl)-thiazole	C6H10NO4PS	223.0068
259	1L-myo-inositol-1-phosphate	C6H13O9P	260.0297
260			
279	linoleic acid	C18H32O2	280.2402
321	dTMP	C10H15N2O8P	322.0566
323	5-enolpyruvyl-shikimate-3-phosphate	C10H13O10P	324.0246

Chromosome 2

Changing Bin	Possible ID	Formula	Accurate Mass
75	glycolic acid	C2H4O3	76.01604
83			
109			
113	3-cyanoalanine	C4H6N2O2	114.0429
117	succinic acid	C4H6O4	118.0266
149	arabinose	C5H10O5	150.0528
159	2-oxoadipate	C6H8O5	160.0372
162			
163	coumaric acid	C9H8O3	164.0473
165	ribonic acid	C5H10O6	166.0477
181	dimethoxybenzoic acid	C9H10O4	182.0579
185	2-phosphoglyceric acid	C3H7O7P	185.9929
195	galactonate	C6H12O7	196.0583
196	3-4-dihydroxy-L-phenylalanine	C9H11NO4	197.0688
207	sinapaldehyde	C11H12O4	208.0736
243	uridine	C9H12N2O6	244.0695
258	glucosamine-1-phosphate	C6H14NO8P	259.0457
260			
275	6-phosphogluconate	C6H13O10P	276.0246
278			
279	linoleic acid	C18H32O2	280.2402
304	2',3'-cyclic CMP	C9H12N3O7P	305.0413
323	5-enolpyruvyl-shikimate-3-phosphate	C10H13O10P	324.0246
341	sucrose and isomers	C12H22O11	342.1162
342			

Chromosome 3

Changing Bin	Possible ID	Formula	Accurate Mass
98			
99			
108			
117	succinic acid	C4H6O4	118.0266
119	erythrose and isomers	C4H8O4	120.0423
125	thymine	C5H6N2O2	126.0429
137	salicylic acid	C7H6O3	138.0317
143	4-guanidino-butanamide	C5H12N4O	144.1011
149	arabinose	C5H10O5	150.0528
153	dihydroxybenzoic acid	C7H6O4	154.0266
161	anabasine	C10H14N2	162.1157
168	1-amino-propan-2-one-3-phosphate	C3H8NO5P	169.014
169	DHAP	C3H7O6P	169.998
181	dimethoxybenzoic acid	C9H10O4	182.0579
185	2-phosphoglyceric acid	C3H7O7P	185.9929
200			
204	lipoamide	C8H15NOS2	205.0595
207	sinapaldehyde	C11H12O4	208.0736
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
221	cystathionine	C7H14N2O4S	222.0674
223	sinapate	C11H12O5	224.0685
273	phloretin	C15H14O5	274.0841
334	dihydroneopterin phosphate	C9H14N5O7P	335.0631
367	orotidine-5'-phosphate	C10H13N2O11P	368.0257

Chromosome 4

Changing Bins	Possible ID	Formula	Accurate Mass
89	oxalic acid	C ₂ H ₂ O ₄	89.99531
91	glycerol	C ₃ H ₈ O ₃	92.04734
107			
117	succinic acid	C ₄ H ₆ O ₄	118.0266
119	erythrose and isomers	C ₄ H ₈ O ₄	120.0423
149	arabinose	C ₅ H ₁₀ O ₅	150.0528
161	anabasin	C ₁₀ H ₁₄ N ₂	162.1157
162			
163	coumaric acid	C ₉ H ₈ O ₃	164.0473
165	ribonic acid	C ₅ H ₁₀ O ₆	166.0477
179	glucose and isomers	C ₆ H ₁₂ O ₆	180.0634
180	tyrosine	C ₉ H ₁₁ NO ₃	181.0739
181	dimethoxybenzoic acid	C ₉ H ₁₀ O ₄	182.0579
185	2-phosphoglyceric acid	C ₃ H ₇ O ₇ P	185.9929
196	3-4-dihydroxy-L-phenylalanine	C ₉ H ₁₁ NO ₄	197.0688
221	cystathionine	C ₇ H ₁₄ N ₂ O ₄ S	222.0674
259	1L-myo-inositol-1-phosphate	C ₆ H ₁₃ O ₉ P	260.0297
260			
279	linoleic acid	C ₁₈ H ₃₂ O ₂	280.2402
299			
300	N-acetyl-D-glucosamine-1-phosphate	C ₈ H ₁₆ NO ₉ P	301.0563
305	2',3'-cyclic UMP	C ₉ H ₁₁ N ₂ O ₈ P	306.0253
309	ribulose-1,5-bisphosphate	C ₅ H ₁₂ O ₁₁ P ₂	309.9855
323	5-enolpyruvyl-shikimate-3-phosphate	C ₁₀ H ₁₃ O ₁₀ P	324.0246
393	ergosta-5,7,22,24(28)-tetraen-3-b-ol	C ₂₈ H ₄₂ O	394.3236

Chromosome 5

Changing Bin	Possible ID	Formula	Accurate Mass
75	glycolic acid	C2H4O3	76.01604
98			
117	succinic acid	C4H6O4	118.0266
125	thymine	C5H6N2O2	126.0429
135	hypoxanthine	C5H4N4O	136.0385
136	4-aminobenzoate	C7H7NO2	137.0477
143	4-guanidino-butanamide	C5H12N4O	144.1011
149	arabinose	C5H10O5	150.0528
150	guanine	C5H5N5O	151.0494
153	dihydroxybenzoic acid	C7H6O4	154.0266
159	2-oxoadipate	C6H8O5	160.0372
165	ribonic acid	C5H10O6	166.0477
195	galactonate	C6H12O7	196.0583
225	chorismate	C10H10O6	226.0477
239	cystine	C6H12N2O4S2	240.0238
251	deoxyinosine	C10H12N4O4	252.0859
265	2,3-bisphospho-D-glycerate	C3H8O10P2	265.9593
267	inosine	C10H12N4O5	268.0808
285	kaempferol	C15H10O6	286.0477
286	indole-3-glycerol-phosphate	C11H14NO6P	287.0559
297			
309	ribulose-1,5-bisphosphate	C5H12O11P2	309.9855
323	5-enolpyruvyl-shikimate-3-phosphate	C10H13O10P	324.0246
393	ergosta-5,7,22,24(28)-tetraen-3-b-ol	C28H42O	394.3236
394			

Chromosome 6

Changing Bin	Possible ID	Formula	Accurate Mass
99	#N/A	#N/A	#N/A
107	#N/A	#N/A	#N/A
113	3-cyanoalanine	C4H6N2O2	114.0429
136	4-aminobenzoate	C7H7NO2	137.0477
143	4-guanidino-butanamide	C5H12N4O	144.1011
149	arabinose	C5H10O5	150.0528
165	ribonic acid	C5H10O6	166.0477
181	dimethoxybenzoic acid	C9H10O4	182.0579
200	#N/A	#N/A	#N/A
213	2-oxo-3-hydroxy-4-phosphobutanoate	C4H7O8P	213.9879
215	erythronate-4-phosphate	C4H9O8P	216.0035
216	#N/A	#N/A	#N/A
217	#N/A	#N/A	#N/A
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
221	cystathionine	C7H14N2O4S	222.0674
222	4-methyl-5-(2-phosphoethyl)-thiazole	C6H10NO4PS	223.0068
258	glucosamine-1-phosphate	C6H14NO8P	259.0457
279	linoleic acid	C18H32O2	280.2402
337	1-(5'-phosphoribosyl)-5-amino-4-imidazolecarboxamide	C9H15N4O8P	338.0627
353	5-amino-6-(5'-phosphoribosylamino)-uracil	C9H15N4O9P	354.0577
354	2-amino-7,8-dihydro-4-hydroxy-6-(diphosphooxymethyl)-pteridine	C7H11N5O8P2	355.0083
377	GA17	C20H26O7	378.1679
379	#N/A	#N/A	#N/A
395	ergocalciferol	C28H44O	396.3392

Chromosome 7

Changing Bin	Possible ID	Formula	Accurate Mass
87	pyruvate	C3H4O3	88.01604
89	oxalic acid	C2H2O4	89.99531
90			
99			
105	glyceric acid	C3H6O4	106.0266
107			
111	uracil	C4H4N2O2	112.0273
113	3-cyanoalanine	C4H6N2O2	114.0429
117	succinic acid	C4H6O4	118.0266
125	thymine	C5H6N2O2	126.0429
135	hypoxanthine	C5H4N4O	136.0385
143	4-guanidino-butanamide	C5H12N4O	144.1011
149	arabinose	C5H10O5	150.0528
150	guanine	C5H5N5O	151.0494
163	coumaric acid	C9H8O3	164.0473
181	dimethoxybenzoic acid	C9H10O4	182.0579
185	2-phosphoglyceric acid	C3H7O7P	185.9929
200			
215	erythronate-4-phosphate	C4H9O8P	216.0035
217			
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
279	linoleic acid	C18H32O2	280.2402
305	2',3'-cyclic UMP	C9H11N2O8P	306.0253
337	1-(5'-phosphoribosyl)-5-amino-4-imidazolecarboxamide	C9H15N4O8P	338.0627
394			

Chromosome 8

Changing Bin	Possible ID	Formula	Accurate Mass
89	oxalic acid	C2H2O4	89.99531
90			
99			
107			
117	succinic acid	C4H6O4	118.0266
129	itaconate	C5H6O4	130.0266
137	salicylic acid	C7H6O3	138.0317
138	hydroxynicotinic acid	C6H5NO3	139.0269
143	4-guanidino-butanamide	C5H12N4O	144.1011
163	coumaric acid	C9H8O3	164.0473
168	1-amino-propan-2-one-3-phosphate	C3H8NO5P	169.014
181	dimethoxybenzoic acid	C9H10O4	182.0579
191	citric acid	C6H8O7	192.027
192			
200			
213	2-oxo-3-hydroxy-4-phosphobutanoate	C4H7O8P	213.9879
215	erythronate-4-phosphate	C4H9O8P	216.0035
216			
217			
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
286	indole-3-glycerol-phosphate	C11H14NO6P	287.0559
353	5-amino-6-(5'-phosphoribosylamino)-uracil	C9H15N4O9P	354.0577
354	2-amino-7,8-dihydro-4-hydroxy-6-(diphosphoxymethyl)-pteridine	C7H11N5O8P2	355.0083
381	trans,trans-farnesyl diphosphate	C15H28O7P2	382.131

Chromosome 9

Changing Bin	Possible ID	Formula	Accurate Mass
107			
111	uracil	C4H4N2O2	112.0273
117	succinic acid	C4H6O4	118.0266
125	thymine	C5H6N2O2	126.0429
129	itaconate	C5H6O4	130.0266
135	hypoxanthine	C5H4N4O	136.0385
136	4-aminobenzoate	C7H7NO2	137.0477
143	4-guanidino-butanamide	C5H12N4O	144.1011
149	arabinose	C5H10O5	150.0528
165	ribonic acid	C5H10O6	166.0477
181	dimethoxybenzoic acid	C9H10O4	182.0579
215	erythronate-4-phosphate	C4H9O8P	216.0035
216			
217			
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
222	4-methyl-5-(2-phosphoethyl)-thiazole	C6H10NO4PS	223.0068
228	5-phosphoribosylamine	C5H12NO7P	229.0351
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
265	2,3-bisphospho-D-glycerate	C3H8O10P2	265.9593
286	indole-3-glycerol-phosphate	C11H14NO6P	287.0559
309	ribulose-1,5-bisphosphate	C5H12O11P2	309.9855
353	5-amino-6-(5'-phosphoribosylamino)-uracil	C9H15N4O9P	354.0577
354	2-amino-7,8-dihydro-4-hydroxy-6-(diphosphooxymethyl)-pteridine	C7H11N5O8P2	355.0083
393	ergosta-5,7,22,24(28)-tetraen-3-b-ol	C28H42O	394.3236
395	ergocalciferol	C28H44O	396.3392

Chromosome 10

Changing Bin	Possible ID	Formula	Accurate Mass
73	glyoxylic acid	C2H2O3	74.00039
91	glycerol	C3H8O3	92.04734
98			
100			
111	uracil	C4H4N2O2	112.0273
117	succinic acid	C4H6O4	118.0266
135	hypoxanthine	C5H4N4O	136.0385
138	hydroxynicotinic acid	C6H5NO3	139.0269
142	5-(2-hydroxyethyl)-4-methylthiazole	C6H9NOS	143.0405
149	arabinose	C5H10O5	150.0528
151	alloxanthine	C5H4N4O2	152.0334
163	coumaric acid	C9H8O3	164.0473
181	dimethoxybenzoic acid	C9H10O4	182.0579
200			
215	erythronate-4-phosphate	C4H9O8P	216.0035
216			
217			
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
261	mannitol-1-phosphate	C6H15O9P	262.0454
279	linoleic acid	C18H32O2	280.2402
323	5-enolpyruvyl-shikimate-3-phosphate	C10H13O10P	324.0246
373			
393	ergosta-5,7,22,24(28)-tetraen-3-b-ol	C28H42O	394.3236
394			
395	ergocalciferol	C28H44O	396.3392

Chromosome 11

Changing Bin	Possible ID	Formula	Accurate Mass
75	glycolic acid	C2H4O3	76.01604
90			
101	2-oxobutanoate	C4H6O3	102.0317
107			
117	succinic acid	C4H6O4	118.0266
119	erythrose and isomers	C4H8O4	120.0423
138	hydroxynicotinic acid	C6H5NO3	139.0269
143	4-guanidino-butanamide	C5H12N4O	144.1011
149	arabinose	C5H10O5	150.0528
161	anabasine	C10H14N2	162.1157
179	glucose and isomers	C6H12O6	180.0634
180	tyrosine	C9H11NO3	181.0739
181	dimethoxybenzoic acid	C9H10O4	182.0579
196	3-4-dihydroxy-L-phenylalanine	C9H11NO4	197.0688
200			
201	spermine	C10H26N4	202.2157
204	lipoamide	C8H15NOS2	205.0595
205	homocitrate	C7H10O7	206.0427
214	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
215	erythronate-4-phosphate	C4H9O8P	216.0035
217			
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
323	5-enolpyruvyl-shikimate-3-phosphate	C10H13O10P	324.0246
337	1-(5'-phosphoribosyl)-5-amino-4-imidazolecarboxamide	C9H15N4O8P	338.0627
395	ergocalciferol	C28H44O	396.3392

Chromosome 12

Changing Bin	Possible ID	Formula	Accurate Mass
89	oxalic acid	C2H2O4	89.99531
90			
107			
143	4-guanidino-butanamide	C5H12N4O	144.1011
149	arabinose	C5H10O5	150.0528
153	dihydroxybenzoic acid	C7H6O4	154.0266
161	anabasine	C10H14N2	162.1157
181	dimethoxybenzoic acid	C9H10O4	182.0579
185	2-phosphoglyceric acid	C3H7O7P	185.9929
199	erythrose-4-phosphate	C4H9O7P	200.0086
211			
227	(R)-5-phosphomevalonate	C6H13O7P	228.0399
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
241	thymidine	C10H14N2O5	242.0903
251	deoxyinosine	C10H12N4O4	252.0859
259	1L-myo-inositol-1-phosphate	C6H13O9P	260.0297
299			
303	pentahydroxyflavanone	C15H12O7	304.0583
305	2',3'-cyclic UMP	C9H11N2O8P	306.0253
309	ribulose-1,5-bisphosphate	C5H12O11P2	309.9855
323	5-enolpyruvyl-shikimate-3-phosphate	C10H13O10P	324.0246
353	5-amino-6-(5'-phosphoribosylamino)-uracil	C9H15N4O9P	354.0577
354	2-amino-7,8-dihydro-4-hydroxy-6-(diphosphooxymethyl)-pteridine	C7H11N5O8P2	355.0083
355	5-amino-6-(5'-phosphoribitylamino)-uracil	C9H17N4O9P	356.0733
393	ergosta-5,7,22,24(28)-tetraen-3-b-ol	C28H42O	394.3236