

Changing Metabolites for Ripe Tomato Introgression Lines (with Possible Identification)

Seeds of *L. esculentum* M82 and *L. pennellii* and 50 introgression lines were obtained from the Tomato Genetic Resource Centre, University of California, Davis. Nine plants of each line were grown in pots in a glasshouse under ambient conditions, in Levington M3 compost with supplemented nutrients (Osmocote, Scotts Ltd, UK). Plants were watered daily and fed weekly with a proprietary tomato food (Tomato Liquid, LBS Horticulture, Lancs, UK) after flowering.

For this study samples were extracted from 3 ripe fruit per plant, 3 plants per line. These extracts were directly injected into a Waters Micromass LCT Mass Spectrometer. Data was collected for three minutes per sample. The data was obtained from the mass spectrum as a peak list (mass to 4 decimal places vs ion counts) and transferred into Microsoft Excel. A minimisation of low intensity metabolite peaks (noise reduction) was carried out and then the data summed into 1 mass unit 'bins'

This binned data was analysed by Principal Components Analysis (PCA) using SPSS software in order to show discrimination between introgression lines. The following data shows the 20 largest changing metabolites for each introgression line as compared to the 2 parents. The data is tabulated for each line individually and the data shown is for aqueous extracts run in positive mode on the mass spectrometer.

3476 Chromosome 1-1

Changing Bin	Possible ID	Formula	Accurate Mass
131	itaconate	C5H6O4	130.0266
189	7,8-diaminononanoate	C9H20N2O2	188.1525
353	prostaglandin D2	C20H32O5	352.225
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
552			
555			
557			
562			
563	protoporphyrin	C34H34N4O4	562.258
565	canthaxanthin	C40H52O2	564.3967
568			
576			
579	deserpidine	C32H38N2O8	578.2628

3478 Chromosome 1-3

Changing Bin	Possible ID	Formula	Accurate Mass
189	7,8-diaminononanoate	C9H20N2O2	188.1525
296	aminoimidazole ribotide	C8H14N3O7P	295.0569
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
545			
546	phytoene	C40H64	544.5008
552			
555			
557			
559			
565	canthaxanthin	C40H52O2	564.3967
568			
576			
579	deserpidine	C32H38N2O8	578.2628

3482 Chromosome 2-3

Changing Bin	Possible ID	Formula	Accurate Mass
117	fumaric acid	C4H4O4	116.011
131	itaconate	C5H6O4	130.0266
189	7,8-diaminononanoate	C9H20N2O2	188.1525
223	cystathionine	C7H14N2O4S	222.0674
235			
257	2-(3-carboxy-3-aminopropyl)-L-histidine	C10H16N4O4	256.1172
511			
528			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
546	phytoene	C40H64	544.5008
552			
555			
557			
563	protoporphyrin	C34H34N4O4	562.258
568			
576			

3483 Chromosome 2-4

Changing Bin	Possible ID	Formula	Accurate Mass
74	3-aminopropanal	C3H7NO2	73.05276
116	proline	C5H9NO2	115.0633
189	7,8-diaminononanoate	C9H20N2O2	188.1525
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
552			
555			
557			
558			
563	protoporphyrin	C34H34N4O4	562.258
565	canthaxanthin	C40H52O2	564.3967
568			
576			
579	deserpidine	C32H38N2O8	578.2628

3488 Chromosome 3-3

Changing Bin	Possible ID	Formula	Accurate Mass
72			
131	itaconate	C5H6O4	130.0266
150	methionine	C5H11NO2S	149.051
189	7,8-diaminononanoate	C9H20N2O2	188.1525
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
545			
546	phytoene	C40H64	544.5008
552			
555			
557			
563	protoporphyrin	C34H34N4O4	562.258
568			
576			
579	deserpidine	C32H38N2O8	578.2628

3489 Chromosome 3-4

Changing Bin	Possible ID	Formula	Accurate Mass
72			
131	itaconate	C5H6O4	130.0266
189	7,8-diaminononanoate	C9H20N2O2	188.1525
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
545			
546	phytoene	C40H64	544.5008
552			
555			
557			
565	canthaxanthin	C40H52O2	564.3967
568			
576			
579	deserpidine	C32H38N2O8	578.2628

3492 Chromosome 4-2

Changing Bin	Possible ID	Formula	Accurate Mass
131	itaconate	C5H6O4	130.0266
171	DHAP	C3H7O6P	169.998
189	7,8-diaminononanoate	C9H20N2O2	188.1525
223	cystathionine	C7H14N2O4S	222.0674
235			
511			
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
552			
555			
557			
562			
568			
576			

3494 Chromosome 4-4

Changing Bin	Possible ID	Formula	Accurate Mass
189	7,8-diaminononanoate	C9H20N2O2	188.1525
223	cystathionine	C7H14N2O4S	222.0674
225	sinapate	C11H12O5	224.0685
257	2-(3-carboxy-3-aminopropyl)-L-histidine	C10H16N4O4	256.1172
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
545			
546	phytoene	C40H64	544.5008
552			
557			
563	protoporphyrin	C34H34N4O4	562.258
568			
576			
657			

3501 Chromosome 6-2

Changing Bin	Possible ID	Formula	Accurate Mass
119	succinic acid	C4H6O4	118.0266
131	itaconate	C5H6O4	130.0266
189	7,8-diaminononanoate	C9H20N2O2	188.1525
235			
305	pentahydroxyflavanone	C15H12O7	304.0583
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
552			
555			
557			
565	canthaxanthin	C40H52O2	564.3967
568			
576			
579	deserpidine	C32H38N2O8	578.2628

3505 Chromosome 7-2

Changing Bin	Possible ID	Formula	Accurate Mass
131	itaconate	C ₅ H ₆ O ₄	130.0266
189	7,8-diaminononanoate	C ₉ H ₂₀ N ₂ O ₂	188.1525
528			
533	calotropin	C ₂₉ H ₄₀ O ₉	532.2672
534			
535			
536			
537	alpha-carotene	C ₄₀ H ₅₆	536.4382
538			
539	neurosporene	C ₄₀ H ₅₈	538.4539
545			
546	phytoene	C ₄₀ H ₆₄	544.5008
552			
555			
557			
558			
565	canthaxanthin	C ₄₀ H ₅₂ O ₂	564.3967
568			
576			
579	deserpidine	C ₃₂ H ₃₈ N ₂ O ₈	578.2628

3518 Chromosome 11-1

Changing Bin	Possible ID	Formula	Accurate Mass
116	proline	C ₅ H ₉ NO ₂	115.0633
119	succinic acid	C ₄ H ₆ O ₄	118.0266
131	itaconate	C ₅ H ₆ O ₄	130.0266
150	methionine	C ₅ H ₁₁ NO ₂ S	149.051
157	orotate	C ₅ H ₄ N ₂ O ₄	156.0171
189	7,8-diaminononanoate	C ₉ H ₂₀ N ₂ O ₂	188.1525
194			
257	2-(3-carboxy-3-aminopropyl)-L-histidine	C ₁₀ H ₁₆ N ₄ O ₄	256.1172
534			
535			
536			
537	alpha-carotene	C ₄₀ H ₅₆	536.4382
538			
539	neurosporene	C ₄₀ H ₅₈	538.4539
552			
555			
557			
565	canthaxanthin	C ₄₀ H ₅₂ O ₂	564.3967
568			
576			

4031 Chromosome 1-2

Changing Bin	Possible ID	Formula	Accurate Mass
120	allothreonine	C4H9NO3	119.0582
131	itaconate	C5H6O4	130.0266
189	7,8-diaminononanoate	C9H20N2O2	188.1525
223	cystathionine	C7H14N2O4S	222.0674
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
552			
555			
557			
558			
565	canthaxanthin	C40H52O2	564.3967
566			
568			
576			
579	deserpidine	C32H38N2O8	578.2628

4033 Chromosome 1-1

Changing Bin	Possible ID	Formula	Accurate Mass
131	itaconate	C5H6O4	130.0266
225	sinapate	C11H12O5	224.0685
511			
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
545			
546	phytoene	C40H64	544.5008
552			
555			
557			
559			
568			
576			
579	deserpidine	C32H38N2O8	578.2628

4035 Chromosome 2-1

Changing Bin	Possible ID	Formula	Accurate Mass
74	3-aminopropanal	C3H7NO2	73.05276
119	succinic acid	C4H6O4	118.0266
120	allothreonine	C4H9NO3	119.0582
131	itaconate	C5H6O4	130.0266
184	normetanephrine	C9H13NO3	183.0895
189	7,8-diaminononanoate	C9H20N2O2	188.1525
206	lipoamide	C8H15NOS2	205.0595
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
552			
555			
557			
565	canthaxanthin	C40H52O2	564.3967
568			
576			
579	deserpidine	C32H38N2O8	578.2628

4037 Chromosome 2-2

Changing Bin	Possible ID	Formula	Accurate Mass
189	7,8-diaminononanoate	C9H20N2O2	188.1525
223	cystathionine	C7H14N2O4S	222.0674
235			
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
545			
546	phytoene	C40H64	544.5008
552			
555			
557			
565	canthaxanthin	C40H52O2	564.3967
568			
576			
579	deserpidine	C32H38N2O8	578.2628

4040 Chromosome 2-5

Changing Bin	Possible ID	Formula	Accurate Mass
152	guanine	C ₅ H ₅ N ₅ O	151.0494
157	orotate	C ₅ H ₄ N ₂ O ₄	156.0171
159	(S)-dihydroorotate	C ₅ H ₆ N ₂ O ₄	158.0328
235			
257	2-(3-carboxy-3-aminopropyl)-L-histidine	C ₁₀ H ₁₆ N ₄ O ₄	256.1172
262			
511			
528			
534			
535			
536			
537	alpha-carotene	C ₄₀ H ₅₆	536.4382
538			
539	neurosporene	C ₄₀ H ₅₈	538.4539
552			
555			
557			
568			
576			
579	deserpidine	C ₃₂ H ₃₈ N ₂ O ₈	578.2628

4041 Chromosome 2-6

Changing Bin	Possible ID	Formula	Accurate Mass
189	7,8-diaminononanoate	C ₉ H ₂₀ N ₂ O ₂	188.1525
223	cystathionine	C ₇ H ₁₄ N ₂ O ₄ S	222.0674
262			
528			
533	calotropin	C ₂₉ H ₄₀ O ₉	532.2672
534			
535			
536			
537	alpha-carotene	C ₄₀ H ₅₆	536.4382
538			
539	neurosporene	C ₄₀ H ₅₈	538.4539
545			
546	phytoene	C ₄₀ H ₆₄	544.5008
552			
555			
557			
565	canthaxanthin	C ₄₀ H ₅₂ O ₂	564.3967
568			
576			
579	deserpidine	C ₃₂ H ₃₈ N ₂ O ₈	578.2628

4043 Chromosome 3-1

Changing Bin	Possible ID	Formula	Accurate Mass
111			
131	itaconate	C5H6O4	130.0266
152	guanine	C5H5N5O	151.0494
159	(S)-dihydroorotate	C5H6N2O4	158.0328
168	pyridine-2,3-dicarboxylate	C7H5NO4	167.0219
189	7,8-diaminononanoate	C9H20N2O2	188.1525
375			
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
552			
555			
557			
565	canthaxanthin	C40H52O2	564.3967
568			
576			
579	deserpidine	C32H38N2O8	578.2628

4044 Chromosome 3-2

Changing Bin	Possible ID	Formula	Accurate Mass
189	7,8-diaminononanoate	C9H20N2O2	188.1525
535			
552			
528			
576			
537	alpha-carotene	C40H56	536.4382
557			
533	calotropin	C29H40O9	532.2672
536			
545			
563	protoporphyrin	C34H34N4O4	562.258
538			
546	phytoene	C40H64	544.5008
539	neurosporene	C40H58	538.4539
568			
131	itaconate	C5H6O4	130.0266
149	2-methylmalic acid	C5H8O5	148.0372
534			
555			
559			

4047 Chromosome 3-5

Changing Bin	Possible ID	Formula	Accurate Mass
122	cysteine	C3H7NO2S	121.0197
131	itaconate	C5H6O4	130.0266
189	7,8-diaminononanoate	C9H20N2O2	188.1525
207	homoisocitrate	C7H10O7	206.0427
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
552			
555			
557			
565	canthaxanthin	C40H52O2	564.3967
568			
576			
579	deserpidine	C32H38N2O8	578.2628
670			

4048 Chromosome 4-1

Changing Bin	Possible ID	Formula	Accurate Mass
189	7,8-diaminononanoate	C9H20N2O2	188.1525
262			
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
545			
546	phytoene	C40H64	544.5008
552			
555			
557			
562			
563	protoporphyrin	C34H34N4O4	562.258
568			
576			
579	deserpidine	C32H38N2O8	578.2628

4051 Chromosome 4-3

Changing Bin	Possible ID	Formula	Accurate Mass
157	orotate	C ₅ H ₄ N ₂ O ₄	156.0171
189	7,8-diaminononanoate	C ₉ H ₂₀ N ₂ O ₂	188.1525
223	cystathionine	C ₇ H ₁₄ N ₂ O ₄ S	222.0674
528			
533	calotropin	C ₂₉ H ₄₀ O ₉	532.2672
534			
535			
536			
537	alpha-carotene	C ₄₀ H ₅₆	536.4382
538			
539	neurosporene	C ₄₀ H ₅₈	538.4539
545			
546	phytoene	C ₄₀ H ₆₄	544.5008
552			
555			
557			
563	protoporphyrin	C ₃₄ H ₃₄ N ₄ O ₄	562.258
565	canthaxanthin	C ₄₀ H ₅₂ O ₂	564.3967
568			
576			

4054 Chromosome 5-1

Changing Bin	Possible ID	Formula	Accurate Mass
131	itaconate	C ₅ H ₆ O ₄	130.0266
149	2-methylmalic acid	C ₅ H ₈ O ₅	148.0372
150	methionine	C ₅ H ₁₁ N ₂ O ₂ S	149.051
167	ribonic acid	C ₅ H ₁₀ O ₆	166.0477
189	7,8-diaminononanoate	C ₉ H ₂₀ N ₂ O ₂	188.1525
223	cystathionine	C ₇ H ₁₄ N ₂ O ₄ S	222.0674
528			
533	calotropin	C ₂₉ H ₄₀ O ₉	532.2672
534			
535			
536			
537	alpha-carotene	C ₄₀ H ₅₆	536.4382
538			
539	neurosporene	C ₄₀ H ₅₈	538.4539
552			
555			
557			
565	canthaxanthin	C ₄₀ H ₅₂ O ₂	564.3967
568			
576			

4055 Chromosome 5-2

Changing Bin	Possible ID	Formula	Accurate Mass
72			
131	itaconate	C5H6O4	130.0266
150	methionine	C5H11NO2S	149.051
189	7,8-diaminononanoate	C9H20N2O2	188.1525
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
552			
555			
557			
565	canthaxanthin	C40H52O2	564.3967
568			
576			
579	deserpidine	C32H38N2O8	578.2628
674	veratridine	C36H51NO11	673.3462

4056 Chromosome 5-2

Changing Bin	Possible ID	Formula	Accurate Mass
131	itaconate	C5H6O4	130.0266
189	7,8-diaminononanoate	C9H20N2O2	188.1525
511			
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
546	phytoene	C40H64	544.5008
552			
555			
557			
558			
565	canthaxanthin	C40H52O2	564.3967
568			
576			
579	deserpidine	C32H38N2O8	578.2628

4057 Chromosome 5-4

Changing Bin	Possible ID	Formula	Accurate Mass
189	7,8-diaminononanoate	C ₉ H ₂₀ N ₂ O ₂	188.1525
225	sinapate	C ₁₁ H ₁₂ O ₅	224.0685
528			
533	calotropin	C ₂₉ H ₄₀ O ₉	532.2672
534			
535			
536			
537	alpha-carotene	C ₄₀ H ₅₆	536.4382
538			
539	neurosporene	C ₄₀ H ₅₈	538.4539
546	phytoene	C ₄₀ H ₆₄	544.5008
552			
555			
557			
559			
563	protoporphyrin	C ₃₄ H ₃₄ N ₄ O ₄	562.258
565	canthaxanthin	C ₄₀ H ₅₂ O ₂	564.3967
568			
576			
579	deserpidine	C ₃₂ H ₃₈ N ₂ O ₈	578.2628

4058 Chromosome 5-5

Changing Bin	Possible ID	Formula	Accurate Mass
131	itaconate	C ₅ H ₆ O ₄	130.0266
157	orotate	C ₅ H ₄ N ₂ O ₄	156.0171
189	7,8-diaminononanoate	C ₉ H ₂₀ N ₂ O ₂	188.1525
194			
257	2-(3-carboxy-3-aminopropyl)-L-histidine	C ₁₀ H ₁₆ N ₄ O ₄	256.1172
528			
533	calotropin	C ₂₉ H ₄₀ O ₉	532.2672
534			
535			
536			
537	alpha-carotene	C ₄₀ H ₅₆	536.4382
538			
539	neurosporene	C ₄₀ H ₅₈	538.4539
552			
555			
557			
565	canthaxanthin	C ₄₀ H ₅₂ O ₂	564.3967
568			
576			
579	deserpidine	C ₃₂ H ₃₈ N ₂ O ₈	578.2628

4059 Chromosome 6-1

Changing Bin	Possible ID	Formula	Accurate Mass
131	itaconate	C5H6O4	130.0266
150	methionine	C5H11NO2S	149.051
189	7,8-diaminononanoate	C9H20N2O2	188.1525
511			
528			
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
545			
546	phytoene	C40H64	544.5008
552			
555			
557			
565	canthaxanthin	C40H52O2	564.3967
568			
576			
579	deserpidine	C32H38N2O8	578.2628

4062 Chromosome 6-3

Changing Bin	Possible ID	Formula	Accurate Mass
72			
131	itaconate	C5H6O4	130.0266
150	methionine	C5H11NO2S	149.051
156	histidine	C6H9N3O2	155.0695
157	orotate	C5H4N2O4	156.0171
189	7,8-diaminononanoate	C9H20N2O2	188.1525
235			
257	2-(3-carboxy-3-aminopropyl)-L-histidine	C10H16N4O4	256.1172
528			
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
552			
555			
557			
568			
576			

4063 Chromosome 6-4

Changing Bin	Possible ID	Formula	Accurate Mass
131	itaconate	C5H6O4	130.0266
189	7,8-diaminononanoate	C9H20N2O2	188.1525
223	cystathionine	C7H14N2O4S	222.0674
262			
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
552			
555			
557			
563	protoporphyrin	C34H34N4O4	562.258
565	canthaxanthin	C40H52O2	564.3967
568			
576			
579	deserpidine	C32H38N2O8	578.2628

4064 Chromosome 7-1

Changing Bin	Possible ID	Formula	Accurate Mass
72			
131	itaconate	C5H6O4	130.0266
189	7,8-diaminononanoate	C9H20N2O2	188.1525
223	cystathionine	C7H14N2O4S	222.0674
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
545			
546	phytoene	C40H64	544.5008
552			
555			
557			
565	canthaxanthin	C40H52O2	564.3967
568			
576			

4066 Chromosome 7-3

Changing Bin	Possible ID	Formula	Accurate Mass
119	succinic acid	C4H6O4	118.0266
131	itaconate	C5H6O4	130.0266
189	7,8-diaminononanoate	C9H20N2O2	188.1525
223	cystathionine	C7H14N2O4S	222.0674
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
545			
546	phytoene	C40H64	544.5008
552			
555			
557			
563	protoporphyrin	C34H34N4O4	562.258
576			
657			

4067 Chromosome 7-3

Changing Bin	Possible ID	Formula	Accurate Mass
119	succinic acid	C4H6O4	118.0266
131	itaconate	C5H6O4	130.0266
152	guanine	C5H5N5O	151.0494
189	7,8-diaminononanoate	C9H20N2O2	188.1525
223	cystathionine	C7H14N2O4S	222.0674
528			
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
552			
555			
557			
565	canthaxanthin	C40H52O2	564.3967
568			
576			
579	deserpidine	C32H38N2O8	578.2628
674	veratridine	C36H51NO11	673.3462

4069 Chromosome 7-5

Changing Bin	Possible ID	Formula	Accurate Mass
72			
131	itaconate	C5H6O4	130.0266
189	7,8-diaminononanoate	C9H20N2O2	188.1525
305	pentahydroxyflavanone	C15H12O7	304.0583
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
545			
546	phytoene	C40H64	544.5008
552			
555			
557			
565	canthaxanthin	C40H52O2	564.3967
568			
576			

4071 Chromosome 8-1

Changing Bin	Possible ID	Formula	Accurate Mass
152	guanine	C5H5N5O	151.0494
167	ribonic acid	C5H10O6	166.0477
168	pyridine-2,3-dicarboxylate	C7H5NO4	167.0219
187	2-phosphoglyceric acid	C3H7O7P	185.9929
189	7,8-diaminononanoate	C9H20N2O2	188.1525
223	cystathionine	C7H14N2O4S	222.0674
511			
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
552			
555			
557			
565	canthaxanthin	C40H52O2	564.3967
568			
576			
579	deserpidine	C32H38N2O8	578.2628

4074 Chromosome 8-2

Changing Bin	Possible ID	Formula	Accurate Mass
189	7,8-diaminononanoate	C ₉ H ₂₀ N ₂ O ₂	188.1525
511			
528			
533	calotropin	C ₂₉ H ₄₀ O ₉	532.2672
534			
535			
536			
537	alpha-carotene	C ₄₀ H ₅₆	536.4382
538			
539	neurosporene	C ₄₀ H ₅₈	538.4539
552			
555			
557			
559			
562			
563	protoporphyrin	C ₃₄ H ₃₄ N ₄ O ₄	562.258
565	canthaxanthin	C ₄₀ H ₅₂ O ₂	564.3967
568			
576			
579	deserpidine	C ₃₂ H ₃₈ N ₂ O ₈	578.2628

4076 Chromosome 8-3

Changing Bin	Possible ID	Formula	Accurate Mass
131	itaconate	C ₅ H ₆ O ₄	130.0266
189	7,8-diaminononanoate	C ₉ H ₂₀ N ₂ O ₂	188.1525
528			
533	calotropin	C ₂₉ H ₄₀ O ₉	532.2672
534			
535			
536			
537	alpha-carotene	C ₄₀ H ₅₆	536.4382
538			
539	neurosporene	C ₄₀ H ₅₈	538.4539
545			
552			
555			
557			
559			
562			
565	canthaxanthin	C ₄₀ H ₅₂ O ₂	564.3967
568			
576			
579	deserpidine	C ₃₂ H ₃₈ N ₂ O ₈	578.2628

4078 Chromosome 9-1

Changing Bin	Possible ID	Formula	Accurate Mass
72			
131	itaconate	C5H6O4	130.0266
189	7,8-diaminononanoate	C9H20N2O2	188.1525
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
545			
546	phytoene	C40H64	544.5008
552			
555			
557			
565	canthaxanthin	C40H52O2	564.3967
568			
576			
579	deserpidine	C32H38N2O8	578.2628

4081 Chromosome 9-2

Changing Bin	Possible ID	Formula	Accurate Mass
131	itaconate	C5H6O4	130.0266
147	2-oxoglutarate	C5H6O5	146.0215
189	7,8-diaminononanoate	C9H20N2O2	188.1525
194			
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
545			
546	phytoene	C40H64	544.5008
552			
555			
557			
565	canthaxanthin	C40H52O2	564.3967
568			
576			

4084 Chromosome 9-3

Changing Bin	Possible ID	Formula	Accurate Mass
72			
131	itaconate	C5H6O4	130.0266
189	7,8-diaminononanoate	C9H20N2O2	188.1525
223	cystathionine	C7H14N2O4S	222.0674
511			
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
545			
546	phytoene	C40H64	544.5008
555			
557			
565	canthaxanthin	C40H52O2	564.3967
576			
579	deserpidine	C32H38N2O8	578.2628

4087 Chromosome 10-1

Changing Bin	Possible ID	Formula	Accurate Mass
72			
119	succinic acid	C4H6O4	118.0266
124	nicotinic acid	C6H5NO2	123.032
131	itaconate	C5H6O4	130.0266
156	histidine	C6H9N3O2	155.0695
157	orotate	C5H4N2O4	156.0171
189	7,8-diaminononanoate	C9H20N2O2	188.1525
257	2-(3-carboxy-3-aminopropyl)-L-histidine	C10H16N4O4	256.1172
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
552			
568			
670			
674	veratridine	C36H51NO11	673.3462

4089 Chromosome 10-2

Changing Bin	Possible ID	Formula	Accurate Mass
189	7,8-diaminononanoate	C9H20N2O2	188.1525
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
545			
546	phytoene	C40H64	544.5008
552			
555			
557			
559			
562			
565	canthaxanthin	C40H52O2	564.3967
568			
576			
579	deserpidine	C32H38N2O8	578.2628

4091 Chromosome 10-3

Changing Bin	Possible ID	Formula	Accurate Mass
131	itaconate	C5H6O4	130.0266
189	7,8-diaminononanoate	C9H20N2O2	188.1525
235			
262			
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
552			
555			
557			
558			
562			
568			
576			
579	deserpidine	C32H38N2O8	578.2628

4093 Chromosome 11-2

Changing Bin	Possible ID	Formula	Accurate Mass
72			
167	ribonic acid	C5H10O6	166.0477
189	7,8-diaminononanoate	C9H20N2O2	188.1525
235			
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
552			
555			
557			
558			
565	canthaxanthin	C40H52O2	564.3967
568			
576			
579	deserpidine	C32H38N2O8	578.2628

4094 Chromosome 11-3

Changing Bin	Possible ID	Formula	Accurate Mass
131	itaconate	C5H6O4	130.0266
159	(S)-dihydroorotate	C5H6N2O4	158.0328
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
552			
555			
557			
562			
563	protoporphyrin	C34H34N4O4	562.258
565	canthaxanthin	C40H52O2	564.3967
568			
576			
579	deserpidine	C32H38N2O8	578.2628
586			

4095 Chromosome 11-4

Changing Bin	Possible ID	Formula	Accurate Mass
131	itaconate	C ₅ H ₆ O ₄	130.0266
189	7,8-diaminononanoate	C ₉ H ₂₀ N ₂ O ₂	188.1525
235			
528			
533	calotropin	C ₂₉ H ₄₀ O ₉	532.2672
534			
535			
536			
537	alpha-carotene	C ₄₀ H ₅₆	536.4382
538			
539	neurosporene	C ₄₀ H ₅₈	538.4539
545			
546	phytoene	C ₄₀ H ₆₄	544.5008
552			
555			
557			
565	canthaxanthin	C ₄₀ H ₅₂ O ₂	564.3967
568			
576			
579	deserpidine	C ₃₂ H ₃₈ N ₂ O ₈	578.2628

4097 Chromosome 12-1

Changing Bin	Possible ID	Formula	Accurate Mass
189	7,8-diaminononanoate	C ₉ H ₂₀ N ₂ O ₂	188.1525
296	aminoimidazole ribotide	C ₈ H ₁₄ N ₃ O ₇ P	295.0569
511			
528			
533	calotropin	C ₂₉ H ₄₀ O ₉	532.2672
534			
535			
536			
537	alpha-carotene	C ₄₀ H ₅₆	536.4382
538			
539	neurosporene	C ₄₀ H ₅₈	538.4539
545			
546	phytoene	C ₄₀ H ₆₄	544.5008
552			
555			
557			
563	protoporphyrin	C ₃₄ H ₃₄ N ₄ O ₄	562.258
568			
576			
579	deserpidine	C ₃₂ H ₃₈ N ₂ O ₈	578.2628

4099 Chromosome 12-2

Changing Bin	Possible ID	Formula	Accurate Mass
72			
131	itaconate	C ₅ H ₆ O ₄	130.0266
150	methionine	C ₅ H ₁₁ NO ₂ S	149.051
189	7,8-diaminononanoate	C ₉ H ₂₀ N ₂ O ₂	188.1525
194			
223	cystathionine	C ₇ H ₁₄ N ₂ O ₄ S	222.0674
511			
528			
533	calotropin	C ₂₉ H ₄₀ O ₉	532.2672
534			
535			
536			
537	alpha-carotene	C ₄₀ H ₅₆	536.4382
538			
539	neurosporene	C ₄₀ H ₅₈	538.4539
552			
555			
557			
568			
576			

4100 Chromosome 12-3

Changing Bin	Possible ID	Formula	Accurate Mass
72			
119	succinic acid	C ₄ H ₆ O ₄	118.0266
131	itaconate	C ₅ H ₆ O ₄	130.0266
189	7,8-diaminononanoate	C ₉ H ₂₀ N ₂ O ₂	188.1525
194			
223	cystathionine	C ₇ H ₁₄ N ₂ O ₄ S	222.0674
528			
533	calotropin	C ₂₉ H ₄₀ O ₉	532.2672
534			
535			
536			
537	alpha-carotene	C ₄₀ H ₅₆	536.4382
538			
539	neurosporene	C ₄₀ H ₅₈	538.4539
545			
552			
557			
559			
568			
576			

4102 Chromosome 12-4

Changing Bin	Possible ID	Formula	Accurate Mass
119	succinic acid	C4H6O4	118.0266
120	allothreonine	C4H9NO3	119.0582
150	methionine	C5H11NO2S	149.051
189	7,8-diaminononanoate	C9H20N2O2	188.1525
528			
533	calotropin	C29H40O9	532.2672
534			
535			
536			
537	alpha-carotene	C40H56	536.4382
538			
539	neurosporene	C40H58	538.4539
545			
552			
555			
557			
565	canthaxanthin	C40H52O2	564.3967
568			
576			
579	deserpidine	C32H38N2O8	578.2628