

Table S1: LC-MS/MS MRM transitions and compound specific parameters

Compound Name	Precursor Ion	Product Ion	Fragmentor (V)	Collision Energy (V)	Ret Time (min)	Polarity
<sup>13</sup> C <sub>6</sub> -Fructose (Internal std)	<b>185.1<sup>z</sup></b>	<b>61.2</b>	<b>69</b>	<b>10</b>	<b>4.8</b>	<b>Negative</b>
	185.1	92.1	69	10	4.8	Negative
5-Methyluridine	<b>259.1</b>	<b>127</b>	<b>166</b>	<b>5</b>	<b>3.9</b>	<b>Positive</b>
	259.1	110	166	37	3.9	Positive
Adenosine	<b>268.1</b>	<b>136.1</b>	<b>100</b>	<b>17</b>	<b>2.2</b>	<b>Positive</b>
	268.1	119.1	100	57	2.2	Positive
Arabinose	<b>149</b>	<b>59.2</b>	<b>66</b>	<b>12</b>	<b>4.9</b>	<b>Negative</b>
	149	89.1	66	4	4.9	Negative
Citric acid	<b>191</b>	<b>111</b>	<b>81</b>	<b>10</b>	<b>13.2</b>	<b>Negative</b>
	191	87	81	14	13.2	Negative
Cytidine	<b>244.1</b>	<b>112.1</b>	<b>140</b>	<b>13</b>	<b>4.4</b>	<b>Positive</b>
	244.1	95.1	140	53	4.4	Positive
Fructose	<b>179.1</b>	<b>88.9</b>	<b>69</b>	<b>5</b>	<b>4.8</b>	<b>Negative</b>
	179.1	59	69	13	4.8	Negative
Galactose	<b>179.1</b>	<b>89.1</b>	<b>70</b>	<b>10</b>	<b>6.9</b>	<b>Negative</b>
	179.1	59.2	70	14	6.9	Negative
Galacturonic acid	<b>193</b>	<b>59.1</b>	<b>166</b>	<b>17</b>	<b>11.4</b>	<b>Negative</b>
	193	113	166	9	11.4	Negative
Glucose	<b>179.1</b>	<b>89.1</b>	<b>69</b>	<b>5</b>	<b>6.4</b>	<b>Negative</b>
	179.1	59.1	69	9	6.4	Negative
Guanosine	<b>284.1</b>	<b>152</b>	<b>80</b>	<b>13</b>	<b>4.9</b>	<b>Positive</b>
	284.1	135	80	49	4.9	Positive
Inosine	<b>267.1</b>	<b>135</b>	<b>144</b>	<b>22</b>	<b>3.5</b>	<b>Negative</b>
	267.1	108	144	44	3.5	Negative
L-Alanine	<b>90.1</b>	<b>44.2</b>	<b>40</b>	<b>13</b>	<b>9.2</b>	<b>Positive</b>
	90.1	29.3	40	57	9.2	Positive
L-Arginine	<b>175.1</b>	<b>70.1</b>	<b>100</b>	<b>24</b>	<b>14.5</b>	<b>Positive</b>
	175.1	60.1	100	12	14.5	Positive
L-Aspartic acid	<b>132</b>	<b>88.1</b>	<b>70</b>	<b>9</b>	<b>11.6</b>	<b>Negative</b>
	132	115	70	9	11.6	Negative
L-Cysteine	<b>122</b>	<b>76</b>	<b>65</b>	<b>13</b>	<b>9.3</b>	<b>Positive</b>
	122	59.1	65	29	9.3	Positive
L-Glutamic acid	<b>146</b>	<b>102.1</b>	<b>80</b>	<b>13</b>	<b>11.6</b>	<b>Negative</b>
	146	128.1	80	9	11.6	Negative
L-Glutamine	<b>147.1</b>	<b>84.1</b>	<b>80</b>	<b>17</b>	<b>10.2</b>	<b>Positive</b>
	147.1	130.1	80	9	10.2	Positive
L-Glycine	<b>76</b>	<b>30.1</b>	<b>35</b>	<b>9</b>	<b>10.0</b>	<b>Positive</b>
	76	28.1	35	53	10.0	Positive
L-Isoleucine	<b>132.1</b>	<b>86.1</b>	<b>75</b>	<b>25</b>	<b>6.2</b>	<b>Positive</b>
	132.1	44.2	75	25	6.2	Positive
L-Leucine	<b>132.1</b>	<b>86.1</b>	<b>75</b>	<b>9</b>	<b>5.9</b>	<b>Positive</b>
	132.1	30.3	75	17	5.9	Positive
L-Lysine	<b>147.1</b>	<b>84.1</b>	<b>75</b>	<b>17</b>	<b>14.8</b>	<b>Positive</b>
	147.1	130.1	75	9	14.8	Positive
L-Methionine	<b>150.1</b>	<b>56.2</b>	<b>80</b>	<b>17</b>	<b>6.6</b>	<b>Positive</b>
	150.1	104.1	80	9	6.6	Positive
L-Phenylalanine	<b>164.1</b>	<b>147</b>	<b>80</b>	<b>9</b>	<b>5.6</b>	<b>Negative</b>
	164.1	103	80	15	5.6	Negative
L-Proline	<b>116.1</b>	<b>70.1</b>	<b>75</b>	<b>37</b>	<b>7.6</b>	<b>Positive</b>
	116.1	43.2	75	37	7.6	Positive
L-Serine	<b>106.1</b>	<b>42.2</b>	<b>67</b>	<b>24</b>	<b>10.2</b>	<b>Positive</b>
	106.1	88.1	67	8	10.2	Positive
L-Threonine	<b>120.1</b>	<b>74.2</b>	<b>80</b>	<b>9</b>	<b>9.6</b>	<b>Positive</b>
	120.1	56.2	80	17	9.6	Positive
L-Tryptophan	<b>205.1</b>	<b>146</b>	<b>80</b>	<b>20</b>	<b>6.2</b>	<b>Positive</b>
	205.1	188	80	8	6.2	Positive
L-Tyrosine	<b>182.1</b>	<b>91.1</b>	<b>85</b>	<b>33</b>	<b>7.3</b>	<b>Positive</b>
	182.1	136.1	85	33	7.3	Positive
L-Valine	<b>118.1</b>	<b>72.2</b>	<b>60</b>	<b>9</b>	<b>7.3</b>	<b>Positive</b>
	118.1	55.2	60	25	7.3	Positive
Malic acid	<b>133</b>	<b>115</b>	<b>76</b>	<b>8</b>	<b>11.9</b>	<b>Negative</b>
	133	71.1	76	14	11.9	Negative

Mannose	<b>179.1</b>	<b>59.2</b>	<b>66</b>	<b>16</b>	<b>5.4</b>	<b>Negative</b>
	179.1	89	66	4	5.4	Negative
Rhamnose	<b>163.1</b>	<b>103</b>	<b>166</b>	<b>5</b>	<b>2.7</b>	<b>Negative</b>
	163.1	119	166	5	2.7	Negative
Succinic acid	<b>117</b>	<b>99</b>	<b>166</b>	<b>9</b>	<b>12.3</b>	<b>Negative</b>
	117	73.1	166	9	12.3	Negative
Sucrose	<b>341.1</b>	<b>89.1</b>	<b>140</b>	<b>21</b>	<b>9.2</b>	<b>Negative</b>
	341.1	179	140	13	9.2	Negative
Tartronic Acid	<b>119</b>	<b>57.1</b>	<b>65</b>	<b>10</b>	<b>11.8</b>	<b>Negative</b>
	119	75.1	65	10	11.8	Negative
Uridine	<b>243.1</b>	<b>200.1</b>	<b>100</b>	<b>9</b>	<b>2.1</b>	<b>Negative</b>
	243.1	110.1	100	17	2.1	Negative
Vitamin B1	<b>265.1</b>	<b>122.1</b>	<b>90</b>	<b>13</b>	<b>7.8</b>	<b>Positive</b>
	265.1	81.1	90	37	7.8	Positive
Vitamin B2	<b>377.2</b>	<b>243</b>	<b>150</b>	<b>21</b>	<b>2.6</b>	<b>Positive</b>
	377.2	172.1	150	41	2.6	Positive
Vitamin B3	<b>124</b>	<b>78.1</b>	<b>135</b>	<b>25</b>	<b>4.9</b>	<b>Positive</b>
	124	53.2	135	37	4.9	Positive
Vitamin B5	<b>220.1</b>	<b>90.1</b>	<b>84</b>	<b>10</b>	<b>6.6</b>	<b>Positive</b>
	220.1	72.1	84	18	6.6	Positive
Vitamin B6	<b>170.1</b>	<b>152</b>	<b>100</b>	<b>13</b>	<b>1.8</b>	<b>Positive</b>
	170.1	134	100	21	1.8	Positive
Vitamin B7	<b>245.1</b>	<b>227</b>	<b>100</b>	<b>13</b>	<b>6.6</b>	<b>Positive</b>
	245.1	97	100	29	6.6	Positive
Vitamin B12	<b>678.3</b>	<b>359.1</b>	<b>165</b>	<b>26</b>	<b>11</b>	<b>Positive</b>
	678.3	635.8	165	22	11	Positive
Vitamin C	<b>177</b>	<b>95</b>	<b>65</b>	<b>9</b>	<b>6.8</b>	<b>Positive</b>
	177	141	65	5	6.8	Positive
Xylose	<b>149</b>	<b>71.1</b>	<b>69</b>	<b>5</b>	<b>4.0</b>	<b>Negative</b>
	149	59.1	69	13	4.0	Negative

<sup>z</sup>Transitions used for quantification are bolded.