

Supplemental Material Table S1.

Specific compound-dependent MS parameters for selected reaction monitoring (SRM).

Compounds	Parent ion ([M-H] <sup>-</sup> )		Collision energy (ev)	Preferred product ion		Internal standard added (μM)
	formula	mass		formula	mass	
Glyoxylate	C <sub>2</sub> H <sub>3</sub> O <sub>3</sub> <sup>-</sup>	73	10	-CO	45	
Glycolate	C <sub>2</sub> H <sub>3</sub> O <sub>3</sub> <sup>-</sup>	75	10	-CO	47	
Pyruvate	C <sub>3</sub> H <sub>3</sub> O <sub>3</sub> <sup>-</sup>	87	10	-CO <sub>2</sub>	43	
Glycerate	C <sub>3</sub> H <sub>5</sub> O <sub>4</sub> <sup>-</sup>	105	10	C <sub>2</sub> H <sub>3</sub> O <sub>3</sub> <sup>-</sup>	75	
Succinate	C <sub>4</sub> H <sub>5</sub> O <sub>4</sub> <sup>-</sup>	117	10	-CO <sub>2</sub>	73	
Aspartate	C <sub>4</sub> H <sub>6</sub> NO <sub>4</sub> <sup>-</sup>	132	10	-CO <sub>2</sub>	88.1	
Malate	C <sub>4</sub> H <sub>5</sub> O <sub>5</sub> <sup>-</sup>	133	10	-H <sub>2</sub> O	115	
2-OG	C <sub>5</sub> H <sub>5</sub> O <sub>5</sub> <sup>-</sup>	145	10	-CO <sub>2</sub>	100.9	
Glutamate	C <sub>5</sub> H <sub>8</sub> NO <sub>4</sub> <sup>-</sup>	146	10	-H <sub>2</sub> O	128	
PEP	C <sub>3</sub> H <sub>4</sub> O <sub>6</sub> P <sup>-</sup>	167	27	[PO <sub>3</sub> ] <sup>-</sup>	79	
GAP/DHAP	C <sub>3</sub> H <sub>6</sub> O <sub>6</sub> P <sup>-</sup>	169	10	[H <sub>2</sub> PO <sub>4</sub> ] <sup>-</sup>	97	
G3P	C <sub>3</sub> H <sub>6</sub> O <sub>6</sub> P <sup>-</sup>	171	27	[PO <sub>3</sub> ] <sup>-</sup>	79	
Aconitate	C <sub>6</sub> H <sub>5</sub> O <sub>6</sub> <sup>-</sup>	173	17	-2CO <sub>2</sub>	85	
Shikimate	C <sub>7</sub> H <sub>9</sub> O <sub>5</sub> <sup>-</sup>	173	28	C <sub>6</sub> H <sub>5</sub> O <sup>-</sup>	93	
2PGA/3PGA	C <sub>3</sub> H <sub>6</sub> O <sub>7</sub> P <sup>-</sup>	185	26	[PO <sub>3</sub> ] <sup>-</sup>	79	
Citrate	C <sub>6</sub> H <sub>7</sub> O <sub>7</sub> <sup>-</sup>	191	22	-a	87	
Isocitrate	C <sub>6</sub> H <sub>7</sub> O <sub>7</sub> <sup>-</sup>	191	28	-a	73	
E4P	C <sub>4</sub> H <sub>8</sub> O <sub>7</sub> P <sup>-</sup>	199	10	[PO <sub>3</sub> ] <sup>-</sup>	79	
R5P/X5P/Ru5P	C <sub>5</sub> H <sub>10</sub> O <sub>8</sub> P <sup>-</sup>	229	10	[H <sub>2</sub> PO <sub>4</sub> ] <sup>-</sup>	97	
G6P/F6P	C <sub>6</sub> H <sub>12</sub> O <sub>9</sub> P <sup>-</sup>	259	22	[H <sub>2</sub> PO <sub>4</sub> ] <sup>-</sup>	97	
G1P	C <sub>6</sub> H <sub>12</sub> O <sub>9</sub> P <sup>-</sup>	259	31	[PO <sub>3</sub> ] <sup>-</sup>	79	
6PG	C <sub>6</sub> H <sub>12</sub> O <sub>10</sub> P <sup>-</sup>	275	22	[PO <sub>3</sub> ] <sup>-</sup>	79	
S7P	C <sub>7</sub> H <sub>14</sub> O <sub>10</sub> P <sup>-</sup>	289	20	[H <sub>2</sub> PO <sub>4</sub> ] <sup>-</sup>	97	
RuBP	C <sub>5</sub> H <sub>11</sub> O <sub>11</sub> P <sub>2</sub> <sup>-</sup>	309	22	[H <sub>2</sub> PO <sub>4</sub> ] <sup>-</sup>	97	
F26BP	C <sub>6</sub> H <sub>13</sub> O <sub>12</sub> P <sub>2</sub> <sup>-</sup>	339	22	-[H <sub>3</sub> PO <sub>4</sub> ]	241	
FBP	C <sub>6</sub> H <sub>13</sub> O <sub>12</sub> P <sub>2</sub> <sup>-</sup>	339	27	[H <sub>2</sub> PO <sub>4</sub> ] <sup>-</sup>	97	
AMP	C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>7</sub> P <sup>-</sup>	346.1	21	[PO <sub>3</sub> ] <sup>-</sup>	79	
SBP	C <sub>7</sub> H <sub>15</sub> O <sub>13</sub> P <sub>2</sub> <sup>-</sup>	369	29	[H <sub>2</sub> PO <sub>4</sub> ] <sup>-</sup>	97	
T6P/S6P	C <sub>12</sub> H <sub>22</sub> O <sub>14</sub> P <sup>-</sup>	421	41	[PO <sub>3</sub> ] <sup>-</sup>	79	
ADP	C <sub>10</sub> H <sub>14</sub> N <sub>5</sub> O <sub>10</sub> P <sub>2</sub> <sup>-</sup>	426.1	24	C <sub>5</sub> H <sub>4</sub> N <sub>5</sub> <sup>-</sup>	134	
ATP	C <sub>10</sub> H <sub>15</sub> N <sub>5</sub> O <sub>13</sub> P <sub>3</sub> <sup>-</sup>	506.2	21	C <sub>10</sub> H <sub>12</sub> N <sub>5</sub> O <sub>9</sub> P <sub>2</sub> <sup>-</sup>	408	
UDPG	C <sub>15</sub> H <sub>23</sub> N <sub>2</sub> O <sub>17</sub> P <sub>2</sub> <sup>-</sup>	565	28	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>9</sub> P <sup>-</sup>	323.1	
ADPG	C <sub>16</sub> H <sub>24</sub> N <sub>5</sub> O <sub>15</sub> P <sub>2</sub> <sup>-</sup>	588	28	C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>7</sub> P <sup>-</sup>	346.1	
NAD	C <sub>21</sub> H <sub>26</sub> N <sub>7</sub> O <sub>14</sub> P <sub>2</sub> <sup>-</sup>	662.3	22	C <sub>15</sub> H <sub>20</sub> N <sub>5</sub> O <sub>13</sub> P <sub>2</sub> <sup>-</sup>	540.1	
NADP	C <sub>21</sub> H <sub>27</sub> N <sub>7</sub> O <sub>17</sub> P <sub>3</sub> <sup>-</sup>	742.2	22	C <sub>15</sub> H <sub>20</sub> N <sub>5</sub> O <sub>16</sub> P <sub>3</sub> <sup>-</sup>	620.1	
[2,3,3- <sup>2</sup> H <sub>3</sub> ]glycerate	C <sub>3</sub> H <sub>2</sub> <sup>2</sup> H <sub>3</sub> O <sub>4</sub> <sup>-</sup>	108	11	C <sub>2</sub> H <sub>2</sub> <sup>2</sup> H <sub>1</sub> O <sub>3</sub> <sup>-</sup>	76	1
[2,2,3,3- <sup>13</sup> C <sub>4</sub> ]succinate	<sup>13</sup> C <sub>4</sub> H <sub>5</sub> O <sub>4</sub> <sup>-</sup>	121	10	- <sup>13</sup> CO <sub>2</sub>	76	1
[2,3,3- <sup>2</sup> H <sub>3</sub> ]aspartate	C <sub>4</sub> H <sub>3</sub> <sup>2</sup> H <sub>3</sub> NO <sub>4</sub> <sup>-</sup>	135	13	-CO <sub>2</sub>	91	10
[2,3,3- <sup>2</sup> H <sub>3</sub> ]malate	C <sub>4</sub> H <sub>2</sub> <sup>2</sup> H <sub>3</sub> O <sub>5</sub> <sup>-</sup>	136	13	-H <sup>2</sup> HO	117	20
[2,3,3- <sup>2</sup> H <sub>3</sub> ]glutamate	C <sub>5</sub> H <sub>5</sub> <sup>2</sup> H <sub>3</sub> NO <sub>4</sub> <sup>-</sup>	149	14	-H <sup>2</sup> HO	130	15
[1,2,3,4- <sup>13</sup> C <sub>4</sub> ]2-OG	C <sup>13</sup> C <sub>4</sub> H <sub>5</sub> O <sub>5</sub> <sup>-</sup>	149	12	-CO <sub>2</sub>	105	0.75
[1,1,2,3,3- <sup>2</sup> H <sub>5</sub> ]G3P	C <sub>3</sub> H <sub>3</sub> <sup>2</sup> H <sub>5</sub> O <sub>6</sub> P <sup>-</sup>	176	27	[PO <sub>3</sub> ] <sup>-</sup>	79	0.5
[6,6- <sup>2</sup> H <sub>5</sub> ]G6P	C <sub>6</sub> H <sub>10</sub> <sup>2</sup> H <sub>2</sub> O <sub>6</sub> P <sup>-</sup>	261	22	[H <sub>2</sub> PO <sub>4</sub> ] <sup>-</sup>	97	1

a The fragmentation pattern is unknown