

Compound	Formula	Mass	RT (min)	Adduct	<sup>b</sup> ID level	Analytical platform	DET	Fragments	FO LDPE VS FO GLU			FE LDPE VS FE GLU				
									<sup>c</sup> Fold Change	<sup>d</sup> VIP	<sup>f</sup> p value with FDR	<sup>c</sup> Fold Change	<sup>d</sup> VIP	<sup>f</sup> p value with FDR		
<b>Amines</b>																
Triethanolamine	C <sub>6</sub> H <sub>15</sub> NO <sub>3</sub>	149.1882	14.24	-	2	GM-GC-QTOF-MS	-	-	-	-	-	0.51	1.51	7.53E-04†		
<b>Amino acids, peptides</b>																
Valine	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub>	117.1463	6.68	-	2	GM-LC-QTOF-MS GM-GC-QTOF-MS	ESI+	-	1.29	1.14	-	0.52	1.18	1.58E-02†		
Ala Thr Gln	C <sub>12</sub> H <sub>22</sub> N <sub>4</sub> O <sub>6</sub>	318.1539	0.62	M-H	3	GM-LC-QTOF-MS	ESI -	-	0.07	1.27	3.36E-05†	-	-	-		
Pyroglutamyl-serine	C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>5</sub>	216.0746	0.64	M-H	3	GM-LC-QTOF-MS	ESI -	-	1.53	1.17	4.37E-04†	0.87	-	4.64E-02†		
UDP-acetyl-alpha-galactosamine	C <sub>17</sub> H <sub>27</sub> N <sub>3</sub> O <sub>17</sub> P <sub>2</sub>	607.0816	0.66	M-H	3	GM-LC-QTOF-MS	ESI -	-	3.02	-	4.15E-02†	-	-	-		
Pyro-glutaminy-glutamine	C <sub>10</sub> H <sub>15</sub> N <sub>3</sub> O <sub>5</sub>	257.1012	0.85	M-H	3	GM-LC-QTOF-MS	ESI -	-	-	-	-	0.91	-	3.85E-03†		
Pyroglutamic acid	C <sub>5</sub> H <sub>7</sub> NO <sub>3</sub>	129.0426	0.91	M-H	2	GM-LC-QTOF-MS GM-GC-QTOF-MS	ESI - / ESI +	82.0328	2.08	1.30	1.10E-05†	0.88	1.03	2.35E-03†		
Hydroxy-phenylalanine	C <sub>9</sub> H <sub>11</sub> NO <sub>3</sub>	181.0739	1.03	M-H	2	GM-LC-QTOF-MS	ESI -	72.0077, 119.0490, 163.0390	2.67	1.18	3.99E-04†	0.46	1.20	7.74E-05†		
Isoleucyl-glutamine	C <sub>11</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>	230.1630	1.13	M+H	2	GM-LC-QTOF-MS	ESI +	70.0692, 86.0964, 130.0501, 147.0760	0.07	1.15	1.11E-03†	1.66	1.15	1.11E-03†		
Leucine	C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>	131.1729	7.99	-	2	GM-GC-QTOF-MS	-	-	-	-	-	0.68	-	0.030582		
Isoleucine	C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>	131.1729	8.31	-	2	GM-GC-QTOF-MS	-	-	1.51	1.57	5.17E-03	0.45	1.33	5.72E-03†		
Leu Ala	C <sub>9</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	202.1317	1.44	M-H	3	GM-LC-QTOF-MS	ESI -	-	0.05	1.07	3.14E-03†	2.99	1.31	4.72E-07†		
Valyl-Valine	C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>	216.1474	1.85	M-H	3	GM-LC-QTOF-MS	ESI -	-	0.41	-	1.65E-02†	2.84	1.29	4.78E-06†		
Phenylalanyl-Threonine	C <sub>13</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub>	266.1267	2.09	M-H	3	GM-LC-QTOF-MS	ESI -	-	0.37	1.15	1.13E-03†	1.68	1.29	4.44E-06†		
Phenylalanine	C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>	165.0790	2.12	M-H	2	GM-LC-QTOF-MS GM-GC-QTOF-MS	ESI -	72.0091, 103.0554, 147.0452	1.91	1.29	1.84E-05†	1.17	-	9.67E-03†		
Ala Ile	C <sub>9</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	202.1317	2.65	M-H	3	GM-LC-QTOF-MS	ESI -	-	-	<i>Only in FO GLU group</i>	1.22	2.35E-04†	2.37	1.29	1.58E-06†	
Val Ile	C <sub>11</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>	230.1630	3.17	M-H	2	GM-LC-QTOF-MS GM-GC-QTOF-MS	ESI - / ESI +	86.0969, 116.0706	0.15	1.08	2.01E-03†	3.88	1.31	2.22E-07†		
valyl-lysyl-glycyl-alanyl-aspartyl-glutamic acid	C <sub>25</sub> H <sub>43</sub> N <sub>7</sub> O <sub>11</sub>	617.3021	3.27	M-H-H <sub>2</sub> O	3	GM-LC-QTOF-MS	ESI -	-	0.63	1.00	5.43E-03†	1.26	1.08	7.79E-04†		
Tryptophyl-Glutamine	C <sub>16</sub> H <sub>20</sub> N <sub>4</sub> O <sub>4</sub>	332.1485	3.30	M-H	3	GM-LC-QTOF-MS	ESI -	-	0.23	1.27	3.88E-05†	1.22	-	1.41E-02†		
Tyrosyl-Proline	C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub>	278.1267	3.39	M-H	3	GM-LC-QTOF-MS	ESI -	-	4.73	1.25	2.80E-05†	0.32	1.17	1.08E-04†		
Proline	C <sub>5</sub> H <sub>9</sub> NO <sub>2</sub>	115.0633	3.53	M+H	2	GM-LC-QTOF-MS	ESI +	70.0654, 116.0714	7.61	1.19	6.58E-04†	0.12	1.19	6.58E-04		
Methyl Proline	C <sub>6</sub> H <sub>11</sub> NO <sub>2</sub>	129.1570	8.17	-	2	GM-GC-QTOF-MS	-	-	-	-	-	0.57	1.25	1.27E-02†		
Pyroglutamylvaline	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub>	228.1110	3.74	M-H	3	GM-LC-QTOF-MS	ESI -	-	1.70	1.24	9.47E-05†	0.89	-	1.82E-02†		
Hydroxyprolyl-Proline	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub>	228.1110	3.81	M+H	3	GM-LC-QTOF-MS	ESI +	-	-	<i>Only in FO GLU group</i>	1.15	9.77E-04†	1.70	1.15	9.77E-04†	
Leucylproline	C <sub>11</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>	228.1474	4.04	M+H	2	GM-LC-QTOF-MS GM-GC-QTOF-MS	ESI - / ESI +	70.0649, 86.0984, 116.0703	1.53	1.26	1.66E-04	0.89	1.26	1.66E-04†		
Maculosin	C <sub>14</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>	260.1161	4.62	M-H	2	GM-LC-QTOF-MS GM-GC-QTOF-MS	ESI - / ESI +	125.0343, 153.0657	1.80	1.28	3.18E-05†	-	-	-		

Pyroglutamyl-Isoleucine	C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub>	242.1267	5.83	M-H	2	GM-LC-QTOF-MS	ESI -	710.0283, 109.0377, 141.1037,197.1292	-	-	-	0.91	-	1.38E-02†
Cyclo(leucylprolyl)	C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>	210.1368	6.60	M+H	2	GM-LC-QTOF-MS GM-GC-QTOF-MS	ESI +	70.0644, 86.0969, 98.0573, 114.0906, 138.1271, 183.1468	<i>Only in FO GLU group</i>	1.00	8.49E-03†	2.22	1.00	8.49E-03†
Prolylphenylalanine	C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	262.1317	7.12	M+H	3	GM-LC-QTOF-MS	ESI +	-	0.25	1.16	9.71E-04†	1.50	1.16	9.71E-04†
Isoleucylproline	C <sub>11</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>	228.1474	8.29	M+H	2	GM-LC-QTOF-MS	ESI +	86.0894, 116.0720	0.28	1.29	4.98E-05†	1.56	1.29	4.98E-05†
Palmitoyl-Phe(b-OH,4-NO <sub>2</sub> )-ol	C <sub>25</sub> H <sub>42</sub> N <sub>2</sub> O <sub>5</sub>	450.3094	19.77	M-H	3	GM-LC-QTOF-MS	ESI -	-	-	-	-	<i>Only in FE GLU group</i>	1.28	6.54E-06†
3-Aminoisobutanoic Acid	C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub>	103.1198	8.81	-	2	GM-GC-QTOF-MS	-	-	-	-	-	37.19	1.45	1.15E-03†
Pipecolic Acid	C <sub>6</sub> H <sub>11</sub> NO <sub>2</sub>	129.1570	9.57	-	2	GM-GC-QTOF-MS	-	-	2.10	1.64	3.99E-03	-	-	-
Glycine	C <sub>2</sub> H <sub>3</sub> NO <sub>2</sub>	75.0666	10.22	-	2	GM-GC-QTOF-MS	-	-	0.55	1.03	-	-	-	-
2-Aminooctanoic Acid	C <sub>8</sub> H <sub>17</sub> NO <sub>2</sub>	159.2261	11.07	-	2	GM-GC-QTOF-MS	-	-	-	-	-	0.42	1.26	1.27E-02†
4-Guanidinobutanoic Acid	C <sub>5</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub>	145.1597	12.87	-	2	GM-GC-QTOF-MS	-	-	0.11	1.11	3.66E-02	4.12	1.28	8.04E-03†
Methionine	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub> S	149.2110	12.96	-	2	GM-GC-QTOF-MS	-	-	0.75	1.07	-	1.30	-	3.70E-02
Glutamic Acid	C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub>	147.1293	13.00	-	2	GM-GC-QTOF-MS	-	-	0.86	1.15	-	-	-	-
Methyl Glutamic Acid	C <sub>6</sub> H <sub>11</sub> NO <sub>4</sub>	161.1558	13.06	-	2	GM-GC-QTOF-MS	-	-	-	-	-	0.48	1.30	8.04E-03†
5-Aminopentanoic Acid	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub>	117.1463	14.54	-	2	GM-GC-QTOF-MS	-	-	0.80	1.14	-	-	-	-
Cysteinylglycine	C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> S	178.2100	16.07	-	2	GM-GC-QTOF-MS	-	-	0.41	1.29	-	-	-	-
Ornithine	C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	132.1610	16.10	-	2	GM-GC-QTOF-MS	-	-	0.56	1.20	2.19E-02	1.64	1.18	1.54E-02†
Glycylvaline	C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>	174.2000	16.85	-	2	GM-GC-QTOF-MS	-	-	0.18	1.40	9.26E-03	3.61	1.28	8.23E-03†
Glucosaminic Acid	C <sub>6</sub> H <sub>13</sub> NO <sub>6</sub>	195.1705	18.37	-	2	GM-GC-QTOF-MS	-	-	0.88	-	-	1.66	1.13	2.67E-02†
Cystine	C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub> S <sub>2</sub>	240.3000	20.52	-	2	GM-GC-QTOF-MS	-	-	0.31	1.35	2.10E-02	2.24	1.21	1.27E-02†
<b>Benzenoids</b>														
4-Methylcatechol	C <sub>7</sub> H <sub>8</sub> O <sub>2</sub>	124.0524	2.27	M+H-H <sub>2</sub> O	2	GM-LC-QTOF-MS	ESI +	77.0389, 79.0547, 95.0495, 105.460	0.20	1.22	3.74E-04	1.38	1.22	3.74E-04†
1,5-Naphthalenediamine	C <sub>10</sub> H <sub>10</sub> N <sub>2</sub>	158.0844	3.92	M+H	2	GM-LC-QTOF-MS	ESI +	115.0537, 132.0805, 142.0658, 143.0675, 158.0826,159.0920	0.31	1.19	5.30E-04†	1.37	1.19	5.30E-04†
2-Phenylacetamide	C <sub>8</sub> H <sub>9</sub> NO	135.0684	4.62	M+H	2	GM-LC-QTOF-MS	ESI +	65.0385, 91.0540	0.02	1.17	5.15E-04†	1.38	1.17	5.15E-04†
3-Oxo-2,4-bis(3-phenylpropyl)pentanedioic acid	C <sub>23</sub> H <sub>26</sub> O <sub>5</sub>	382.1780	21.18	M-H	3	GM-LC-QTOF-MS	ESI -	-	3.47	-	4.11E-03†	0.32	1.04	2.59E-03†
Benzoic Acid	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	122.1230	9.32	-	2	GM-GC-QTOF-MS	-	-	-	-	-	1.44	1.18	2.10E-02†
4-Hydroxybenzoic Acid	C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>	138.1220	14.20	-	2	GM-GC-QTOF-MS	-	-	0.55	1.60	2.44E-03	-	-	-
Dimethylbenzimidazole	C <sub>9</sub> H <sub>10</sub> N <sub>2</sub>	146.1891	16.02	-	2	GM-GC-QTOF-MS	-	-	-	-	-	1.66	1.11	2.80E-02†
Anisomycin	C <sub>14</sub> H <sub>19</sub> NO <sub>4</sub>	265.3090	19.33	-	2	GM-GC-QTOF-MS	-	-	0.49	1.57	3.56E-03	-	-	-
<b>Carbohydrates and carbohydrate conjugates</b>														
Xylulose	C <sub>5</sub> H <sub>10</sub> O <sub>5</sub>	150.1300	14.67	-	2	GM-GC-QTOF-MS	-	-	1.48	1.13	-	-	-	-
Ribonolactone	C <sub>5</sub> H <sub>8</sub> O <sub>5</sub>	148.1140	14.68	-	2	GM-GC-QTOF-MS	-	-	-	-	-	1.87	1.14	1.89E-02†
Xylitol/Ribitol	C <sub>5</sub> H <sub>12</sub> O <sub>5</sub>	152.1458	14.98	-	2	GM-GC-QTOF-MS	-	-	0.43	1.53	9.49E-03	0.65	1.04	3.56E-02†
3-Phosphoglyceric Acid	C <sub>3</sub> H <sub>7</sub> O <sub>7</sub> P	186.0572	15.86	-	2	GM-GC-QTOF-MS	-	-	1.36	-	-	2.12	1.31	6.45E-03†

Methyl Galactopyranoside	C <sub>7</sub> H <sub>14</sub> O <sub>6</sub>	194.1825	16.44	-	2	GM-GC-QTOF-MS	-	-	0.37	1.59	4.04E-03	1.55	1.06	3.70E-02†	
Gluconolactone	C <sub>6</sub> H <sub>10</sub> O <sub>6</sub>	178.1400	16.95	-	2	GM-GC-QTOF-MS	-	-	-	-	-	1.84	1.19	1.54E-02†	
Fructose	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	180.1559	17.11	-	2	GM-GC-QTOF-MS	-	-	0.64	1.18	-	0.68	1.24	9.86E-03†	
Sedoheptulose	C <sub>7</sub> H <sub>14</sub> O <sub>7</sub>	210.1800	17.23	-	2	GM-GC-QTOF-MS	-	-	0.14	1.29	3.84E-02	9.88	1.39	3.23E-03†	
Beta-D-Galactose	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	180.1559	17.32	-	2	GM-GC-QTOF-MS	-	-	1.89	1.17	-	-	-	-	
Glucose	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	180.1559	17.38	-	2	GM-GC-QTOF-MS	-	-	0.63	1.17	-	0.73	1.15	1.54E-02†	
2-Keto Gluconate	C <sub>6</sub> H <sub>10</sub> O <sub>7</sub>	194.1394	17.57	-	2	GM-GC-QTOF-MS	-	-	0.59	1.16	-	-	-	-	
Gluconic Acid	C <sub>6</sub> H <sub>12</sub> O <sub>7</sub>	196.1553	17.71	-	2	GM-GC-QTOF-MS	-	-	1.70	1.21	3.50E-02	4.04	1.47	7.20E-04†	
Glucaric Acid	C <sub>6</sub> H <sub>10</sub> O <sub>8</sub>	210.1388	18.11	-	2	GM-GC-QTOF-MS	-	-	-	-	-	1.74	1.02	3.52E-02†	
Acetylneuraminic Acid	C <sub>11</sub> H <sub>19</sub> NO <sub>9</sub>	309.2699	23.80	-	2	GM-GC-QTOF-MS	-	-	0.42	1.21	4.85E-02	1.88	1.23	1.23E-02†	
Cellobiose	C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>	342.2965	24.30	-	2	GM-GC-QTOF-MS	-	-	0.31	1.32	7.05E-03	0.38	-	-	
Maltose	C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>	342.2965	24.30	-	2	GM-GC-QTOF-MS	-	-	1.29	1.15	-	0.51	1.18	1.58E-02†	
Isomaltose	C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>	342.2965	25.56	-	2	GM-GC-QTOF-MS	-	-	0.26	1.86	-	0.74	1.12	1.27E-02†	
<b>Diazines</b>															
Uracil	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	112.0868	10.64	-	2	GM-GC-QTOF-MS	-	-	0.73	1.28	-	-	-	-	
Thymine	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	126.1133	11.03	-	2	GM-GC-QTOF-MS	-	-	-	-	-	1.37	-	0.04727	
<b>Carnitines</b>															
CAR 2:0	C <sub>9</sub> H <sub>17</sub> NO <sub>4</sub>	203.1158	0.82	M+H	2	GM-LC-QTOF-MS	ESI +	53.0341, 58.0650, 84.0808, 85.0291,	<i>Only in FO GLU group</i>	1.07	3.79E-03†	1.91	1.07	3.79E-03†	
<b>Fatty acid esters of hydroxyl fatty acids</b>															
FAHFA 38:6	C <sub>38</sub> H <sub>62</sub> O <sub>4</sub>	582.4648	20.26	M-H	2	GM-LC-QTOF-MS	ESI -	279.2354	3.20	1.15	3.05E-04†	0.44	1.10	2.80E-04†	
FAHFA 38:4	C <sub>38</sub> H <sub>60</sub> O <sub>4</sub>	586.4961	21.18	M-H	2	GM-LC-QTOF-MS	ESI -	281.2485	3.65	-	8.86E-03†	0.28	-	6.79E-03†	
<b>Fatty Acyls</b>															
13-Hydroxyoctadecadienoic acid (13-HODE)	C <sub>18</sub> H <sub>32</sub> O <sub>3</sub>	296.2351	16.42	M-H	3	GM-LC-QTOF-MS	ESI -	-	4.13	1.02	4.35E-03†	-	-	-	
Dimorphecolic acid	C <sub>18</sub> H <sub>32</sub> O <sub>3</sub>	296.2351	17.08	M-H	3	GM-LC-QTOF-MS	ESI -	-	3.60	-	4.66E-02†	0.24	-	1.43E-02†	
11-Deoxyprostaglandin E2	C <sub>21</sub> H <sub>34</sub> O <sub>4</sub>	350.2457	19.44	M-H-H <sub>2</sub> O	3	GM-LC-QTOF-MS	ESI -	-	4.68	1.15	7.10E-04†	-	-	-	
Linoleic acid	C <sub>18</sub> H <sub>32</sub> O <sub>2</sub>	280.2402	20.27	M-H	2	GM-LC-QTOF-MS GM-GC-QTOF-MS	ESI -	279.233	2.88	1.16	2.38E-04†	0.47	1.15	1.75E-04†	
Palmitic acid	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>	256.2402	21.02	M-H	2	GM-LC-QTOF-MS GM-GC-QTOF-MS	ESI -	255.2333	-	-	-	0.32	1.01	4.32E-03†	
Falcarindiol	C <sub>17</sub> H <sub>24</sub> O <sub>2</sub>	260.1776	3.25	M+H-2H <sub>2</sub> O	3		ESI +	-	-	-	-	0.79	-	1.11E-02†	
Mosin C	C <sub>35</sub> H <sub>62</sub> O <sub>7</sub>	594.8626	8.59	-	2	GM-GC-QTOF-MS	-	-	0.57	1.32	3.55E-02	1.57	1.19	1.54E-02†	
Methyltartronic Acid	C <sub>4</sub> H <sub>6</sub> O <sub>5</sub>	134.0900	10.44	-	2	GM-GC-QTOF-MS	-	-	0.82	-	-	0.30	1.60	7.45E-05†	
3-Hydroxymethylglutaric Acid	C <sub>6</sub> H <sub>10</sub> O <sub>5</sub>	162.1406	13.64	-	2	GM-GC-QTOF-MS	-	-	0.55	1.22	3.87E-02	1.67	1.24	1.18E-02†	
Muconic Acid	C <sub>6</sub> H <sub>6</sub> O <sub>4</sub>	142.1094	14.01	-	2	GM-GC-QTOF-MS	-	-	-	-	-	0.26	1.48	1.07E-03†	
Palmitoleic Acid	C <sub>16</sub> H <sub>30</sub> O <sub>2</sub>	254.4082	18.29	-	2	GM-GC-QTOF-MS	-	-	-	-	-	0.26	1.48	1.07E-03†	
Heptadecanoic Acid	C <sub>17</sub> H <sub>34</sub> O <sub>2</sub>	270.4507	19.27	-	2	GM-GC-QTOF-MS	-	-	-	-	-	0.24	1.56	1.29E-04†	
Oleic Acid	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>	282.4614	20.04	-	2	GM-GC-QTOF-MS	-	-	-	-	-	0.32	1.33	6.85E-03†	
13-Octadecenoic Acid	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>	282.4680	20.09	-	2	GM-GC-QTOF-MS	-	-	-	-	-	0.45	-	4.00E-02†	
Arachidic Acid	C <sub>20</sub> H <sub>40</sub> O <sub>2</sub>	312.5304	21.90	-	2	GM-GC-QTOF-MS	-	-	-	-	-	0.30	1.35	3.39E-03†	
Behenic Acid	C <sub>22</sub> H <sub>44</sub> O <sub>2</sub>	340.5836	23.42	-	2	GM-GC-QTOF-MS	-	-	-	-	-	0.22	1.58	7.45E-05†	
Turanose	C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>	342.2965	24.66	-	2	GM-GC-QTOF-MS	-	-	1.68	1.44	1.19E-02	-	-	-	

13-Docosenamide	C <sub>22</sub> H <sub>43</sub> NO	337.5920	24.75	-	2	GM-GC-QTOF-MS	-	-	13.68	1.13	-	2.05	1.31	8.04E-03f	
Nervonic Acid	C <sub>24</sub> H <sub>46</sub> O <sub>2</sub>	366.6208	24.84	-	2	GM-GC-QTOF-MS	-	-	-	-	-	0.07	1.60	4.85E-05f	
<b>Glycerophospholipids</b>															
PG 17:0	C <sub>23</sub> H <sub>45</sub> O <sub>10</sub> P	512.2750	6.17	M-H	3	GM-LC-QTOF-MS	ESI -	-	<i>Only in FO GLU group</i>	1.19	2.72E-04f	1.49	1.13	3.69E-04f	
PG 30:3	C <sub>36</sub> H <sub>65</sub> O <sub>10</sub> P	688.4315	9.33	M-H	3	GM-LC-QTOF-MS	ESI -	-	<i>Only in FO GLU group</i>	1.09	1.78E-03f	1.52	1.00	2.36E-03f	
PI 36:6	C <sub>45</sub> H <sub>75</sub> O <sub>13</sub> P	854.4945	10.22	M-H	3	GM-LC-QTOF-MS	ESI -	-	0.31	1.21	7.44E-05f	-	-	-	
LPE 18:2 <i>iso 1</i>	C <sub>23</sub> H <sub>44</sub> NO <sub>7</sub> P	477.2855	16.18	M-H	2	GM-LC-QTOF-MS	ESI -	279.233	4.89	1.12	6.72E-04f	-	-	-	
LPE 18:2 <i>iso 2</i>	C <sub>23</sub> H <sub>44</sub> NO <sub>7</sub> P	477.2855	16.39	M-H	2	GM-LC-QTOF-MS	ESI -	279.2330, 196.0380	4.68	1.19	2.53E-04f	-	-	-	
LPC 18:2 <i>iso 1</i>	C <sub>26</sub> H <sub>50</sub> NO <sub>7</sub> P	519.3325	16.24	M+COOH	2	GM-LC-QTOF-MS	ESI -/ ESI +	279.233	10.53	-	2.22E-02f	-	-	-	
LPC 18:2 <i>iso 2</i>	C <sub>26</sub> H <sub>50</sub> NO <sub>7</sub> P	519.3325	16.45	M+COOH	2	GM-LC-QTOF-MS	ESI -/ ESI +	279.233	5.44	1.15	5.21E-04f	-	-	-	
LPE 17:1 <i>iso 1</i>	C <sub>22</sub> H <sub>44</sub> NO <sub>7</sub> P	465.2855	16.41	M-H	2	GM-LC-QTOF-MS	ESI -	267.233	2.78	-	2.26E-02f	0.26	1.23	2.08E-05f	
LPE 17:1 <i>iso 2</i>	C <sub>22</sub> H <sub>44</sub> NO <sub>7</sub> P	465.2855	16.65	M-H	2	GM-LC-QTOF-MS	ESI -	267.2330, 214.0486, 196.0380	3.02	-	1.32E-02f	0.08	-	1.43E-02f	
LPE 16:0	C <sub>21</sub> H <sub>44</sub> NO <sub>7</sub> P	453.2855	16.88	M-H	2	GM-LC-QTOF-MS	ESI -	196.0380, 214.0486, 255.2330	3.82	1.01	9.52E-03f	-	-	-	
LPA 18:2	C <sub>21</sub> H <sub>39</sub> O <sub>7</sub> P	434.2433	16.97	M-H	2	GM-LC-QTOF-MS	ESI -	78.9591, 152.9958	3.18	-	1.77E-02f	0.31	1.03	9.87E-04f	
LPE 18:1	C <sub>23</sub> H <sub>46</sub> NO <sub>7</sub> P	479.3012	17.23	M-H	3	GM-LC-QTOF-MS	ESI -	-	3.64	1.04	4.06E-03f	-	-	-	
LPC 18:1	C <sub>26</sub> H <sub>52</sub> NO <sub>7</sub> P	521.3481	17.31	M+COOH	2	GM-LC-QTOF-MS	ESI -	281.2486	6.58	1.14	8.63E-04f	-	-	-	
LPC 16:0	C <sub>24</sub> H <sub>50</sub> NO <sub>7</sub> P	495.3325	17.08	M+H	2	GM-LC-QTOF-MS	ESI +	104.1070, 184.0732	22.58	1.09	3.44E-03f	2.28	1.09	3.44E-03f	
PC 36:4	C <sub>44</sub> H <sub>80</sub> NO <sub>8</sub> P	781.5622	21.71	M+H	2	GM-LC-QTOF-MS	ESI +	184.073	0.42	-	1.38E-02f	1.63	-	1.38E-02f	
<b>Glycerolipids</b>															
Diglycerol	C <sub>6</sub> H <sub>14</sub> O <sub>5</sub>	166.1700	15.46	-	2	GM-GC-QTOF-MS	-	-	-	-	-	2.66	1.42	2.00E-03f	
1,3-Dihydroxypropan-2-yl Octadecanoate	C <sub>21</sub> H <sub>42</sub> O <sub>4</sub>	358.5558	24.27	-	2	GM-GC-QTOF-MS	-	-	-	-	-	0.52	-	4.47E-02f	
2,3-Dihydroxypropyl Octadecanoate	C <sub>21</sub> H <sub>42</sub> O <sub>4</sub>	358.5558	24.51	-	2	GM-GC-QTOF-MS	-	-	0.86	1.19	-	-	-	-	
Glyceryl Monostearate	C <sub>21</sub> H <sub>42</sub> O <sub>4</sub>	358.5558	24.52	-	2	GM-GC-QTOF-MS	-	-	0.89	1.14	-	-	-	-	
<b>Homogeneous non-metal compounds</b>															
Phosphate	H <sub>3</sub> O <sub>4</sub> P	97.9952	9.77	-	2	GM-GC-QTOF-MS	-	-	-	-	-	1.44	1.18	2.10E-02f	
<b>Hydroxy acids and derivatives</b>															
5-Keto-gluconate	C <sub>6</sub> H <sub>10</sub> O <sub>7</sub>	194.0427	0.60	M-H	3	GM-LC-QTOF-MS	ESI -	-	4.27	1.01	6.39E-03f	-	-	-	
<b>Indoles and derivatives</b>															
Indole	C <sub>8</sub> H <sub>7</sub> N	117.0578	3.68	M-H	2	GM-LC-QTOF-MS	ESI -	116.0506	1.82	1.26	7.41E-05f	-	-	-	
Tryptophan	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	204.0899	3.92	M+H	2	GM-LC-QTOF-MS	ESI -/ ESI +	146.0589, 170.0594,	1.84	-	1.61E-02	0.52	-	1.61E-02	
Asperochromamide D	C <sub>16</sub> H <sub>17</sub> N <sub>3</sub> O <sub>4</sub>	315.1219	7.24	M-H	3	GM-LC-QTOF-MS	ESI -	-	1.73	1.07	4.64E-03f	0.83	-	3.71E-03f	
Methyl Tryptophan	C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>	218.2500	18.97	-	2	GM-GC-QTOF-MS	-	-	0.75	1.13	-	-	-	-	
5-Hydroxy Tryptophan	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	220.2246	21.71	-	2	GM-GC-QTOF-MS	-	-	-	-	-	4.15	1.41	2.33E-03f	
<b>Keto acids and derivatives</b>															
Acetoacetate	C <sub>4</sub> H <sub>5</sub> O <sub>3</sub>	101.0820	7.37	-	2	GM-GC-QTOF-MS	-	-	-	-	-	0.41	1.29	1.23E-02f	
Ketoleucine	C <sub>6</sub> H <sub>10</sub> O <sub>3</sub>	130.1418	8.71	-	2	GM-GC-QTOF-MS	-	-	-	-	-	0.36	1.44	3.39E-03f	
<b>Nucleósidos</b>															

5-Methyl-3'-Deoxyuridine	C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>5</sub>	242.2300	21.01	-	2	GM-GC-QTOF-MS	-	-	0.62	1.11	-	0.53	-	-	
<b>Organic acids and derivatives</b>															
Oxalic Acid	C <sub>2</sub> H <sub>2</sub> O <sub>4</sub>	90.0349	7.49	-	2	GM-GC-QTOF-MS	-	-	0.81	-	-	1.95	1.30	9.74E-03†	
3-Hydroxybutyric Acid	C <sub>4</sub> H <sub>8</sub> O <sub>3</sub>	104.1045	8.10	-	2	GM-GC-QTOF-MS	-	-	1.44	1.05	-	0.93	-	-	
Methylmalonic Acid	C <sub>4</sub> H <sub>6</sub> O <sub>4</sub>	118.0880	8.74	-	2	GM-GC-QTOF-MS	-	-	0.62	1.64	2.76E-02†	1.14	-	-	
Maleic Acid	C <sub>4</sub> H <sub>4</sub> O <sub>4</sub>	116.0722	10.03	-	2	GM-GC-QTOF-MS	-	-	1.21	1.40	-	0.83	-	-	
Succinic Acid	C <sub>4</sub> H <sub>6</sub> O <sub>4</sub>	118.0880	10.25	-	2	GM-GC-QTOF-MS	-	-	1.04	-	-	1.47	1.24	1.04E-02†	
Fumaric Acid	C <sub>4</sub> H <sub>4</sub> O <sub>4</sub>	116.0722	10.68	-	2	GM-GC-QTOF-MS	-	-	2.06	1.08	-	-	-	-	
Malonic Acid	C <sub>3</sub> H <sub>4</sub> O <sub>4</sub>	104.0615	11.47	-	2	GM-GC-QTOF-MS	-	-	1.68	1.44	1.22E-02	1.50	-	-	
Malic Acid	C <sub>4</sub> H <sub>6</sub> O <sub>5</sub>	134.0874	12.42	-	2	GM-GC-QTOF-MS	-	-	-	-	-	4.15	1.24	1.18E-02†	
Acetylputrescine	C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O	130.1882	15.52	-	2	GM-GC-QTOF-MS	-	-	0.20	1.12	-	3.33	1.24	1.18E-02†	
Galactonic Acid	C <sub>6</sub> H <sub>12</sub> O <sub>7</sub>	196.1553	16.95	-	2	GM-GC-QTOF-MS	-	-	-	-	-	1.59	-	4.53E-02	
Dehydroascorbic Acid	C <sub>6</sub> H <sub>6</sub> O <sub>6</sub>	174.1082	17.57	-	2	GM-GC-QTOF-MS	-	-	0.70	1.05	-	-	-	-	
<b>Organic oxygen compounds</b>															
2,3-Butanediol	C <sub>4</sub> H <sub>10</sub> O <sub>2</sub>	90.1210	6.13	-	2	GM-GC-QTOF-MS	-	-	-	-	-	0.65	-	3.40E-02	
2-Deoxy Ribose	C <sub>5</sub> H <sub>10</sub> O <sub>4</sub>	134.1310	13.37	-	2	GM-GC-QTOF-MS	-	-	-	-	-	2.37	1.23	1.27E-02†	
Allo-Inositol	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	180.1559	16.69	-	2	GM-GC-QTOF-MS	-	-	0.53	1.46	7.34E-03	1.37	1.09	2.67E-02†	
<b>Organosulfur compounds</b>															
3-(Methylthio)Propylamine	C <sub>4</sub> H <sub>11</sub> NS	105.2000	11.39	-	2	GM-GC-QTOF-MS	-	-	0.60	-	-	3.50	1.45	1.08E-03†	
Cysteamine	C <sub>2</sub> H <sub>7</sub> NS	77.1490	19.89	-	2	GM-GC-QTOF-MS	-	-	0.22	1.27	2.08E-02	2.37	1.17	1.63E-02†	
<b>Phenylpropanoids and polyketides</b>															
2-Hydroxycinnamic Acid	C <sub>9</sub> H <sub>8</sub> O <sub>3</sub>	164.1580	15.98	-	2	GM-GC-QTOF-MS	-	-	5.08	1.25	3.23E-02	-	-	-	
Hydroxyphenyllactic Acid	C <sub>9</sub> H <sub>10</sub> O <sub>4</sub>	182.1733	17.03	-	2	GM-GC-QTOF-MS	-	-	0.70	1.10	3.85E-02	-	-	-	
<b>Pyridines and derivatives</b>															
Nicotinic Acid	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	123.1094	9.96	-	2	GM-GC-QTOF-MS	-	-	0.36	1.45	9.29E-03	-	-	-	
1-Methylnicotinamide	C <sub>7</sub> H <sub>9</sub> N <sub>2</sub> O	137.1592	12.39	-	2	GM-GC-QTOF-MS	-	-	-	-	-	2.05	-	3.29E-02	
<b>Organonitrogen compounds</b>															
Tetradecyldiethanolamine	C <sub>18</sub> H <sub>39</sub> NO <sub>2</sub>	301.2981	15.61	M+H	2	GM-LC-QTOF-MS	ESI +	70.0662, 88.0757, 102.0913, 106.0862, 284.2947	2.99	1.06	2.80E-03†	1.67	1.06	2.80E-03†	
Dimethyldodecylamine	C <sub>14</sub> H <sub>31</sub> N	213.2456	14.36	M-H+H <sub>2</sub> O	2	GM-LC-QTOF-MS	ESI +	58.0653, 62.0596	1.41	1.21	5.50E-04†	0.91	1.21	5.50E-04†	
Phenylethanolamine	C <sub>8</sub> H <sub>11</sub> NO	137.0841	6.78	M-H-H <sub>2</sub> O	2	GM-LC-QTOF-MS	ESI +	91.0536, 93.0692, 95.0485, 103.0534	0.50	1.11	2.04E-03†	1.37	1.11	2.04E-03†	
Phytosphingosine	C <sub>18</sub> H <sub>39</sub> NO <sub>3</sub>	317.2930	14.40	M+H	2	GM-LC-QTOF-MS	ESI +	60.0456, 282.2795, 300.2886	0.08	1.10	2.03E-03†	1.19	1.10	2.03E-03†	
Polanrazine B	C <sub>18</sub> H <sub>23</sub> N <sub>3</sub> O <sub>2</sub> S <sub>2</sub>	377.1232	20.16	M+H	2	GM-LC-QTOF-MS	ESI +	157.1016	1.58	1.01	8.35E-03†	0.93	1.01	8.35E-03†	
<b>Prenol lipids</b>															
Canavalioideside	C <sub>26</sub> H <sub>42</sub> O <sub>12</sub>	528.2589	11.95	M-H	3	GM-LC-QTOF-MS	ESI -	-	-	Only in FO GLU group	1.15	4.81E-04†	-	-	
2H-Oxireno[1,10a]phenanthro[3,2-b]furan-10(11)-one, 5,7-bis(acetyloxy)-decahydro-4,4,7a,11-tetramethyl-	C <sub>24</sub> H <sub>32</sub> O <sub>7</sub>	432.2148	15.57	M-H-H <sub>2</sub> O	2	GM-LC-QTOF-MS	ESI +	91.0536, 107.0849, 119.0854, 120.0885, 135.0811	-	Only in FO GLU group	1.11	2.21E-03†	2.51	1.11	2.21E-03†
Squalene	C <sub>30</sub> H <sub>50</sub>	410.7300	24.83	-	2	GM-GC-QTOF-MS	-	-	-	-	-	0.04	1.51	2.69E-04†	

Loganose	C <sub>17</sub> H <sub>26</sub> O <sub>10</sub>	390.3850	25.77	-	2	GM-GC-QTOF-MS	-	-	0.81	1.03	-	-	-	-	
<b>Purine nucleosides</b>															
Inosine	C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>5</sub>	268.0808	1.69	M-H	2	GM-LC-QTOF-MS	ESI -	92.0256, 108.0210, 135.0304	-	-	-	0.69	-	1.25E-02†	
Guanosine	C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>5</sub>	283.0917	1.75	M-H	2	GM-LC-QTOF-MS	ESI -	108.0202, 133.0157	-	-	-	1.94	1.26	1.39E-05†	
<b>Purines and purine derivatives</b>															
Guanine	C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> O	151.0494	1.66	M+H	2	GM-LC-QTOF-MS	ESI +	55.0284, 110.0342, 135.0312	<i>Only in FO GLU group</i>	1.17	7.32E-04†	1.56	1.17	7.32E-04†	
Hypoxanthine	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O	136.0385	1.13	M+H	2	GM-LC-QTOF-MS	ESI +	55.0291, 67.0287, 110.0352, 119.0347	0.13	1.24	1.95E-04†	1.30	1.24	1.95E-04†	
<b>Pyridines and derivatives</b>															
Isonicotinic acid	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	123.0320	0.81	M+H	2	GM-LC-QTOF-MS	ESI +	53.0384, 78.0335, 80.0499, 96.0441	<i>Only in FO GLU group</i>	1.14	1.27E-03†	1.57	1.14	1.27E-03†	
Nicotinic Acid	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	123.1094	9.96	-	2	GM-GC-QTOF-MS	-	-	0.36	1.45	9.29E-03	-	-	-	
1-Methylnicotinamide	C <sub>7</sub> H <sub>9</sub> N <sub>2</sub> O	137.1592	12.39	-	2	GM-GC-QTOF-MS	-	-	-	-	-	2.05	-	0.032853	
<b>Pyrrolidines</b>															
2-Pyrrolidinone	C <sub>4</sub> H <sub>7</sub> NO	85.1045	7.84	-	2	GM-GC-QTOF-MS	-	-	0.64	1.52	1.42E-02	1.53	1.24	1.18E-02†	
<b>Steroids</b>															
ST 28:1;O5	C <sub>28</sub> H <sub>48</sub> O <sub>5</sub>	464.3502	18.39	M-H-H <sub>2</sub> O	3	GM-LC-QTOF-MS	ESI -	-	5.63	1.18	4.47E-04†	2.40	1.15	3.05E-04†	
ST 28:3;O5	C <sub>28</sub> H <sub>44</sub> O <sub>5</sub>	460.3189	19.30	M-H	3	GM-LC-QTOF-MS	ESI -	-	4.22	1.04	2.67E-03†	-	-	-	
(2-phenylethyl)-4-{4,7,11-trihydroxy-9,11-dimethyl-hexadecahydro-1H-cyclopenta[a]phenanthren-1-yl}pentanamide	C <sub>32</sub> H <sub>49</sub> NO <sub>4</sub>	511.3662	19.42	M-H	3	GM-LC-QTOF-MS	ESI -	-	2.38	-	3.50E-02†	-	-	-	
ST 28:2;O4	C <sub>28</sub> H <sub>46</sub> O <sub>4</sub>	446.3396	19.47	M-H	3	GM-LC-QTOF-MS	ESI -	-	3.38	1.18	2.45E-04†	-	-	-	
Trihydroxyergosta-7,22-Dien-6-One	C <sub>28</sub> H <sub>44</sub> O <sub>4</sub>	444.3240	19.84	M-H	3	GM-LC-QTOF-MS	ESI -	-	4.16	1.13	4.53E-04†	0.54	-	7.39E-03†	
<b>Thiazoles</b>															
4-Methyl-5-Thiazoleethanol	C <sub>6</sub> H <sub>9</sub> NOS	143.2070	11.02	-	2	GM-GC-QTOF-MS	-	-	0.56	1.55	8.67E-03	1.50	1.19	1.69E-02†	
2-Hydroxyatrazine	C <sub>8</sub> H <sub>15</sub> N <sub>5</sub> O	197.2420	15.90	-	2	GM-GC-QTOF-MS	-	-	0.59	1.19	-	1.49	1.25	1.23E-02†	

RT: retention time; <sup>a</sup>CV, coefficient of variation in the metabolites in the QC samples; <sup>b</sup>Fold Change, change in the abundance of the specified comparison calculated as (case/control); <sup>c</sup>*p* value\* correspond to the *p* values calculated by the Benjamini-Hochberg false discovery rate post hoc correction (FDR < 0.05); <sup>d</sup>VIP, variable importance in projection. GM: global metabolomics, LC: liquid chromatography, GC: gas chromatography, QTOF-MS: quadrupole time-of-flight mass spectrometer.