

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 negative mode on the mass spectrometer.

3476 Chromosome 1-1

Changing Bin	Possible ID	Formula	Accurate Mass
105	glyceric acid	C3H6O4	106.0266
148	methionine	C5H11NO2S	149.0510
165	ribonic acid	C5H10O6	166.0477
182	normetanephine	C9H13NO3	183.0895
192			
208			
215	erythronate-4-phosphate	C4H9O8P	216.0035
217			
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
250	muramic acid	C9H17NO7	251.1005
283	xanthosine	C10H12N4O6	284.0757
526			
695			
760			
765			
773			
789	all-trans-nonaprenyl diphosphate	C45H76O7P2	790.5066

3478 Chromosome 1-3

Changing Bin	Possible ID	Formula	Accurate Mass
71	methylglyoxal	C3H4O2	72.0211
73	glyoxylic acid	C2H2O3	74.0004
75	glycolic acid	C2H4O3	76.0160
98			
105	glyceric acid	C3H6O4	106.0266
142	5-(2-hydroxyethyl)-4-methylthiazole	C6H9NOS	143.0405
154	histidine	C6H9N3O2	155.0695
159	2-oxoadipate	C6H8O5	160.0372
173	aconitic acid	C6H6O6	174.0164
186	8-amino-7-oxononanoate	C9H17NO3	187.1208
208			
211			
213	2-oxo-3-hydroxy-4-phosphobutanoate	C4H7O8P	213.9879
214	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
216			
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
236			
239	cystine	C6H12N2O4S2	240.0238
272	erythroidine	C16H19NO3	273.1365
501			

3482 Chromosome 2-3

Changing Bin	Possible ID	Formula	Accurate Mass
75	glycolic acid	C2H4O3	76.0160
87	pyruvate	C3H4O3	88.0160
88	oxamic acid	C2H3NO3	89.0113
105	glyceric acid	C3H6O4	106.0266
142	5-(2-hydroxyethyl)-4-methylthiazole	C6H9NOS	143.0405
148	methionine	C5H11NO2S	149.0510
154	histidine	C6H9N3O2	155.0695
157	(S)-dihydroorotate	C5H6N2O4	158.0328
159	2-oxoadipate	C6H8O5	160.0372
184	3-phosphoserine	C3H8NO6P	185.0089
207	sinapaldehyde	C11H12O4	208.0736
208			
213	2-oxo-3-hydroxy-4-phosphobutanoate	C4H7O8P	213.9879
214	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
217			
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
501			
526			

3483 Chromosome 2-4

Changing Bin	Possible ID	Formula	Accurate Mass
98			
105	glyceric acid	C3H6O4	106.0266
186	8-amino-7-oxononanoate	C9H17NO3	187.1208
208			
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
246	pyridoxal-5'-phosphate	C8H10NO6P	247.0246
249	gamma-L-glutamyl-L-cysteine	C8H14N2O5S	250.0623
260			
297			
425	(S)-2,3-epoxysqualene	C30H50O	426.3862
427	IDP	C10H14N4O11P2	428.0134
433	6-deoxoteasterone	C28H50O3	434.3760
458			
469			
773			
774			

3488 Chromosome 3-3

Changing Bin	Possible ID	Formula	Accurate Mass
98			
134	homocysteine	C4H9NO2S	135.0354
143	4-guanidino-butanamide	C5H12N4O	144.1011
144	spermidine	C7H19N3	145.1579
161	anabasine	C10H14N2	162.1157
192			
309	ribulose-1,5-bisphosphate	C5H12O11P2	309.9855
317	myricetin	C15H10O8	318.0376
352	2,5-diamino-6-hydroxy-4-(5'-phosphoribosylamino)-pyrimidine	C9H16N5O8P	353.0736
353	5-amino-6-(5'-phosphoribosylamino)-uracil	C9H15N4O9P	354.0577
354	2-amino-7,8-dihydro-4-hydroxy-6-(diphosphoxymethyl)-pteridine	C7H11N5O8P2	355.0083
367	orotidine-5'-phosphate	C10H13N2O11P	368.0257
487			
488			
695			
737			
757			
763			
773			
774			

3489 Chromosome 3-4

Changing Bin	Possible ID	Formula	Accurate Mass
98			
134	homocysteine	C4H9NO2S	135.0354
143	4-guanidino-butanamide	C5H12N4O	144.1011
144	spermidine	C7H19N3	145.1579
161	anabasine	C10H14N2	162.1157
192			
309	ribulose-1,5-bisphosphate	C5H12O11P2	309.9855
317	myricetin	C15H10O8	318.0376
352	2,5-diamino-6-hydroxy-4-(5'-phosphoribosylamino)-pyrimidine	C9H16N5O8P	353.0736
353	5-amino-6-(5'-phosphoribosylamino)-uracil	C9H15N4O9P	354.0577
354	2-amino-7,8-dihydro-4-hydroxy-6-(diphosphoxymethyl)-pteridine	C7H11N5O8P2	355.0083
367	orotidine-5'-phosphate	C10H13N2O11P	368.0257
487			
488			
695			
737			
757			
763			
656			
659			

3492 Chromosome 4-2

Changing Bin	Possible ID	Formula	Accurate Mass
58			
81			
83			
90			
91	glycerol	C3H8O3	92.0473
107			
179	3-(4-hydroxyphenyl)pyruvate	C9H8O4	180.0423
194	glucosaminic acid	C6H13NO6	195.0743
225	chorismate	C10H10O6	226.0477
241	thymidine	C10H14N2O5	242.0903
309	ribulose-1,5-bisphosphate	C5H12O11P2	309.9855
313	5'-phosphoribosyl-N-formylglycinamide	C8H15N2O9P	314.0515
314			
317	myricetin	C15H10O8	318.0376
354	2-amino-7,8-dihydro-4-hydroxy-6-(diphosphoxymethyl)-pteridine	C7H11N5O8P2	355.0083
367	orotidine-5'-phosphate	C10H13N2O11P	368.0257
385	1-sinapoyl-D-glucose	C17H22O10	386.1213
633	rescinamine	C35H42N2O9	634.2890
782			
783			

3494 Chromosome 4-4

Changing Bin	Possible ID	Formula	Accurate Mass
98			
134	homocysteine	C4H9NO2S	135.0354
142	5-(2-hydroxyethyl)-4-methylthiazole	C6H9NOS	143.0405
143	4-guanidino-butanamide	C5H12N4O	144.1011
192			
236			
243	uridine	C9H12N2O6	244.0695
352	2,5-diamino-6-hydroxy-4-(5'-phosphoribosylamino)-pyrimidine	C9H16N5O8P	353.0736
353	5-amino-6-(5'-phosphoribosylamino)-uracil	C9H15N4O9P	354.0577
354	2-amino-7,8-dihydro-4-hydroxy-6-(diphosphooxymethyl)-pteridine	C7H11N5O8P2	355.0083
384			
487			
695			
732			
757			
760			
763			
781			
757			
773			

3501 Chromosome 6-2

Changing Bin	Possible ID	Formula	Accurate Mass
133	malic acid	C4H6O5	134.0215
134	homocysteine	C4H9NO2S	135.0354
143	4-guanidino-butanamide	C5H12N4O	144.1011
180	tyrosine	C9H11NO3	181.0739
192			
194	glucosaminic acid	C6H13NO6	195.0743
309	ribulose-1,5-bisphosphate	C5H12O11P2	309.9855
339	fructose-1,6-bisphosphate	C6H14O12P2	339.9960
352	2,5-diamino-6-hydroxy-4-(5'-phosphoribosylamino)-pyrimidine	C9H16N5O8P	353.0736
353	5-amino-6-(5'-phosphoribosylamino)-uracil	C9H15N4O9P	354.0577
354	2-amino-7,8-dihydro-4-hydroxy-6-(diphosphooxymethyl)-pteridine	C7H11N5O8P2	355.0083
367	orotidine-5'-phosphate	C10H13N2O11P	368.0257
487			
557			
633	rescinamine	C35H42N2O9	634.2890
659			
695			
737			
469			
501			

3505 Chromosome 7-2

Changing Bin	Possible ID	Formula	Accurate Mass
105	glyceric acid	C3H6O4	106.0266
142	5-(2-hydroxyethyl)-4-methylthiazole	C6H9NOS	143.0405
165	ribonic acid	C5H10O6	166.0477
186	8-amino-7-oxononanoate	C9H17NO3	187.1208
208			
214	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
250	muramic acid	C9H17NO7	251.1005
255	2-(3-carboxy-3-aminopropyl)-L-histidine	C10H16N4O4	256.1172
260			
283	xanthosine	C10H12N4O6	284.0757
425	(S)-2,3-epoxysqualene	C30H50O	426.3862
427	IDP	C10H14N4O11P2	428.0134
501			
526			

3518 Chromosome 11-1

Changing Bin	Possible ID	Formula	Accurate Mass
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
249	gamma-L-glutamyl-L-cysteine	C8H14N2O5S	250.0623
250	muramic acid	C9H17NO7	251.1005
255	2-(3-carboxy-3-aminopropyl)-L-histidine	C10H16N4O4	256.1172
272	erythroidine	C16H19NO3	273.1365
283	xanthosine	C10H12N4O6	284.0757
312	3',5'-cyclic dAMP	C10H12N5O5P	313.0576
329	3',5'-cyclic IMP	C10H11N4O7P	330.0365
345	GA24	C20H26O5	346.1780
398			
425	(S)-2,3-epoxysqualene	C30H50O	426.3862
427	IDP	C10H14N4O11P2	428.0134
433	6-deoxoteasterone	C28H50O3	434.3760
469			
469			
501			

4031 Chromosome 1-2

Changing Bin	Possible ID	Formula	Accurate Mass
98			
105	glyceric acid	C3H6O4	106.0266
159	2-oxoadipate	C6H8O5	160.0372
186	8-amino-7-oxononanoate	C9H17NO3	187.1208
208			
214	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
216			
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
245	D3-isopentenyl-PP	C5H12O7P2	246.0058
246	pyridoxal-5'-phosphate	C8H10NO6P	247.0246
283	xanthosine	C10H12N4O6	284.0757
425	(S)-2,3-epoxysqualene	C30H50O	426.3862
427	IDP	C10H14N4O11P2	428.0134
757			
763			

4033 Chromosome 1-4

Changing Bin	Possible ID	Formula	Accurate Mass
98			
161	anabesine	C10H14N2	162.1157
177	pyrophosphate	H4O7P2	177.9432
182	normetanephrene	C9H13NO3	183.0895
191	citric acid	C6H8O7	192.0270
192			
215	erythronate-4-phosphate	C4H9O8P	216.0035
217			
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
352	2,5-diamino-6-hydroxy-4-(5'-phosphoribosylamino)-pyrimidine	C9H16N5O8P	353.0736
353	5-amino-6-(5'-phosphoribosylamino)-uracil	C9H15N4O9P	354.0577
487			
557			
695			
737			
469			
501			

4035 Chromosome 2-1

Changing Bin	Possible ID	Formula	Accurate Mass
105	glyceric acid	C3H6O4	106.0266
214	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
216			
217			
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
239	cystine	C6H12N2O4S2	240.0238
250	muramic acid	C9H17NO7	251.1005
255	2-(3-carboxy-3-aminopropyl)-L-histidine	C10H16N4O4	256.1172
283	xanthosine	C10H12N4O6	284.0757
297			
328	2',3'-cyclic AMP	C10H12N5O6P	329.0525
329	3',5'-cyclic IMP	C10H11N4O7P	330.0365
398			
425	(S)-2,3-epoxysqualene	C30H50O	426.3862
427	IDP	C10H14N4O11P2	428.0134
433	6-deoxoteasterone	C28H50O3	434.3760
458			
789	all-trans-nonaprenyl diphosphate	C45H76O7P2	790.5066
791			

4037 Chromosome 2-2

Changing Bin	Possible ID	Formula	Accurate Mass
134	homocysteine	C4H9NO2S	135.0354
192			
309	ribulose-1,5-bisphosphate	C5H12O11P2	309.9855
352	2,5-diamino-6-hydroxy-4-(5'-phosphoribosylamino)-pyrimidine	C9H16N5O8P	353.0736
353	5-amino-6-(5'-phosphoribosylamino)-uracil	C9H15N4O9P	354.0577
354	2-amino-7,8-dihydro-4-hydroxy-6-(diphosphoxymethyl)-pteridine	C7H11N5O8P2	355.0083
367	orotidine-5'-phosphate	C10H13N2O11P	368.0257
384			
487			
488			
659			
695			
737			
757			
760			
763			
773			
774			
311	icosanoic acid	C20H40O2	312.3028
501			

4040 Chromosome 2-5

Changing Bin	Possible ID	Formula	Accurate Mass
98			
105	glyceric acid	C3H6O4	106.0266
142	5-(2-hydroxyethyl)-4-methylthiazole	C6H9NOS	143.0405
144	spermidine	C7H19N3	145.1579
177	pyrophosphate	H4O7P2	177.9432
182	normetanephine	C9H13NO3	183.0895
186	8-amino-7-oxononanoate	C9H17NO3	187.1208
208			
216			
217			
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
272	erythroidine	C16H19NO3	273.1365
283	xanthosine	C10H12N4O6	284.0757
297			
398			
501			

4041 Chromosome 2-6

Changing Bin	Possible ID	Formula	Accurate Mass
98			
105	glyceric acid	C3H6O4	106.0266
186	8-amino-7-oxononanoate	C9H17NO3	187.1208
208			
214	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
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
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
251	deoxyinosine	C10H12N4O4	252.0859
264			
283	xanthosine	C10H12N4O6	284.0757
297			
469			
501			

4043 Chromosome 3-1

Changing Bin	Possible ID	Formula	Accurate Mass
105	glyceric acid	C3H6O4	106.0266
186	8-amino-7-oxononanoate	C9H17NO3	187.1208
208			
214	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
216			
217			
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
249	gamma-L-glutamyl-L-cysteine	C8H14N2O5S	250.0623
260			
264			
283	xanthosine	C10H12N4O6	284.0757
297			
398			
782			
783			

4044 Chromosome 3-2

Changing Bin	Possible ID	Formula	Accurate Mass
98			
105	glyceric acid	C3H6O4	106.0266
148	methionine	C5H11NO2S	149.0510
177	pyrophosphate	H4O7P2	177.9432
182	normetanephine	C9H13NO3	183.0895
192			
236			
243	uridine	C9H12N2O6	244.0695
352	2,5-diamino-6-hydroxy-4-(5'-phosphoribosylamino)-pyrimidine	C9H16N5O8P	353.0736
353	5-amino-6-(5'-phosphoribosylamino)-uracil	C9H15N4O9P	354.0577
354	2-amino-7,8-dihydro-4-hydroxy-6-(diphosphoxymethyl)-pteridine	C7H11N5O8P2	355.0083
487			
557			
695			
732			
757			
760			
763			
774			
791			

4047 Chromosome 3-5

Changing Bin	Possible ID	Formula	Accurate Mass
134	homocysteine	C4H9NO2S	135.0354
143	4-guanidino-butanamide	C5H12N4O	144.1011
177	pyrophosphate	H4O7P2	177.9432
192			
194	glucosaminic acid	C6H13NO6	195.0743
215	erythronate-4-phosphate	C4H9O8P	216.0035
309	ribulose-1,5-bisphosphate	C5H12O11P2	309.9855
339	fructose-1,6-bisphosphate	C6H14O12P2	339.9960
352	2,5-diamino-6-hydroxy-4-(5'-phosphoribosylamino)-pyrimidine	C9H16N5O8P	353.0736
353	5-amino-6-(5'-phosphoribosylamino)-uracil	C9H15N4O9P	354.0577
354	2-amino-7,8-dihydro-4-hydroxy-6-(diphosphoxymethyl)-pteridine	C7H11N5O8P2	355.0083
367	orotidine-5'-phosphate	C10H13N2O11P	368.0257
487			
695			
737			
757			
763			
773			
526			
773			

4048 Chromosome 4-1

Changing Bin	Possible ID	Formula	Accurate Mass
105	glyceric acid	C3H6O4	106.0266
142	5-(2-hydroxyethyl)-4-methylthiazole	C6H9NOS	143.0405
148	methionine	C5H11NO2S	149.0510
177	pyrophosphate	H4O7P2	177.9432
182	normetanephrine	C9H13NO3	183.0895
191	citric acid	C6H8O7	192.0270
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
250	muramic acid	C9H17NO7	251.1005
270	pelargonidin	C15H11O5	271.0606
272	erythroidine	C16H19NO3	273.1365
283	xanthosine	C10H12N4O6	284.0757
425	(S)-2,3-epoxysqualene	C30H50O	426.3862
433	6-deoxoteasterone	C28H50O3	434.3760
469			
501			
763			
773			

4051 Chromosome 4-3

Changing Bin	Possible ID	Formula	Accurate Mass
177	pyrophosphate	H4O7P2	177.9432
191	citric acid	C6H8O7	192.0270
192			
215	erythronate-4-phosphate	C4H9O8P	216.0035
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
260			
352	2,5-diamino-6-hydroxy-4-(5'-phosphoribosylamino)-pyrimidine	C9H16N5O8P	353.0736
353	5-amino-6-(5'-phosphoribosylamino)-uracil	C9H15N4O9P	354.0577
354	2-amino-7,8-dihydro-4-hydroxy-6-(diphosphooxymethyl)-pteridine	C7H11N5O8P2	355.0083
487			
489			
557			
695			
737			
757			
760			
272	erythroidine	C16H19NO3	273.1365
774			

4054 Chromosome 5-1

Changing Bin	Possible ID	Formula	Accurate Mass
98			
105	glyceric acid	C3H6O4	106.0266
142	5-(2-hydroxyethyl)-4-methylthiazole	C6H9NOS	143.0405
144	spermidine	C7H19N3	145.1579
148	methionine	C5H11NO2S	149.0510
177	pyrophosphate	H4O7P2	177.9432
182	normetanephrine	C9H13NO3	183.0895
191	citric acid	C6H8O7	192.0270
195	galactonate	C6H12O7	196.0583
208			
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
249	gamma-L-glutamyl-L-cysteine	C8H14N2O5S	250.0623
250	muramic acid	C9H17NO7	251.1005
260			
763			
789	all-trans-nonaprenyl diphosphate	C45H76O7P2	790.5066

4055 Chromosome 5-2

Changing Bin	Possible ID	Formula	Accurate Mass
148	methionine	C5H11NO2S	149.0510
149	arabinose	C5H10O5	150.0528
165	ribonic acid	C5H10O6	166.0477
192			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
246	pyridoxal-5'-phosphate	C8H10NO6P	247.0246
247	pyridoxamine phosphate	C8H13N2O5P	248.0562
256			
272	erythroidine	C16H19NO3	273.1365
280			
281	elaidic acid	C18H34O2	282.2559
283	xanthosine	C10H12N4O6	284.0757
526			
695			
724			
737			
283	xanthosine	C10H12N4O6	284.0757
501			

4056 Chromosome 5-3

Changing Bin	Possible ID	Formula	Accurate Mass
75	glycolic acid	C2H4O3	76.0160
98			
105	glyceric acid	C3H6O4	106.0266
142	5-(2-hydroxyethyl)-4-methylthiazole	C6H9NOS	143.0405
157	(S)-dihydroorotate	C5H6N2O4	158.0328
159	2-oxoadipate	C6H8O5	160.0372
177	pyrophosphate	H4O7P2	177.9432
207	sinapaldehyde	C11H12O4	208.0736
208			
214	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
216			
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
239	cystine	C6H12N2O4S2	240.0238
250	muramic acid	C9H17NO7	251.1005
251	deoxyinosine	C10H12N4O4	252.0859
272	erythroidine	C16H19NO3	273.1365
695			
763			

4057 Chromosome 5-4

Changing Bin	Possible ID	Formula	Accurate Mass
165	ribonic acid	C5H10O6	166.0477
177	pyrophosphate	H4O7P2	177.9432
191	citric acid	C6H8O7	192.0270
192			
215	erythronate-4-phosphate	C4H9O8P	216.0035
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
243	uridine	C9H12N2O6	244.0695
256			
280			
281	elaidic acid	C18H34O2	282.2559
352	2,5-diamino-6-hydroxy-4-(5'-phosphoribosylamino)-pyrimidine	C9H16N5O8P	353.0736
353	5-amino-6-(5'-phosphoribosylamino)-uracil	C9H15N4O9P	354.0577
354	2-amino-7,8-dihydro-4-hydroxy-6-(diphosphooxymethyl)-pteridine	C7H11N5O8P2	355.0083
487			
546			
557			
469			
501			

4058 Chromosome 5-5

Changing Bin	Possible ID	Formula	Accurate Mass
142	5-(2-hydroxyethyl)-4-methylthiazole	C6H9NOS	143.0405
148	methionine	C5H11NO2S	149.0510
182	normetanephine	C9H13NO3	183.0895
191	citric acid	C6H8O7	192.0270
192			
208			
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
244			
246	pyridoxal-5'-phosphate	C8H10NO6P	247.0246
256			
260			
283	xanthosine	C10H12N4O6	284.0757
308	N-acetylneuraminic acid	C11H19NO9	309.1060
312	3',5'-cyclic dAMP	C10H12N5O5P	313.0576
326			
469			
501			

4059 Chromosome 6-1

Changing Bin	Possible ID	Formula	Accurate Mass
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
246	pyridoxal-5'-phosphate	C8H10NO6P	247.0246
250	muramic acid	C9H17NO7	251.1005
255	2-(3-carboxy-3-aminopropyl)-L-histidine	C10H16N4O4	256.1172
283	xanthosine	C10H12N4O6	284.0757
312	3',5'-cyclic dAMP	C10H12N5O5P	313.0576
326			
328	2',3'-cyclic AMP	C10H12N5O6P	329.0525
345	GA24	C20H26O5	346.1780
425	(S)-2,3-epoxysqualene	C30H50O	426.3862
427	IDP	C10H14N4O11P2	428.0134
433	6-deoxoteasterone	C28H50O3	434.3760
462	N6-(1,2-dicarboxyethyl)-AMP	C14H18N5O11P	463.0740
501			
526			

4062 Chromosome 6-3

Changing Bin	Possible ID	Formula	Accurate Mass
105	glyceric acid	C3H6O4	106.0266
148	methionine	C5H11NO2S	149.0510
165	ribonic acid	C5H10O6	166.0477
182	normetanephine	C9H13NO3	183.0895
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
246	pyridoxal-5'-phosphate	C8H10NO6P	247.0246
247	pyridoxamine phosphate	C8H13N2O5P	248.0562
256			
260			
270	pelargonidin	C15H11O5	271.0606
280			
284	morphine	C17H19NO3	285.1365
308	N-acetylneuraminic acid	C11H19NO9	309.1060
328	2',3'-cyclic AMP	C10H12N5O6P	329.0525
425	(S)-2,3-epoxysqualene	C30H50O	426.3862
469			
425	(S)-2,3-epoxysqualene	C30H50O	426.3862
501			

4063 Chromosome 6-4

Changing Bin	Possible ID	Formula	Accurate Mass
98			
105			
159	glyceric acid	C3H6O4	106.0266
177	2-oxoadipate	C6H8O5	160.0372
186	pyrophosphate	H4O7P2	177.9432
191	8-amino-7-oxononanoate	C9H17NO3	187.1208
207	citric acid	C6H8O7	192.0270
208	sinapaldehyde	C11H12O4	208.0736
214			
217	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
218			
219	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
236	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
237			
239	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
249	cystine	C6H12N2O4S2	240.0238
251	gamma-L-glutamyl-L-cysteine	C8H14N2O5S	250.0623
283	deoxyinosine	C10H12N4O4	252.0859
272	xanthosine	C10H12N4O6	284.0757
283	erythroidine	C16H19NO3	273.1365
	xanthosine	C10H12N4O6	284.0757

4064 Chromosome 7-1

Changing Bin	Possible ID	Formula	Accurate Mass
75	glycolic acid	C2H4O3	76.0160
98			
105	glyceric acid	C3H6O4	106.0266
117	succinic acid	C4H6O4	118.0266
142	5-(2-hydroxyethyl)-4-methylthiazole	C6H9NOS	143.0405
147	2-methylmalic acid	C5H8O5	148.0372
148	methionine	C5H11NO2S	149.0510
159	2-oxoadipate	C6H8O5	160.0372
207	sinapaldehyde	C11H12O4	208.0736
208			
214	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
239	cystine	C6H12N2O4S2	240.0238
246	pyridoxal-5'-phosphate	C8H10NO6P	247.0246
249	gamma-L-glutamyl-L-cysteine	C8H14N2O5S	250.0623
250	muramic acid	C9H17NO7	251.1005
260			
773			
782			

4066 Chromosome 7-3

Changing Bin	Possible ID	Formula	Accurate Mass
98			
148	methionine	C5H11NO2S	149.0510
161	anabasine	C10H14N2	162.1157
177	pyrophosphate	H4O7P2	177.9432
192			
215	erythronate-4-phosphate	C4H9O8P	216.0035
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
352	2,5-diamino-6-hydroxy-4-(5'-phosphoribosylamino)-pyrimidine	C9H16N5O8P	353.0736
353	5-amino-6-(5'-phosphoribosylamino)-uracil	C9H15N4O9P	354.0577
354	2-amino-7,8-dihydro-4-hydroxy-6-(diphosphooxymethyl)-pteridine	C7H11N5O8P2	355.0083
384			
487			
557			
695			
724			
757			
763			
469			
501			

4067 Chromosome 7-4

Changing Bin	Possible ID	Formula	Accurate Mass
75	glycolic acid	C2H4O3	76.0160
105	glyceric acid	C3H6O4	106.0266
159	2-oxoadipate	C6H8O5	160.0372
182	normetanephine	C9H13NO3	183.0895
186	8-amino-7-oxononanoate	C9H17NO3	187.1208
208			
214	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
216			
217			
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
222	4-methyl-5-(2-phosphoethyl)-thiazole	C6H10NO4PS	223.0068
236			
239	cystine	C6H12N2O4S2	240.0238
250	muramic acid	C9H17NO7	251.1005
251	deoxyinosine	C10H12N4O4	252.0859
283	xanthosine	C10H12N4O6	284.0757
297			
260			
272	erythroidine	C16H19NO3	273.1365

4069 Chromosome 7-5

Changing Bin	Possible ID	Formula	Accurate Mass
75	glycolic acid	C2H4O3	76.0160
98			
105	glyceric acid	C3H6O4	106.0266
142	5-(2-hydroxyethyl)-4-methylthiazole	C6H9NOS	143.0405
144	spermidine	C7H19N3	145.1579
147	2-methylmalic acid	C5H8O5	148.0372
148	methionine	C5H11NO2S	149.0510
159	2-oxoadipate	C6H8O5	160.0372
161	anabasine	C10H14N2	162.1157
208			
214	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
217			
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
239	cystine	C6H12N2O4S2	240.0238
249	gamma-L-glutamyl-L-cysteine	C8H14N2O5S	250.0623
250	muramic acid	C9H17NO7	251.1005
272	erythroidine	C16H19NO3	273.1365
501			

4071 Chromosome 8-1

Changing Bin	Possible ID	Formula	Accurate Mass
98			
105	glyceric acid	C3H6O4	106.0266
148	methionine	C5H11NO2S	149.0510
186	8-amino-7-oxononanoate	C9H17NO3	187.1208
195	galactonate	C6H12O7	196.0583
208			
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
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
249	gamma-L-glutamyl-L-cysteine	C8H14N2O5S	250.0623
250	muramic acid	C9H17NO7	251.1005
260			
214	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249

4074 Chromosome 8-2

Changing Bin	Possible ID	Formula	Accurate Mass
71	methylglyoxal	C3H4O2	72.0211
73	glyoxylic acid	C2H2O3	74.0004
75	glycolic acid	C2H4O3	76.0160
98			
105	glyceric acid	C3H6O4	106.0266
152	3-hydroxyanthranilate	C7H7NO3	153.0426
157	(S)-dihydroorotate	C5H6N2O4	158.0328
159	2-oxoadipate	C6H8O5	160.0372
163	coumaric acid	C9H8O3	164.0473
164	phenylalanine	C9H11NO2	165.0790
184	3-phosphoserine	C3H8NO6P	185.0089
186	8-amino-7-oxononanoate	C9H17NO3	187.1208
197	syringic acid	C9H10O5	198.0528
199	erythrose-4-phosphate	C4H9O7P	200.0086
207	sinapaldehyde	C11H12O4	208.0736
208			
211			
213	2-oxo-3-hydroxy-4-phosphobutanoate	C4H7O8P	213.9879
469			
501			

4076 Chromosome 8-3

Changing Bin	Possible ID	Formula	Accurate Mass
105	glyceric acid	C3H6O4	106.0266
148	methionine	C5H11NO2S	149.0510
159	2-oxoadipate	C6H8O5	160.0372
182	normetanephine	C9H13NO3	183.0895
208			
214	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
246	pyridoxal-5'-phosphate	C8H10NO6P	247.0246
249	gamma-L-glutamyl-L-cysteine	C8H14N2O5S	250.0623
250	muramic acid	C9H17NO7	251.1005
251	deoxyinosine	C10H12N4O4	252.0859
255	2-(3-carboxy-3-aminopropyl)-L-histidine	C10H16N4O4	256.1172
283	xanthosine	C10H12N4O6	284.0757
425	(S)-2,3-epoxysqualene	C30H50O	426.3862
427	IDP	C10H14N4O11P2	428.0134
251	deoxyinosine	C10H12N4O4	252.0859
501			

4078 Chromosome 9-1

Changing Bin	Possible ID	Formula	Accurate Mass
71	methylglyoxal	C3H4O2	72.0211
73	glyoxylic acid	C2H2O3	74.0004
75	glycolic acid	C2H4O3	76.0160
98			
105	glyceric acid	C3H6O4	106.0266
152	3-hydroxyanthranilate	C7H7NO3	153.0426
157	(S)-dihydroorotate	C5H6N2O4	158.0328
159	2-oxoadipate	C6H8O5	160.0372
184	3-phosphoserine	C3H8NO6P	185.0089
186	8-amino-7-oxononanoate	C9H17NO3	187.1208
197	syringic acid	C9H10O5	198.0528
199	erythrose-4-phosphate	C4H9O7P	200.0086
207	sinapaldehyde	C11H12O4	208.0736
208			
211			
213	2-oxo-3-hydroxy-4-phosphobutanoate	C4H7O8P	213.9879
214	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
236			
773			
789	all-trans-nonaprenyl diphosphate	C45H76O7P2	790.5066

4081 Chromosome 9-2

Changing Bin	Possible ID	Formula	Accurate Mass
105	glyceric acid	C3H6O4	106.0266
165	ribonic acid	C5H10O6	166.0477
191	citric acid	C6H8O7	192.0270
195	galactonate	C6H12O7	196.0583
208			
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
250	muramic acid	C9H17NO7	251.1005
255	2-(3-carboxy-3-aminopropyl)-L-histidine	C10H16N4O4	256.1172
260			
283	xanthosine	C10H12N4O6	284.0757
315	isorhamnetin	C16H12O7	316.0583
469			
501			
757			
283	xanthosine	C10H12N4O6	284.0757
501			

4084 Chromosome 9-3

Changing Bin	Possible ID	Formula	Accurate Mass
105	glyceric acid	C3H6O4	106.0266
148	methionine	C5H11NO2S	149.0510
150	guanine	C5H5N5O	151.0494
182	normetanephrine	C9H13NO3	183.0895
191	citric acid	C6H8O7	192.0270
214	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
216			
217			
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
249	gamma-L-glutamyl-L-cysteine	C8H14N2O5S	250.0623
250	muramic acid	C9H17NO7	251.1005
251	deoxyinosine	C10H12N4O4	252.0859
264			
272	erythroidine	C16H19NO3	273.1365
501			
526			

4087 Chromosome 10-1

Changing Bin	Possible ID	Formula	Accurate Mass
165	ribonic acid	C5H10O6	166.0477
182	normetanephrine	C9H13NO3	183.0895
208			
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
283	xanthosine	C10H12N4O6	284.0757
297			
312	3',5'-cyclic dAMP	C10H12N5O5P	313.0576
326			
328	2',3'-cyclic AMP	C10H12N5O6P	329.0525
329	3',5'-cyclic IMP	C10H11N4O7P	330.0365
345	GA24	C20H26O5	346.1780
427	IDP	C10H14N4O11P2	428.0134
462	N6-(1,2-dicarboxyethyl)-AMP	C14H18N5O11P	463.0740
469			
272	erythroidine	C16H19NO3	273.1365
425	(S)-2,3-epoxysqualene	C30H50O	426.3862

4089 Chromosome 10-2

Changing Bin	Possible ID	Formula	Accurate Mass
88	oxamic acid	C2H3NO3	89.0113
98			
105	glyceric acid	C3H6O4	106.0266
142	5-(2-hydroxyethyl)-4-methylthiazole	C6H9NOS	143.0405
148	methionine	C5H11NO2S	149.0510
150	guanine	C5H5N5O	151.0494
165	ribonic acid	C5H10O6	166.0477
182	normetanephine	C9H13NO3	183.0895
186	8-amino-7-oxononanoate	C9H17NO3	187.1208
195	galactonate	C6H12O7	196.0583
214	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
246	pyridoxal-5'-phosphate	C8H10NO6P	247.0246
249	gamma-L-glutamyl-L-cysteine	C8H14N2O5S	250.0623
250	muramic acid	C9H17NO7	251.1005
260			
283	xanthosine	C10H12N4O6	284.0757
501			

4091 Chromosome 10-3

Changing Bin	Possible ID	Formula	Accurate Mass
75	glycolic acid	C2H4O3	76.0160
98			
105	glyceric acid	C3H6O4	106.0266
117	succinic acid	C4H6O4	118.0266
157	(S)-dihydroorotate	C5H6N2O4	158.0328
159	2-oxoadipate	C6H8O5	160.0372
164	phenylalanine	C9H11NO2	165.0790
182	normetanephine	C9H13NO3	183.0895
208			
213	2-oxo-3-hydroxy-4-phosphobutanoate	C4H7O8P	213.9879
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
222	4-methyl-5-(2-phosphoethyl)-thiazole	C6H10NO4PS	223.0068
236			
239	cystine	C6H12N2O4S2	240.0238
249	gamma-L-glutamyl-L-cysteine	C8H14N2O5S	250.0623
250	muramic acid	C9H17NO7	251.1005
251	deoxyinosine	C10H12N4O4	252.0859
272	erythroidine	C16H19NO3	273.1365
782			
789	all-trans-nonaprenyl diphosphate	C45H76O7P2	790.5066

4093 Chromosome 11-2

Changing Bin	Possible ID	Formula	Accurate Mass
105	glyceric acid	C3H6O4	106.0266
142	5-(2-hydroxyethyl)-4-methylthiazole	C6H9NOS	143.0405
148	methionine	C5H11NO2S	149.0510
165	ribonic acid	C5H10O6	166.0477
192			
243	uridine	C9H12N2O6	244.0695
246	pyridoxal-5'-phosphate	C8H10NO6P	247.0246
256			
352	2,5-diamino-6-hydroxy-4-(5'-phosphoribosylamino)-pyrimidine	C9H16N5O8P	353.0736
353	5-amino-6-(5'-phosphoribosylamino)-uracil	C9H15N4O9P	354.0577
354	2-amino-7,8-dihydro-4-hydroxy-6-(diphosphoxymethyl)-pteridine	C7H11N5O8P2	355.0083
487			
489			
557			
695			
757			
763			
773			
782			
789	all-trans-nonaprenyl diphosphate	C45H76O7P2	790.5066

4094 Chromosome 11-3

Changing Bin	Possible ID	Formula	Accurate Mass
165	ribonic acid	C5H10O6	166.0477
192			
215	erythronate-4-phosphate	C4H9O8P	216.0035
217			
243	uridine	C9H12N2O6	244.0695
247	pyridoxamine phosphate	C8H13N2O5P	248.0562
256			
279	linoleic acid	C18H32O2	280.2402
326			
352	2,5-diamino-6-hydroxy-4-(5'-phosphoribosylamino)-pyrimidine	C9H16N5O8P	353.0736
353	5-amino-6-(5'-phosphoribosylamino)-uracil	C9H15N4O9P	354.0577
487			
489			
526			
557			
695			
763			
773			
501			
760			

4095 Chromosome 11-4

Changing Bin	Possible ID	Formula	Accurate Mass
105	glyceric acid	C3H6O4	106.0266
148	methionine	C5H11NO2S	149.0510
165	ribonic acid	C5H10O6	166.0477
182	normetanephine	C9H13NO3	183.0895
191	citric acid	C6H8O7	192.0270
208			
214	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
216			
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
249	gamma-L-glutamyl-L-cysteine	C8H14N2O5S	250.0623
250	muramic acid	C9H17NO7	251.1005
272	erythroidine	C16H19NO3	273.1365
283	xanthosine	C10H12N4O6	284.0757
469			
469			
501			

4097 Chromosome 12-1

Changing Bin	Possible ID	Formula	Accurate Mass
105	glyceric acid	C3H6O4	106.0266
142	5-(2-hydroxyethyl)-4-methylthiazole	C6H9NOS	143.0405
148	methionine	C5H11NO2S	149.0510
177	pyrophosphate	H4O7P2	177.9432
182	normetanephine	C9H13NO3	183.0895
186	8-amino-7-oxononanoate	C9H17NO3	187.1208
208			
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
246	pyridoxal-5'-phosphate	C8H10NO6P	247.0246
250	muramic acid	C9H17NO7	251.1005
270	pelargonidin	C15H11O5	271.0606
272	erythroidine	C16H19NO3	273.1365
283	xanthosine	C10H12N4O6	284.0757
425	(S)-2,3-epoxysqualene	C30H50O	426.3862
501			
526			

4099 Chromosome 12-2

Changing Bin	Possible ID	Formula	Accurate Mass
105	glyceric acid	C3H6O4	106.0266
148	methionine	C5H11NO2S	149.0510
208			
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
243	uridine	C9H12N2O6	244.0695
250	muramic acid	C9H17NO7	251.1005
260			
283	xanthosine	C10H12N4O6	284.0757
312	3',5'-cyclic dAMP	C10H12N5O5P	313.0576
326			
425	(S)-2,3-epoxysqualene	C30H50O	426.3862
427	IDP	C10H14N4O11P2	428.0134
433	6-deoxoteasterone	C28H50O3	434.3760
469			
469			
501			

4100 Chromosome 12-3

4100			
12-3			
98			
105	glyceric acid	C3H6O4	106.0266
182	normetanephrine	C9H13NO3	183.0895
186	8-amino-7-oxononanoate	C9H17NO3	187.1208
208			
214	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
237	erythro-1-(imidazol-4-yl)glycerol-3-phosphate	C6H11N2O6P	238.0355
239	cystine	C6H12N2O4S2	240.0238
246	pyridoxal-5'-phosphate	C8H10NO6P	247.0246
250	muramic acid	C9H17NO7	251.1005
270	pelargonidin	C15H11O5	271.0606
272	erythroidine	C16H19NO3	273.1365
283	xanthosine	C10H12N4O6	284.0757
297			
425	(S)-2,3-epoxysqualene	C30H50O	426.3862
427	IDP	C10H14N4O11P2	428.0134
469			
501			

4102 Chromosome 12-4

Changing Bin	Possible ID	Formula	Accurate Mass
75	glycolic acid	C2H4O3	76.0160
98			
103	hydroxypyruvic acid	C3H4O4	104.0110
105	glyceric acid	C3H6O4	106.0266
157	(S)-dihydroorotate	C5H6N2O4	158.0328
159	2-oxoadipate	C6H8O5	160.0372
186	8-amino-7-oxononanoate	C9H17NO3	187.1208
208			
213	2-oxo-3-hydroxy-4-phosphobutanoate	C4H7O8P	213.9879
214	O-phospho-4-hydroxy-L-threonine	C4H10NO7P	215.0195
218	4-amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	219.0409
219	3-(imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	220.0249
236			
239	cystine	C6H12N2O4S2	240.0238
250	muramic acid	C9H17NO7	251.1005
251	deoxyinosine	C10H12N4O4	252.0859
283	xanthosine	C10H12N4O6	284.0757
297			
469			
501			