

**Supporting Information**

**Metabolomics Profile and Targeted Lipidomics in Multiple Tissues  
Associated with Feed Efficiency in Beef Steers**

Virginia M. Artegoitia<sup>†\*</sup>, Andrew P. Foote<sup>‡</sup>, Ronald M. Lewis<sup>†</sup>, Harvey C. Freetly<sup>‡</sup>,

<sup>†</sup>University of Nebraska-Lincoln, Department of Animal Science, Lincoln NE, 68583, USA.

<sup>‡</sup>USDA, ARS, U.S. Meat Animal Research Center, Clay Center NE 68933,

Table S1- Identification of *longissimus dorsi*, adipose, liver and duodenum metabolites for feed efficiency

Table S2. Results from tissues pathway analysis

Table S1. Identification of longissimus dorsi, adipose, liver and duodenum metabolites for feed efficiency

Metabolites	Formula	Adducts	RT (min)	Ion (m/z)	Mass error (ppm)	ID	Fold change	VIP
<b>Longissimus dorsi</b>								
(5R)-5-Hydroxyhexanoic acid	C <sub>6</sub> H <sub>12</sub> O <sub>3</sub>	M+H	10.75	133.086	1.50	BMDB00409	-1.08	0.49
1,4-beta-D-Glucan	C <sub>18</sub> H <sub>32</sub> O <sub>18</sub>	M-H	2.357	535.153	3.07	BMDB06944	1.19	0.75
13(S)-HODE	C <sub>18</sub> H <sub>32</sub> O <sub>3</sub>	M-H	11.41	295.227	-2.63	BMDB06939	1.22	0.75
3-Deoxy-D-glycero-D-galacto-2-nonulosonic acid	C <sub>9</sub> H <sub>16</sub> O <sub>9</sub>	M+H	2.422	269.086	-4.14	BMDB00425	1.50	0.97
3-Sulfofopyruvic acid	C <sub>3</sub> H <sub>4</sub> O <sub>6</sub> S	M+H	0.437	168.981	2.52	BMDB04045	-1.22	0.65
7-Sulfocholic acid	C <sub>24</sub> H <sub>40</sub> O <sub>8</sub> S	M-H	0.254	487.237	-0.73	BMDB02421	1.18	0.66
8,11,14-Eicosatrienoic acid	C <sub>20</sub> H <sub>34</sub> O <sub>2</sub>	M+H	10.02	307.264	3.48	BMDB02925	-1.12	0.59
Acetoacetic acid	C <sub>4</sub> H <sub>6</sub> O <sub>3</sub>	M-H	0.289	101.024	-2.83	BMDB00060	-1.19	0.70
Adrenic acid	C <sub>22</sub> H <sub>36</sub> O <sub>2</sub>	M+H	13.16	333.279	0.04	BMDB02226	1.11	0.89
Alpha-Linolenic acid	C <sub>18</sub> H <sub>30</sub> O <sub>2</sub>	M+H	11.99	279.231	-3.21	BMDB01388	-1.12	0.55
Bisnorcholic acid	C <sub>22</sub> H <sub>36</sub> O <sub>5</sub>	M+H	9.871	381.263	-2.55	BMDB02082	-1.12	0.58
Butyrylcarnitine	C <sub>11</sub> H <sub>21</sub> NO <sub>4</sub>	M+H	1.237	232.155	1.49	BMDB02013	1.25	0.59
Cholesterol	C <sub>27</sub> H <sub>46</sub> O <sub>4</sub> S	M-H	0.481	465.303	-3.54	BMDB00653	-2.11	1.57
cis-4-Octenedioic acid	C <sub>8</sub> H <sub>12</sub> O <sub>4</sub>	M+H	1.237	173.081	0.48	BMDB04982	-1.17	0.48
Cortolone	C <sub>21</sub> H <sub>34</sub> O <sub>5</sub>	M+H	8.486	367.248	0.58	BMDB03128	-1.09	0.49
Creatine	C <sub>4</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>	M-H	0.254	130.062	-2.18	BMDB00064	1.17	0.61
DG(14:1(9Z)/22:5(4Z,7Z,10Z,13Z,16Z)/0:0)	C <sub>39</sub> H <sub>64</sub> O <sub>5</sub>	M+H	15.07	613.480	-4.05	BMDB07061	-1.15	1.44
DG(16:0/20:1(11Z)/0:0)	C <sub>39</sub> H <sub>74</sub> O <sub>5</sub>	M+H	14.16	623.561	0.82	BMDB07108	-1.86	0.83
DG(20:4(5Z,8Z,11Z,14Z)/16:1(9Z)/0:0)	C <sub>39</sub> H <sub>66</sub> O <sub>5</sub>	M+H	17.99	615.497	-2.92	BMDB07505	-1.33	0.67
DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/16:1(9Z)/0:0)	C <sub>41</sub> H <sub>66</sub> O <sub>5</sub>	M+H	17.74	639.497	-2.82	BMDB07766	-1.22	0.87
Glucose	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	M-H	1.254	179.056	-3.22	BMDB00122	1.50	1.00
acid	C <sub>22</sub> H <sub>34</sub> O <sub>2</sub>	M+H	10.05	331.264	2.09	BMDB01976	-1.17	1.30
Ecgonine	C <sub>9</sub> H <sub>15</sub> NO <sub>3</sub>	M+H	0.289	186.113	1.72	BMDB06548	-1.26	0.73
Eicosadienoic acid	C <sub>20</sub> H <sub>36</sub> O <sub>2</sub>	M+H	10.38	309.28	2.48	BMDB05060	-1.08	0.38
Glycerol 3-phosphate	C <sub>3</sub> H <sub>9</sub> O <sub>6</sub> P	M-H	0.289	171.006	-3.03	BMDB00126	-1.37	0.83
Glycerophosphocholine	C <sub>8</sub> H <sub>20</sub> NO <sub>6</sub> P	M+H	0.289	258.111	3.22	BMDB00086	-1.49	1.09
Glycerolphosphorylethanolamine	C <sub>8</sub> H <sub>14</sub> NO <sub>6</sub> P	M-H	0.254	214.048	-1.23	BMDB00114	-1.50	1.03
Guanidosuccinic acid	C <sub>5</sub> H <sub>9</sub> N <sub>3</sub> O <sub>4</sub>	M+H	1.128	176.067	3.35	BMDB03157	1.20	0.65
Guggulsterone	C <sub>22</sub> H <sub>30</sub> O <sub>3</sub>	M+H	10.28	343.226	-2.48	BMDB02726	-1.07	0.41
L-Acetylcarnitine	C <sub>9</sub> H <sub>17</sub> NO <sub>4</sub>	M+H	0.289	204.124	-1.62	BMDB00201	-1.15	0.48
L-Alanine	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	M-H	0.254	88.040	0.77	BMDB00161	-1.13	0.55
L-Histidine	C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>	M-H	9.035	154.062	-4.02	BMDB00177	4.88	1.81
L-Lactic acid	C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>	M-H	0.323	89.024	-0.52	BMDB00190	-1.18	0.61
LysoPC(15:0)	C <sub>23</sub> H <sub>48</sub> NO <sub>7</sub> P	M-H	15.54	480.309	-0.69	BMDB10381	1.80	2.24
LysoPC(20:4(5Z,8Z,11Z,14Z))	C <sub>28</sub> H <sub>50</sub> NO <sub>7</sub> P	M+H	9.401	544.339	-1.13	BMDB10395	-1.34	0.88
LysoPC(20:5(5Z,8Z,11Z,14Z,17Z))	C <sub>28</sub> H <sub>48</sub> NO <sub>7</sub> P	M+H	9.435	542.322	-3.59	BMDB10397	-1.33	0.87
Malic acid	C <sub>4</sub> H <sub>6</sub> O <sub>5</sub>	M-H	0.289	133.014	3.29	BMDB00744	-1.62	1.05
Oleamide	C <sub>18</sub> H <sub>35</sub> NO	M+H	13.83	282.280	2.06	BMDB02117	1.18	0.59
Palmitic amide	C <sub>16</sub> H <sub>33</sub> NO	M+H	9.871	256.264	2.22	BMDB12273	4.06	2.03
PC(14:0/22:5(4Z,7Z,10Z,13Z,16Z))	C <sub>44</sub> H <sub>78</sub> NO <sub>8</sub> P	M+H	14.56	780.553	4.16	BMDB07890	1.38	1.14
PC(14:0/P-18:0)	C <sub>40</sub> H <sub>80</sub> NO <sub>7</sub> P	M+H	15.36	718.575	1.11	BMDB07896	1.33	0.96
PC(14:0/P-18:1(9Z))	C <sub>40</sub> H <sub>78</sub> NO <sub>7</sub> P	M+H	14.89	716.559	3.51	BMDB07898	-1.34	0.86
PC(14:1(9Z)/20:0)	C <sub>42</sub> H <sub>82</sub> NO <sub>8</sub> P	M+H	16.75	760.586	1.49	BMDB07911	-1.36	1.06
PC(15:0/16:0)	C <sub>39</sub> H <sub>78</sub> NO <sub>8</sub> P	M+H	13.86	720.556	3.28	BMDB07935	1.38	0.92
PC(16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C <sub>46</sub> H <sub>80</sub> NO <sub>8</sub> P	M+H	15.04	806.567	-2.52	BMDB07991	-1.32	0.84
PC(18:0/14:1(9Z))	C <sub>40</sub> H <sub>78</sub> NO <sub>8</sub> P	M+H	11.81	732.554	0.63	BMDB08032	1.45	1.04
PC(18:0/18:4(6Z,9Z,12Z,15Z))	C <sub>44</sub> H <sub>80</sub> NO <sub>8</sub> P	M+H	16.75	782.568	-1.56	BMDB08042	1.46	1.16
PC(18:1(9Z)/P-16:0)	C <sub>42</sub> H <sub>82</sub> NO <sub>7</sub> P	M+H	16.39	744.591	3.84	BMDB08126	-1.41	1.04
PC(18:2(9Z,12Z)/20:5(5Z,8Z,11Z,14Z,17Z))	C <sub>46</sub> H <sub>78</sub> NO <sub>8</sub> P	M+H	14.34	804.553	-1.55	BMDB08149	1.49	1.11
PC(18:3(9Z,12Z,15Z)/P-16:0)	C <sub>42</sub> H <sub>78</sub> NO <sub>7</sub> P	M+H	13.97	740.560	1.13	BMDB08225	1.46	1.10
PC(18:4(6Z,9Z,12Z,15Z)/dm18:0)	C <sub>44</sub> H <sub>80</sub> NO <sub>7</sub> P	M+H	15.62	766.574	-0.26	BMDB08259	1.51	1.21
PC(22:5(7Z,10Z,13Z,16Z,19Z)/16:0)	C <sub>46</sub> H <sub>82</sub> NO <sub>8</sub> P	M+H	17.99	808.583	-2.15	BMDB08692	-1.37	0.83
PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C <sub>48</sub> H <sub>80</sub> NO <sub>8</sub> P	M+H	14.92	830.566	-3.62	BMDB08730	1.32	1.13
PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/P-18:1(11Z))	C <sub>48</sub> H <sub>82</sub> NO <sub>7</sub> P	M+H	17.85	816.587	-4.02	BMDB08753	1.60	1.06
PC(P-16:0/18:2(9Z,12Z))	C <sub>42</sub> H <sub>80</sub> NO <sub>7</sub> P	M+H	15.87	742.575	1.87	BMDB11211	-1.33	0.94
PC(P-16:0/18:4(6Z,9Z,12Z,15Z))	C <sub>42</sub> H <sub>76</sub> NO <sub>7</sub> P	M+H	14.89	738.541	-3.93	BMDB11214	-1.43	1.07
PC(P-16:0/20:3(5Z,8Z,11Z))	C <sub>44</sub> H <sub>80</sub> NO <sub>7</sub> P	M+H	17.08	768.590	0.28	BMDB11218	1.41	1.22
PC(P-16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C <sub>46</sub> H <sub>80</sub> NO <sub>7</sub> P	M+H	17.08	790.573	-1.78	BMDB11229	1.51	1.12
PC(P-18:0/18:4(6Z,9Z,12Z,15Z))	C <sub>44</sub> H <sub>80</sub> NO <sub>7</sub> P	M+H	16.42	766.572	-2.76	BMDB11247	1.50	0.97
PC(P-18:0/20:5(5Z,8Z,11Z,14Z,17Z))	C <sub>46</sub> H <sub>82</sub> NO <sub>7</sub> P	M+H	16.27	792.589	-1.78	BMDB11255	1.41	0.72

PC(P-18:0/22:5(4Z,7Z,10Z,13Z,16Z))	C <sub>48</sub> H <sub>86</sub> NO <sub>7</sub> P	M+H	17.55	820.619	-2.45	BMDB11260	1.28	1.03	
PC(P-18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C <sub>44</sub> H <sub>78</sub> NO <sub>7</sub> P	M+H	15.87	764.557	-1.89	BMDB11280	-1.44	1.15	
PC(P-18:1(11Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C <sub>48</sub> H <sub>82</sub> NO <sub>7</sub> P	M+H	16.90	816.586	-4.85	BMDB11295	1.57	1.14	
PE(16:0/20:5(5Z,8Z,11Z,14Z,17Z))	C <sub>41</sub> H <sub>72</sub> NO <sub>8</sub> P	M+H	14.63	738.506	-0.62	BMDB08939	1.22	1.20	
PE(18:0/P-18:1(11Z))	C <sub>41</sub> H <sub>80</sub> NO <sub>7</sub> P	M+H	16.54	730.574	-0.21	BMDB09017	-1.40	0.97	
PE(18:1(11Z)/20:0)	C <sub>43</sub> H <sub>84</sub> NO <sub>8</sub> P	M+H	17.99	774.602	0.73	BMDB09031	-1.41	0.98	
PE(20:2(11Z,14Z)/P-18:0)	C <sub>43</sub> H <sub>82</sub> NO <sub>7</sub> P	M+H	17.08	756.591	0.72	BMDB09313	-1.35	0.94	
PE(20:4(5Z,8Z,11Z,14Z)/18:0)	C <sub>43</sub> H <sub>78</sub> NO <sub>8</sub> P	M+H	15.04	768.557	3.41	BMDB09387	-1.36	0.87	
PE(20:4(5Z,8Z,11Z,14Z)/18:0)	C <sub>43</sub> H <sub>78</sub> NO <sub>8</sub> P	M+H	17.88	768.557	3.97	BMDB09387	1.30	1.01	
PE(20:5(5Z,8Z,11Z,14Z,17Z)/P-16:0)	C <sub>41</sub> H <sub>72</sub> NO <sub>7</sub> P	M+H	16.05	722.51	0.55	BMDB09477	-1.30	0.97	
PE(22:2(13Z,16Z)/15:0)	C <sub>42</sub> H <sub>80</sub> NO <sub>8</sub> P	M+H	14.56	758.571	0.56	BMDB09549	-1.32	0.89	
PE(22:5(7Z,10Z,13Z,16Z,19Z)/P-18:0)	C <sub>45</sub> H <sub>80</sub> NO <sub>7</sub> P	M+H	17.08	778.573	-2.49	BMDB09676	-1.41	0.86	
PE(dm18:0/18:0)	C <sub>41</sub> H <sub>80</sub> NO <sub>7</sub> P	M+H	17.08	732.591	1.25	BMDB11373	-1.36	1.06	
PE(P-16:0/18:3(6Z,9Z,12Z))	C <sub>39</sub> H <sub>72</sub> NO <sub>7</sub> P	M+H	14.19	698.512	0.07	BMDB11344	-1.42	0.96	
PE(P-16:0/20:2(11Z,14Z))	C <sub>41</sub> H <sub>78</sub> NO <sub>7</sub> P	M+H	14.34	728.56	2.09	BMDB11349	-1.37	0.81	
PE(P-16:0/22:5(4Z,7Z,10Z,13Z,16Z))	C <sub>43</sub> H <sub>76</sub> NO <sub>7</sub> P	M+H	16.42	750.544	0.52	BMDB11359	-1.28	1.04	
PE(P-16:0e/18:1(9Z))	C <sub>39</sub> H <sub>78</sub> NO <sub>7</sub> P	M+H	15.87	704.559	0.22	BMDB11157	-1.37	0.87	
PE-NMe2(16:0/18:1(9Z))	C <sub>41</sub> H <sub>80</sub> NO <sub>8</sub> P	M+H	15.07	746.572	-3.38	BMDB10568	-1.38	0.95	
Phosphite	HO <sub>3</sub> P <sub>2</sub>	M-H	0.289	78.959	2.87	BMDB01443	-1.16	0.54	
PI(18:1(9Z)/20:4(8Z,11Z,14Z,17Z))	C <sub>47</sub> H <sub>81</sub> O <sub>13</sub> P	M+H	16.20	885.545	-3.78	BMDB09845	-4.27	2.65	
PI(22:4(10Z,13Z,16Z,19Z)/16:0)	C <sub>47</sub> H <sub>83</sub> O <sub>13</sub> P	M+H	16.27	887.562	-2.95	BMDB09912	1.55	0.95	
Pristanal	C <sub>19</sub> H <sub>38</sub> O	M-H	14.44	281.285	1.43	BMDB01958	1.17	0.65	
Proline betaine	C <sub>7</sub> H <sub>13</sub> NO <sub>2</sub>	M+H	0.289	144.102	3.91	BMDB04827	1.19	0.59	
PS(18:3(9Z,12Z,15Z)/18:0)	C <sub>42</sub> H <sub>76</sub> NO <sub>10</sub> P	M+H	14.52	786.531	3.86	BMDB12411	-1.33	0.93	
PS(20:4(5Z,8Z,11Z,14Z)/16:1(9Z))	C <sub>42</sub> H <sub>72</sub> NO <sub>10</sub> P	M+H	14.34	782.494	-3.64	BMDB12432	-1.36	0.99	
Pyruvaldehyde	C <sub>3</sub> H <sub>4</sub> O <sub>2</sub>	M-H	0.323	71.014	3.29	BMDB01167	-1.16	0.61	
SM(d18:0/18:0)	C <sub>41</sub> H <sub>85</sub> N <sub>2</sub> O <sub>6</sub> P	M+H	17.45	733.622	-1.15	BMDB12087	1.33	0.97	
SM(d18:0/18:1(9Z))	C <sub>41</sub> H <sub>83</sub> N <sub>2</sub> O <sub>6</sub> P	M+H	15.87	731.607	1.12	BMDB12089	1.33	1.20	
Taurine	C <sub>2</sub> H <sub>7</sub> NO <sub>3</sub> S	M-H	0.254	124.007	-4.28	BMDB00251	1.34	0.82	
Ubiquinol	C <sub>49</sub> H <sub>78</sub> O <sub>4</sub>	M+H	15.32	731.597	-0.29	BMDB01060	-1.34	0.88	
Undecanedioic acid	C <sub>11</sub> H <sub>20</sub> O <sub>4</sub>	M-H	5.662	215.128	-4.28	BMDB00888	1.27	1.31	
Uric acid	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>3</sub>	M-H	0.289	167.02	-4.52	BMDB00289	-1.54	0.91	
Uridine 5'-diphosphate	C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O <sub>12</sub> P <sub>2</sub>	M-H	0.357	402.997	4.81	BMDB00295	-1.21	0.63	
<b>Adipose</b>									
(R)-3-Hydroxydecanoic acid	C <sub>10</sub> H <sub>20</sub> O <sub>3</sub>	M-H	14.92	187.133	-4.01	BMDB10725	-1.13	1.16	
2-Hydroxymyristic acid	C <sub>14</sub> H <sub>28</sub> O <sub>3</sub>	M-H	16.79	243.196	-2.54	BMDB02261	-1.08	1.05	
3b-Allotetrahydrocortisol	C <sub>21</sub> H <sub>34</sub> O <sub>5</sub>	M-H	14.37	365.234	0.87	BMDB00314	-1.05	1.05	
3-Methyl-2-butenal	C <sub>5</sub> H <sub>8</sub> O	M-H	16.18	83.05	-1.60	BMDB12157	-1.09	1.05	
5-Methylthioribose 1-phosphate	C <sub>6</sub> H <sub>13</sub> O <sub>7</sub> PS	M+H	0.289	261.019	-2.38	BMDB00963	1.17	1.01	
5-Phenylvaleric acid	C <sub>11</sub> H <sub>14</sub> O <sub>2</sub>	M-H	9.767	177.092	-3.01	BMDB02043	-1.20	0.87	
Alpha-Linolenic acid	C <sub>18</sub> H <sub>30</sub> O <sub>2</sub>	M-H	12.79	279.256	-2.01	BMDB01388	-1.24	1.41	
Arachidic acid	C <sub>20</sub> H <sub>40</sub> O <sub>2</sub>	M-H	15.43	311.295	-2.56	BMDB02212	-1.06	1.18	
But-2-enoic acid	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	M-H	0.254	85.029	-0.69	BMDB10720	1.79	1.06	
CE(18:2(9Z,12Z))	C <sub>45</sub> H <sub>76</sub> O <sub>2</sub>	M-H	17.81	647.577	0.21	BMDB00610	-1.09	1.42	
CPA(18:2(9Z,12Z)/0:0)	C <sub>21</sub> H <sub>37</sub> O <sub>6</sub> P	M-H	17.66	415.226	2.06	BMDB07007	-1.03	1.21	
Hexacosanoic acid	C <sub>26</sub> H <sub>52</sub> O <sub>2</sub>	M-H	17.55	395.388	-3.51	BMDB02356	-1.07	1.09	
Hyodeoxycholic acid	C <sub>24</sub> H <sub>40</sub> O <sub>4</sub>	M-H	9.001	391.284	-4.24	BMDB00733	1.99	0.63	
L-Alanine	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	M-H	0.254	88.040	-1.11	BMDB00161	2.25	1.09	
L-Lactic acid	C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>	M-H	0.323	89.024	-3.02	BMDB00190	-1.58	1.33	
L-Serine	C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub>	M-H	0.254	104.035	-3.91	BMDB00187	-2.06	1.30	
LysoPC(18:1(9Z))	C <sub>26</sub> H <sub>52</sub> NO <sub>7</sub> P	M+H	11.05	522.354	-3.52	BMDB02815	1.29	1.16	
LysoPC(18:3(9Z,12Z,15Z))	C <sub>26</sub> H <sub>48</sub> NO <sub>7</sub> P	M+H	11.05	518.323	-2.40	BMDB10388	1.15	1.00	
LysoPE(0:0/18:0)	C <sub>23</sub> H <sub>48</sub> NO <sub>7</sub> P	M-H	11.38	480.309	-1.84	BMDB11129	1.26	1.03	
LysoPE(20:1(11Z)/0:0)	C <sub>25</sub> H <sub>50</sub> NO <sub>7</sub> P	M-H	11.41	506.325	-1.36	BMDB11512	1.40	1.08	
Maltotriose	C <sub>18</sub> H <sub>32</sub> O <sub>16</sub>	M-H	0.254	503.16	-4.11	BMDB01262	1.76	0.98	
Methyl propenyl ketone	C <sub>5</sub> H <sub>8</sub> O	M-H	15.35	83.050	-2.33	BMDB01184	-1.09	1.06	
Myristic acid	C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>	M-H	11.41	227.201	-1.98	BMDB00806	-1.05	1.06	
N-Acetylcystathionine	C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> O <sub>5</sub> S	M-H	0.254	263.071	2.35	BMDB02381	1.42	1.01	
Oleic acid	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>	M-H	11.41	281.248	-1.47	BMDB00207	1.37	1.35	
Palmitelaic acid	C <sub>16</sub> H <sub>30</sub> O <sub>2</sub>	M-H	9.584	253.217	-1.79	BMDB12328	1.32	0.99	
Palmitic acid	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>	M-H	13.09	255.232	-2.65	BMDB00220	-1.05	1.30	
Palmitoylethanolamide	C <sub>18</sub> H <sub>37</sub> NO <sub>2</sub>	M+H	9.652	300.29	0.92	BMDB02100	-1.04	0.85	
PC(14:0/22:1(13Z))	C <sub>44</sub> H <sub>86</sub> NO <sub>8</sub> P	M+H	16.71	788.615	-2.39	BMDB07887	1.44	0.69	
PC(14:0/22:5(4Z,7Z,10Z,13Z,16Z))	C <sub>44</sub> H <sub>78</sub> NO <sub>8</sub> P	M+H	14.59	780.555	1.20	BMDB07890	1.44	1.04	
PC(14:1(9Z)/22:2(13Z,16Z))	C <sub>44</sub> H <sub>82</sub> NO <sub>8</sub> P	M+H	15.11	784.586	0.67	BMDB07921	1.74	0.22	

PC(18:2(9Z,12Z)/20:4(5Z,8Z,11Z,14Z))	C <sub>46</sub> H <sub>80</sub> NO <sub>8</sub> P	M+H	15.10	806.567	-3.28	BMDB08147	1.55	0.25	
PC(18:3(6Z,9Z,12Z)/22:5(4Z,7Z,10Z,13Z,16Z))	C <sub>48</sub> H <sub>80</sub> NO <sub>8</sub> P	M+H	14.92	830.573	4.20	BMDB08187	1.46	0.38	
PC(20:2(11Z,14Z)/18:2(9Z,12Z))	C <sub>46</sub> H <sub>84</sub> NO <sub>8</sub> P	M+H	16.75	810.600	-0.49	BMDB08336	1.64	1.14	
PC(20:2(11Z,14Z)/18:2(9Z,12Z))	C <sub>46</sub> H <sub>84</sub> NO <sub>8</sub> P	M+H	17.82	810.604	3.62	BMDB08336	2.15	0.06	
PC(20:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C <sub>46</sub> H <sub>82</sub> NO <sub>8</sub> P	M+H	17.99	808.583	-2.27	BMDB08369	1.75	0.18	
PE(18:0/18:1(9Z))	C <sub>41</sub> H <sub>80</sub> NO <sub>8</sub> P	M-H	17.55	744.554	-1.59	BMDB08993	2.46	1.04	
PE(18:1(11Z)/20:4(5Z,8Z,11Z,14Z))	C <sub>43</sub> H <sub>78</sub> NO <sub>8</sub> P	M+H	14.99	766.538	-0.77	BMDB09036	1.61	0.15	
PE(18:1(9Z)/20:0)	C <sub>43</sub> H <sub>84</sub> NO <sub>8</sub> P	M-H	18.00	772.585	-1.07	BMDB09064	2.59	1.08	
PE(18:1(9Z)/20:3(8Z,11Z,14Z))	C <sub>43</sub> H <sub>78</sub> NO <sub>8</sub> P	M+H	17.92	768.556	2.86	BMDB09068	1.87	0.28	
PE(20:0/20:3(8Z,11Z,14Z))	C <sub>45</sub> H <sub>84</sub> NO <sub>8</sub> P	M-H	17.82	796.584	-3.02	BMDB09233	1.72	0.98	
PE(20:1(11Z)/18:3(9Z,12Z,15Z))	C <sub>43</sub> H <sub>78</sub> NO <sub>8</sub> P	M-H	17.63	766.542	3.39	BMDB09260	2.15	1.06	
PE(20:3(8Z,11Z,14Z)/18:0)	C <sub>43</sub> H <sub>80</sub> NO <sub>8</sub> P	M-H	17.37	768.556	1.15	BMDB09354	2.24	1.04	
PE(20:4(8Z,11Z,14Z,17Z)/16:0)	C <sub>41</sub> H <sub>78</sub> NO <sub>8</sub> P	M+H	14.44	740.52	-4.00	BMDB09418	1.41	0.29	
PE(22:4(7Z,10Z,13Z,16Z)/P-18:1(9Z))	C <sub>45</sub> H <sub>80</sub> NO <sub>7</sub> P	M+H	16.27	778.574	-0.06	BMDB09612	1.41	1.06	
PE(P-18:1(9Z)/16:1(9Z))	C <sub>39</sub> H <sub>76</sub> NO <sub>7</sub> P	M+H	16.09	700.527	-1.22	BMDB11438	1.10	1.01	
Pentacosanoic acid	C <sub>25</sub> H <sub>50</sub> O <sub>2</sub>	M-H	17.18	381.372	-4.07	BMDB02361	-1.05	0.57	
PG(18:1(11Z)/18:0)	C <sub>42</sub> H <sub>81</sub> O <sub>10</sub> P	M+H	14.56	777.563	-1.86	BMDB10617	1.12	1.30	
Pyruvaldehyde	C <sub>3</sub> H <sub>4</sub> O <sub>2</sub>	M-H	0.254	71.014	2.07	BMDB01167	2.22	1.21	
S-Adenosylhomocysteine	C <sub>14</sub> H <sub>20</sub> N <sub>6</sub> O <sub>5</sub> S	M-H	0.254	383.115	2.54	BMDB00939	1.46	1.10	
Stearic acid	C <sub>18</sub> H <sub>36</sub> O <sub>2</sub>	M-H	12.95	283.264	-2.45	BMDB00827	1.20	0.92	
<b>Liver</b>									
11-Oxo-androsterone glucuronide	C <sub>25</sub> H <sub>36</sub> O <sub>9</sub>	M+H	10.35	481.25	3.40	BMDB10338	-1.44	1.31	
1-Pyrroline-2-carboxylic acid	C <sub>5</sub> H <sub>7</sub> NO <sub>2</sub>	M+H	8.303	114.055	3.93	BMDB06875	1.91	0.99	
20-Hydroxy-PGF2a	C <sub>20</sub> H <sub>34</sub> O <sub>6</sub>	M-H	1.603	369.227	-2.49	BMDB04049	-1.72	1.16	
3 alpha,7 alpha,26-Trihydroxy-5beta-cholestane	C <sub>27</sub> H <sub>46</sub> O <sub>3</sub>	M-H	13.46	419.352	-3.37	BMDB12455	1.25	1.11	
3-O-Sulfogalactosylceramide (d18:1/24:0)	C <sub>48</sub> H <sub>93</sub> NO <sub>11</sub> S	M+H	1.911	892.654	2.88	BMDB00024	1.20	0.82	
4a-Carboxy-4b-methyl-5a-cholesta-8,24-dien-3b-ol	C <sub>29</sub> H <sub>46</sub> O <sub>3</sub>	M-H	2.602	441.337	1.20	BMDB01181	1.51	0.75	
4a-Methylzymosterol-4-carboxylic acid	C <sub>29</sub> H <sub>46</sub> O <sub>3</sub>	M-H	8.269	441.337	-1.19	BMDB06927	1.64	0.65	
APGPR Enterostatin	C <sub>21</sub> H <sub>36</sub> N <sub>8</sub> O <sub>6</sub>	M+H	10.20	497.284	0.01	BMDB06117	-1.25	0.95	
Arabinosylhypoxanthine	C <sub>10</sub> H <sub>13</sub> N <sub>4</sub> O <sub>5</sub>	M-H	11.96	267.073	0.32	BMDB03040	-2.08	1.04	
Caproic acid	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	M+H	1.502	117.091	1.60	BMDB00535	1.49	0.61	
Cortolone	C <sub>21</sub> H <sub>34</sub> O <sub>5</sub>	M-H	11.33	365.232	0.23	BMDB03128	-2.49	0.91	
CPA(18:1(11Z)/0:0)	C <sub>21</sub> H <sub>30</sub> O <sub>6</sub> P	M+H	12.11	419.255	-2.01	BMDB07005	-1.35	1.00	
CPA(18:1(9Z)/0:0)	C <sub>21</sub> H <sub>30</sub> O <sub>6</sub> P	M+H	14.31	419.256	-0.26	BMDB07006	-1.28	1.42	
Cysteinylglycine	C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> S	M+H	11.48	179.049	0.41	BMDB00078	-2.07	0.96	
DG(18:4(6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z)/0:0)	C <sub>39</sub> H <sub>66</sub> O <sub>5</sub>	M+H	4.244	609.448	-3.13	BMDB07338	-1.47	0.76	
DG(20:4(5Z,8Z,11Z,14Z)/18:1(9Z)/0:0)	C <sub>41</sub> H <sub>70</sub> O <sub>5</sub>	M+H	13.76	643.528	-2.88	BMDB07508	-2.48	0.78	
Glucosamine	C <sub>6</sub> H <sub>14</sub> NO <sub>6</sub> P	M+H	13.24	260.053	1.16	BMDB01514	-1.57	0.64	
Glutathione	C <sub>10</sub> H <sub>17</sub> N <sub>3</sub> O <sub>6</sub> S	M+H	12.84	308.091	0.04	BMDB00125	-2.07	1.22	
Glycerylphosphorylethanolamine	C <sub>5</sub> H <sub>14</sub> NO <sub>6</sub> P	M-H	8.086	214.048	-1.90	BMDB00114	1.13	0.79	
Guanosine	C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>5</sub>	M-H	7.586	282.083	-4.12	BMDB00133	-1.51	1.08	
Heptadecanoyl carnitine	C <sub>24</sub> H <sub>47</sub> NO <sub>4</sub>	M+H	1.911	414.357	-1.08	BMDB06210	1.58	1.05	
Homocysteine	C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> S	M+H	10.23	136.043	1.00	BMDB00742	1.42	1.14	
Hypoxanthine	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O	M-H	10.28	135.031	-0.68	BMDB00157	1.60	1.02	
Inosine	C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>5</sub>	M+H	1.322	269.089	-1.32	BMDB00195	-3.51	0.85	
Isocaproic acid	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	M+H	1.451	117.091	1.60	BMDB00689	1.32	0.68	
Lithocholic acid glycine conjugate	C <sub>26</sub> H <sub>43</sub> NO <sub>4</sub>	M-H	2.933	432.311	-0.57	BMDB00698	1.57	1.15	
Lithocholyltaurine	C <sub>26</sub> H <sub>45</sub> NO <sub>5</sub> S	M-H	11.01	482.295	-2.51	BMDB00722	2.18	1.20	
L-phenylalanyl-L-hydroxyproline	C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub>	M-H	7.057	277.119	-1.06	BMDB11176	1.72	1.42	
LysoPC(20:1(11Z))	C <sub>28</sub> H <sub>56</sub> NO <sub>7</sub> P	M+H	6.577	550.386	-2.63	BMDB10391	-1.55	1.05	
LysoPE(0:0/16:0)	C <sub>21</sub> H <sub>44</sub> NO <sub>7</sub> P	M+H	11.81	454.293	-0.37	BMDB11473	-1.25	0.87	
LysoPE(0:0/20:1(11Z))	C <sub>25</sub> H <sub>50</sub> NO <sub>7</sub> P	M-H	13.03	506.326	-0.47	BMDB11482	-1.22	1.18	
LysoPE(0:0/22:0)	C <sub>27</sub> H <sub>56</sub> NO <sub>7</sub> P	M+H	11.01	538.387	1.54	BMDB11490	-1.38	1.20	
LysoPE(22:1(13Z)/0:0)	C <sub>27</sub> H <sub>54</sub> NO <sub>7</sub> P	M+H	11.69	536.371	-2.64	BMDB11521	-1.29	1.13	
Methyl bisnorbiotinyl ketone	C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> S	M+H	13.28	215.085	-2.42	BMDB04822	1.32	1.03	
Oleamide	C <sub>18</sub> H <sub>35</sub> NO	M+H	11.96	282.279	-0.34	BMDB02117	1.27	0.81	
PA(20:4(5Z,8Z,11Z,14Z)e/2:0)	C <sub>25</sub> H <sub>43</sub> O <sub>7</sub> P	M-H	8.371	485.270	-2.49	BMDB11156	1.49	1.04	
PC(14:1(9Z)/18:3(6Z,9Z,12Z))	C <sub>40</sub> H <sub>72</sub> NO <sub>8</sub> P	M+H	11.20	726.510	-0.43	BMDB07908	1.51	0.95	
PC(15:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C <sub>45</sub> H <sub>78</sub> NO <sub>8</sub> P	M+H	12.29	792.555	-0.55	BMDB07958	1.42	0.94	
PC(16:0/18:3(9Z,12Z,15Z))	C <sub>42</sub> H <sub>78</sub> NO <sub>8</sub> P	M+H	15.54	756.552	0.90	BMDB07975	1.61	0.93	
PC(16:0/18:3(9Z,12Z,15Z))	C <sub>42</sub> H <sub>78</sub> NO <sub>8</sub> P	M+H	14.04	756.557	0.45	BMDB07975	1.54	0.89	
PC(16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C <sub>46</sub> H <sub>80</sub> NO <sub>8</sub> P	M+H	16.02	806.568	4.69	BMDB07991	1.54	0.98	
PC(18:0/15:0)	C <sub>41</sub> H <sub>82</sub> NO <sub>8</sub> P	M+H	15.07	748.584	4.66	BMDB08033	1.59	0.84	
PC(18:0/18:2(9Z,12Z))	C <sub>44</sub> H <sub>84</sub> NO <sub>8</sub> P	M+H	15.54	786.602	0.12	BMDB08039	1.88	1.26	
PC(18:1(11Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C <sub>44</sub> H <sub>82</sub> NO <sub>8</sub> P	M+H	17.23	832.584	1.71	BMDB08090	1.89	1.20	

PC(18:2(9Z,12Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C <sub>48</sub> H <sub>80</sub> NO <sub>8</sub> P	M+H	17.88	830.569	1.83	BMDB08156	1.75	0.82	
PC(18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C <sub>44</sub> H <sub>74</sub> NO <sub>8</sub> P	M+H	16.97	776.524	-2.67	BMDB08174	-1.59	0.98	
PC(18:3(9Z,12Z,15Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C <sub>48</sub> H <sub>78</sub> NO <sub>8</sub> P	M+H	14.88	828.552	-1.63	BMDB08222	-1.55	0.81	
PC(20:4(8Z,11Z,14Z,17Z)/16:0)	C <sub>44</sub> H <sub>80</sub> NO <sub>8</sub> P	M+H	17.05	782.570	0.39	BMDB08462	1.61	0.81	
PC(22:4(7Z,10Z,13Z,16Z)/16:0)	C <sub>46</sub> H <sub>84</sub> NO <sub>8</sub> P	M+H	14.04	810.602	0.74	BMDB08626	-1.64	0.91	
PC(22:5(7Z,10Z,13Z,16Z,19Z)/16:0)	C <sub>46</sub> H <sub>82</sub> NO <sub>8</sub> P	M+H	14.34	808.583	-1.64	BMDB08692	1.33	0.87	
PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/16:0)	C <sub>46</sub> H <sub>80</sub> NO <sub>8</sub> P	M+H	17.70	806.570	0.55	BMDB08725	-1.63	0.99	
PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/16:1(9Z))	C <sub>46</sub> H <sub>78</sub> NO <sub>8</sub> P	M+H	14.04	804.553	0.70	BMDB08726	1.80	1.09	
PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C <sub>48</sub> H <sub>80</sub> NO <sub>8</sub> P	M+H	14.04	830.568	0.82	BMDB08730	1.59	1.09	
PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:2(11Z,14Z))	C <sub>50</sub> H <sub>84</sub> NO <sub>8</sub> P	M+H	14.31	858.598	0.99	BMDB08736	1.70	1.07	
PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:3(5Z,8Z,11Z))	C <sub>50</sub> H <sub>82</sub> NO <sub>8</sub> P	M+H	15.66	856.584	0.46	BMDB08737	1.66	0.87	
PC(P-16:0/15:0)	C <sub>39</sub> H <sub>78</sub> NO <sub>7</sub> P	M+H	14.04	704.559	-0.95	BMDB11205	-1.47	0.98	
PE(16:0/18:1(9Z))	C <sub>39</sub> H <sub>76</sub> NO <sub>8</sub> P	M+H	17.34	718.541	-0.64	BMDB08927	-1.56	1.04	
PE(16:1(9Z)/20:0)	C <sub>41</sub> H <sub>80</sub> NO <sub>8</sub> P	M+H	15.29	746.571	-1.41	BMDB08965	-1.86	0.98	
PE(18:0/16:0)	C <sub>39</sub> H <sub>78</sub> NO <sub>8</sub> P	M+H	16.90	720.555	-1.01	BMDB08989	-1.68	0.86	
PE(18:0/20:3(5Z,8Z,11Z))	C <sub>43</sub> H <sub>80</sub> NO <sub>8</sub> P	M+H	15.04	770.570	1.45	BMDB09001	-1.52	0.88	
PE(18:0/P-18:1(11Z))	C <sub>41</sub> H <sub>80</sub> NO <sub>7</sub> P	M+H	14.44	730.573	1.28	BMDB09017	-1.50	1.18	
PE(18:2(9Z,12Z)/18:0))	C <sub>41</sub> H <sub>78</sub> NO <sub>8</sub> P	M+H	14.04	744.557	1.31	BMDB09090	1.96	1.12	
PE(18:4(6Z,9Z,12Z,15Z)/P-18:0)	C <sub>41</sub> H <sub>74</sub> NO <sub>7</sub> P	M+H	15.84	724.528	-2.93	BMDB09214	-1.82	0.74	
PE(20:0/15:0)	C <sub>40</sub> H <sub>80</sub> NO <sub>8</sub> P	M+H	10.35	734.571	3.65	BMDB09219	-1.45	1.06	
PE(20:0/20:4(8Z,11Z,14Z,17Z))	C <sub>45</sub> H <sub>82</sub> NO <sub>8</sub> P	M+H	15.11	796.585	-1.58	BMDB09235	-1.77	0.88	
PE(20:2(11Z,14Z)/P-18:0)	C <sub>43</sub> H <sub>82</sub> NO <sub>7</sub> P	M+H	16.02	756.587	-0.57	BMDB09313	-1.53	0.90	
PE(20:3(8Z,11Z,14Z)/20:0)	C <sub>45</sub> H <sub>84</sub> NO <sub>8</sub> P	M+H	15.29	798.601	-2.51	BMDB09361	-1.45	1.04	
PE(20:4(5Z,8Z,11Z,14Z)/18:0)	C <sub>43</sub> H <sub>78</sub> NO <sub>8</sub> P	M+H	17.15	768.556	-1.06	BMDB09387	-2.61	0.92	
PE(20:5(5Z,8Z,11Z,14Z,17Z)/20:5(5Z,8Z,11Z,14Z,17Z))	C <sub>45</sub> H <sub>70</sub> NO <sub>8</sub> P	M-H	17.37	782.474	-2.63	BMDB09467	-1.26	1.07	
PE(22:1(13Z)/20:5(5Z,8Z,11Z,14Z,17Z))	C <sub>47</sub> H <sub>82</sub> NO <sub>8</sub> P	M+H	17.92	820.584	-0.37	BMDB09533	-1.61	1.10	
PE(22:4(7Z,10Z,13Z,16Z)/22:5(4Z,7Z,10Z,13Z,16Z))	C <sub>49</sub> H <sub>80</sub> NO <sub>8</sub> P	M+H	15.80	842.569	-0.47	BMDB09603	-1.26	0.84	
PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:2(11Z,14Z))	C <sub>47</sub> H <sub>78</sub> NO <sub>8</sub> P	M+H	17.37	816.553	1.54	BMDB09693	-1.77	1.34	
PE(P-16:0e/0:0)	C <sub>21</sub> H <sub>44</sub> NO <sub>6</sub> P	M+H	13.43	438.296	-2.64	BMDB11152	-1.35	0.97	
PE(P-18:0/20:3(5Z,8Z,11Z))	C <sub>43</sub> H <sub>80</sub> NO <sub>7</sub> P	M+H	10.46	754.572	-2.42	BMDB11383	-1.40	0.86	
PE(P-18:0/22:4(7Z,10Z,13Z,16Z))	C <sub>45</sub> H <sub>82</sub> NO <sub>7</sub> P	M+H	11.56	780.587	-0.34	BMDB11391	-1.40	1.08	
PE(P-18:1(11Z)/14:0)	C <sub>37</sub> H <sub>72</sub> NO <sub>7</sub> P	M+H	15.32	674.513	-2.49	BMDB11401	-1.71	0.95	
PE(P-18:1(9Z)/14:1(9Z))	C <sub>37</sub> H <sub>70</sub> NO <sub>7</sub> P	M+H	15.95	672.497	-0.43	BMDB11435	2.25	0.76	
PE(P-18:1(9Z)/22:4(7Z,10Z,13Z,16Z))	C <sub>45</sub> H <sub>80</sub> NO <sub>7</sub> P	M+H	15.04	778.575	-0.55	BMDB11457	-1.40	0.64	
PE-NMMe(16:0/16:0)	C <sub>38</sub> H <sub>76</sub> NO <sub>8</sub> P	M+H	17.82	706.541	0.90	BMDB10567	-2.56	0.65	
Pristanal	C <sub>19</sub> H <sub>38</sub> O	M-H	14.19	281.284	0.45	BMDB01958	1.69	1.24	
PS(14:0/14:0)	C <sub>34</sub> H <sub>66</sub> NO <sub>10</sub> P	M+H	11.96	680.449	4.69	BMDB12330	-1.51	1.49	
PS(14:1(9Z)/14:0)	C <sub>34</sub> H <sub>64</sub> NO <sub>10</sub> P	M+H	11.48	678.434	4.66	BMDB12341	-1.26	1.21	
PS(18:0/22:5(7Z,10Z,13Z,16Z,19Z))	C <sub>46</sub> H <sub>80</sub> NO <sub>10</sub> P	M+H	11.93	838.558	0.12	BMDB10166	-1.40	1.02	
PS(18:3(9Z,12Z,15Z)/18:1(9Z))	C <sub>42</sub> H <sub>74</sub> NO <sub>10</sub> P	M+H	11.08	784.509	-0.25	BMDB12412	-1.63	0.88	
Saccharopine	C <sub>11</sub> H <sub>20</sub> N <sub>2</sub> O <sub>6</sub>	M+H	17.70	277.141	-2.30	BMDB00279	1.17	1.17	
SM(d18:0/18:1(11Z))	C <sub>41</sub> H <sub>83</sub> N <sub>2</sub> O <sub>6</sub> P	M+H	14.92	731.604	-0.26	BMDB12088	-1.48	0.75	
Taurine	C <sub>2</sub> H <sub>7</sub> NO <sub>2</sub> S	M+H	6.988	126.022	0.29	BMDB00251	2.36	0.97	
Taurocholic acid	C <sub>26</sub> H <sub>45</sub> NO <sub>7</sub> S	M-H	15.84	514.284	0.86	BMDB00036	1.65	0.72	
Taurodeoxycholic acid	C <sub>26</sub> H <sub>45</sub> NO <sub>6</sub> S	M-H	9.069	498.290	-0.77	BMDB00896	1.93	1.05	
Tauroursodeoxycholic acid	C <sub>26</sub> H <sub>45</sub> NO <sub>6</sub> S	M+H	3.032	500.304	-0.25	BMDB00874	2.22	1.04	
Thymidine	C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>5</sub>	M+H	6.623	243.098	3.21	BMDB00273	1.41	1.12	
<b>Duodenum</b>									
2-Arachidonylglycerol	C <sub>23</sub> H <sub>38</sub> O <sub>4</sub>	M-H	6.291	377.268	-3.53	BMDB04666	-3.5	1.34	
3,7-Dihydroxy-12-oxocholanoic acid	C <sub>24</sub> H <sub>38</sub> O <sub>5</sub>	M-H	4.861	405.264	-0.93	BMDB00400	-1.65	0.76	
3a,6b,7a,12a-Tetrahydroxy-5b-cholanoic acid	C <sub>24</sub> H <sub>40</sub> O <sub>6</sub>	M-H	5.342	423.274	-2.48	BMDB00399	-2.47	0.63	
3a,7b,12a-Trihydroxyoxocholanyl-Glycine	C <sub>26</sub> H <sub>43</sub> NO <sub>6</sub>	M+H	8.341	466.317	-0.86	BMDB00331	-3.52	0.94	
3-Methylcrotonylglycine	C <sub>7</sub> H <sub>11</sub> NO <sub>3</sub>	M+H	9.042	158.081	-3.80	BMDB00459	-2.34	0.76	
3-O-Sulfogalactosylceramide (d18:1/16:0)	C <sub>40</sub> H <sub>77</sub> NO <sub>11</sub> S	M+H	16.72	780.529	0.10	BMDB12313	-2.69	1.23	
3-Oxo-4,6-choladienoic acid	C <sub>24</sub> H <sub>34</sub> O <sub>3</sub>	M-H	4.864	369.243	-2.50	BMDB00476	-2.05	1.44	
3-Oxohexadecanoic acid	C <sub>16</sub> H <sub>30</sub> O <sub>3</sub>	M+H	9.254	271.227	2.07	BMDB10733	1.31	0.57	
3-Sulfodeoxycholic acid	C <sub>23</sub> H <sub>38</sub> O <sub>7</sub> S	M-H	7.461	457.227	1.47	BMDB02504	-2.32	0.97	
4a-Methylzosterol-4-carboxylic acid	C <sub>29</sub> H <sub>46</sub> O <sub>3</sub>	M-H	8.379	441.336	-3.71	BMDB06927	-3.12	1.03	
4-Hydroxydebrisoquine	C <sub>10</sub> H <sub>13</sub> N <sub>3</sub> O	M-H	4.225	190.099	2.45	BMDB06468	1.19	1.10	
5,6-trans-25-Hydroxyvitamin D3	C <sub>27</sub> H <sub>44</sub> O <sub>2</sub>	M+H	13.86	401.341	0.01	BMDB06721	-1.34	0.73	
5b-Cyprinol sulfate	C <sub>27</sub> H <sub>48</sub> O <sub>3</sub> S	M-H	7.274	531.298	-3.55	BMDB06888	-2.04	0.95	
Adrenic acid	C <sub>22</sub> H <sub>36</sub> O <sub>2</sub>	M+H	13.31	333.28	4.67	BMDB02226	-1.41	0.98	
Aerobactin	C <sub>22</sub> H <sub>36</sub> N <sub>4</sub> O <sub>13</sub>	M-H	5.561	563.221	0.43	BMDB04051	-1.80	0.89	
Alpha-Linolenic acid	C <sub>18</sub> H <sub>30</sub> O <sub>2</sub>	M-H	11.61	277.217	-2.09	BMDB01388	-1.08	1.02	

Biliverdin	C <sub>30</sub> H <sub>54</sub> NO <sub>7</sub> P	M+H	9.551	583.255	0.31	BMDB01008	-1.74	0.95
Boldione	C <sub>19</sub> H <sub>24</sub> O <sub>2</sub>	M+H	7.914	285.186	3.23	BMDB03422	-1.53	0.83
Bovinic acid	C <sub>18</sub> H <sub>32</sub> O <sub>2</sub>	M-H	10.38	279.233	-1.43	BMDB03797	1.25	1.21
Chenodeoxyglycocholic acid	C <sub>26</sub> H <sub>43</sub> NO <sub>5</sub>	M+H	3.291	450.321	-1.63	BMDB06898	-2.53	1.01
Cholestane-3,7,12,25-tetrol-3-glucuronide	C <sub>33</sub> H <sub>56</sub> O <sub>10</sub>	M-H	9.325	611.378	-2.89	BMDB10355	-2.49	0.70
Cholesterol sulfate	C <sub>27</sub> H <sub>46</sub> O <sub>4</sub> S	M-H	1.514	465.302	-4.6	BMDB00653	1.85	1.29
Cortisol	C <sub>21</sub> H <sub>30</sub> O <sub>5</sub>	M+H	8.325	363.215	-3.04	BMDB00063	1.23	0.66
Cystathionine sulfoxide	C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> S	M-H	5.854	237.054	-4.01	BMDB02399	1.29	0.80
D-Alanine	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	M-H	6.187	88.04	-1.24	BMDB01310	-1.86	0.74
DG(22:5(7Z,10Z,13Z,16Z,19Z)/20:3(5Z,8Z,11Z)/0:0)	C <sub>45</sub> H <sub>72</sub> O <sub>5</sub>	M+H	13.53	693.543	-3.68	BMDB07748	1.27	1.35
Elaidic carnitine	C <sub>25</sub> H <sub>47</sub> NO <sub>4</sub>	M+H	10.22	426.358	0.31	BMDB06464	-1.91	1.25
Ercalcitriol	C <sub>28</sub> H <sub>44</sub> O <sub>3</sub>	M-H	13.43	427.32	-3.34	BMDB06225	1.26	1.20
Estrone	C <sub>18</sub> H <sub>22</sub> O <sub>2</sub>	M+H	7.996	271.17	1.62	BMDB00145	-1.69	0.75
Gamma-glutamyl-L-putrescine	C <sub>9</sub> H <sub>19</sub> N <sub>3</sub> O <sub>3</sub>	M+H	0.689	218.151	4.18	BMDB12230	-1.49	1.05
Glycine	C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>	M-H	5.566	74.025	-1.42	BMDB00123	-2.21	0.95
Glycocholic acid	C <sub>26</sub> H <sub>43</sub> NO <sub>6</sub>	M-H	4.144	464.3	-4.73	BMDB00138	-2.73	0.95
Glycoursodeoxycholic acid	C <sub>26</sub> H <sub>43</sub> NO <sub>5</sub>	M-H	7.462	448.306	-0.64	BMDB00708	-2.34	1.07
L-Alanine	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	M-H	8.044	88.04	-2.91	BMDB00161	-1.74	0.85
Lithocholic acid glycine conjugate	C <sub>26</sub> H <sub>43</sub> NO <sub>4</sub>	M-H	8.824	432.311	-3.19	BMDB00698	-2.04	1.04
Lithocholyltaurine	C <sub>26</sub> H <sub>45</sub> NO <sub>5</sub> S	M-H	7.578	482.292	-4.9	BMDB00722	-1.72	0.93
LPA(P-16:0e/0:0)	C <sub>19</sub> H <sub>39</sub> O <sub>6</sub> P	M+H	8.154	395.256	-0.05	BMDB11154	-1.75	0.72
L-Palmitoylcarnitine	C <sub>23</sub> H <sub>45</sub> NO <sub>4</sub>	M+H	9.984	400.342	-0.65	BMDB00222	-1.47	1.25
L-Urobilinogen	C <sub>15</sub> H <sub>24</sub> N <sub>2</sub> O <sub>17</sub> P <sub>2</sub>	M-H	7.751	595.348	3.19	BMDB04157	-2.75	0.69
LysoPC(14:0)	C <sub>22</sub> H <sub>46</sub> NO <sub>7</sub> P	M+H	10.14	468.308	-0.09	BMDB10379	-1.39	1.12
LysoPC(16:0)	C <sub>24</sub> H <sub>50</sub> NO <sub>7</sub> P	M+H	4.023	496.34	-0.43	BMDB10382	-1.57	0.79
LysoPC(18:1(9Z))	C <sub>26</sub> H <sub>52</sub> NO <sub>7</sub> P	M+H	3.959	522.356	0.79	BMDB02815	-1.78	0.78
LysoPC(18:3(6Z,9Z,12Z))	C <sub>26</sub> H <sub>48</sub> NO <sub>7</sub> P	M-H	9.556	516.307	-4.56	BMDB10387	-2.18	1.08
LysoPC(20:2(11Z,14Z))	C <sub>28</sub> H <sub>54</sub> NO <sub>7</sub> P	M+H	11.74	548.372	0.89	BMDB10392	-1.31	1.11
LysoPC(20:4(8Z,11Z,14Z,17Z))	C <sub>28</sub> H <sub>50</sub> NO <sub>7</sub> P	M+H	3.965	544.338	-2.65	BMDB10396	-1.88	1.00
LysoPC(22:4(7Z,10Z,13Z,16Z))	C <sub>30</sub> H <sub>54</sub> NO <sub>7</sub> P	M+H	11.52	572.371	-4.21	BMDB10401	-1.27	1.01
LysoPC(O-18:0)	C <sub>26</sub> H <sub>56</sub> NO <sub>6</sub> P	M+H	13.39	510.392	0.48	BMDB11149	-1.43	0.55
LysoPC(P-16:0)	C <sub>24</sub> H <sub>50</sub> NO <sub>6</sub> P	M+H	3.876	480.345	0.02	BMDB10407	-2.62	0.98
LysoPE(0:0/16:0)	C <sub>21</sub> H <sub>44</sub> NO <sub>7</sub> P	M+H	9.228	454.291	-1.41	BMDB11473	-2.42	1.13
LysoPE(0:0/18:3(6Z,9Z,12Z))	C <sub>23</sub> H <sub>42</sub> NO <sub>7</sub> P	M+H	9.221	476.276	-1.59	BMDB11478	-1.68	1.22
LysoPE(0:0/20:1(11Z))	C <sub>25</sub> H <sub>50</sub> NO <sub>7</sub> P	M-H	4.263	506.323	-1.36	BMDB11482	-3.81	1.11
LysoPE(0:0/20:2(11Z,14Z))	C <sub>25</sub> H <sub>48</sub> NO <sub>7</sub> P	M-H	10.32	504.309	-1.85	BMDB11483	1.25	0.70
LysoPE(0:0/22:4(7Z,10Z,13Z,16Z))	C <sub>26</sub> H <sub>43</sub> NO <sub>8</sub> S	M-H	11.81	528.307	3.72	BMDB11493	-1.19	0.79
LysoPE(16:0/0:0)	C <sub>21</sub> H <sub>44</sub> NO <sub>7</sub> P	M+H	3.523	454.292	-1.41	BMDB11503	-2.52	0.85
LysoPE(18:1(11Z)/0:0)	C <sub>23</sub> H <sub>46</sub> NO <sub>7</sub> P	M+H	3.482	480.308	-0.58	BMDB11505	-2.34	0.99
LysoPE(18:2(9Z,12Z)/0:0)	C <sub>23</sub> H <sub>44</sub> NO <sub>7</sub> P	M-H	10.42	476.277	-3.26	BMDB11507	1.26	1.23
LysoPE(18:4(6Z,9Z,12Z,15Z)/0:0)	C <sub>23</sub> H <sub>40</sub> NO <sub>7</sub> P	M+H	8.348	474.26	-2.81	BMDB11510	-1.62	1.08
LysoPE(22:4(7Z,10Z,13Z,16Z)/0:0)	C <sub>27</sub> H <sub>48</sub> NO <sub>8</sub> P	M-H	7.465	528.309	-1.91	BMDB11523	-2.55	1.11
Metanephrine	C <sub>10</sub> H <sub>15</sub> NO <sub>3</sub>	M+H	8.341	198.113	2.27	BMDB04063	-2.24	0.79
MG(20:4(5Z,8Z,11Z,14Z)/0:0/0:0)	C <sub>23</sub> H <sub>38</sub> O <sub>4</sub>	M-H	7.724	377.268	-4.15	BMDB11578	-2.61	0.90
N-[(3a,5b,7a)-3-hydroxy-24-oxo-7-(sulfooxy)cholan-24-yl]-Glycine	C <sub>26</sub> H <sub>43</sub> NO <sub>8</sub> S	M-H	5.561	528.266	3.72	BMDB02496	-1.93	0.90
Oleamide	C <sub>18</sub> H <sub>35</sub> NO	M+H	9.555	282.28	1.96	BMDB02117	-1.33	1.22
PC(15:0/20:2(11Z,14Z))	C <sub>43</sub> H <sub>82</sub> NO <sub>8</sub> P	M+H	15.07	772.582	-3.56	BMDB07946	2.11	1.16
PC(16:0/18:4(6Z,9Z,12Z,15Z))	C <sub>42</sub> H <sub>76</sub> NO <sub>8</sub> P	M+H	17.08	754.541	4.16	BMDB07976	1.33	0.92
PC(18:1(9Z)e/2:0)	C <sub>28</sub> H <sub>56</sub> NO <sub>7</sub> P	M+H	12.88	550.387	0.22	BMDB11148	-1.31	1.21
PC(22:5(7Z,10Z,13Z,16Z,19Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C <sub>52</sub> H <sub>82</sub> NO <sub>8</sub> P	M-H	7.064	878.573	3.17	BMDB08715	2.52	1.02
PE(16:0/15:0)	C <sub>36</sub> H <sub>72</sub> NO <sub>8</sub> P	M+H	16.39	678.508	1.2	BMDB08922	-1.51	0.82
PE(18:0/18:3(6Z,9Z,12Z))	C <sub>41</sub> H <sub>76</sub> NO <sub>8</sub> P	M-H	3.151	740.523	-0.39	BMDB08995	2.17	0.73
PE(22:2(13Z,16Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C <sub>49</sub> H <sub>82</sub> NO <sub>8</sub> P	M+H	16.79	844.583	-2.71	BMDB09573	-1.65	1.58
PE(O-18:1(1Z)/20:4(5Z,8Z,11Z,14Z))	C <sub>43</sub> H <sub>78</sub> NO <sub>7</sub> P	M-H	2.991	750.545	1.27	BMDB05779	1.59	1.13
PE(P-16:0/20:4(5Z,8Z,11Z,14Z))	C <sub>41</sub> H <sub>74</sub> NO <sub>7</sub> P	M-H	3.024	722.513	2.5	BMDB11352	1.42	1.12
PE(P-16:0e/0:0)	C <sub>21</sub> H <sub>44</sub> NO <sub>6</sub> P	M+H	11.63	438.297	-2.05	BMDB11152	-1.33	0.90
PE(P-16:0e/0:0)	C <sub>21</sub> H <sub>44</sub> NO <sub>6</sub> P	M+H	3.385	438.297	-2.05	BMDB11152	3.05	0.66
Prostaglandin F2a	C <sub>20</sub> H <sub>34</sub> O <sub>5</sub>	M+H	8.375	355.246	-4.52	BMDB01139	1.23	0.95
PS(14:0/20:3(8Z,11Z,14Z))	C <sub>40</sub> H <sub>72</sub> NO <sub>10</sub> P	M+H	14.85	758.495	-2.27	BMDB12338	-1.30	0.82
PS(18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C <sub>46</sub> H <sub>78</sub> NO <sub>10</sub> P	M+H	15.59	836.547	4.28	BMDB10167	-1.31	0.80
Safrole	C <sub>10</sub> H <sub>10</sub> O <sub>2</sub>	M+H	7.314	163.076	3.9	BMDB02333	1.31	1.38
Stearidonyl carnitine	C <sub>25</sub> H <sub>41</sub> NO <sub>4</sub>	M-H	3.731	418.295	-2.23	BMDB06463	-2.63	0.81
Sulfolithocholylglycine	C <sub>26</sub> H <sub>43</sub> NO <sub>7</sub> S	M-H	1.723	512.267	-3.46	BMDB02639	-2.22	0.82
Taurallocholic acid	C <sub>26</sub> H <sub>45</sub> NO <sub>7</sub> S	M+H	1.731	516.389	1.35	BMDB00922	-1.49	0.81

Taurocholic acid	C <sub>26</sub> H <sub>45</sub> NO <sub>7</sub> S	M-H	5.446	514.284	-2.78	BMDB00036	-1.70	1.20
Taurodeoxycholic acid	C <sub>26</sub> H <sub>45</sub> NO <sub>6</sub> S	M-H	5.045	498.288	-3.25	BMDB00896	-2.35	0.93
Tauroursodeoxycholic acid	C <sub>26</sub> H <sub>45</sub> NO <sub>6</sub> S	M+H	1.147	500.304	-0.3	BMDB00874	-1.63	0.83
Tetracosatetraenoic acid (24:4n-6)	C <sub>24</sub> H <sub>40</sub> O <sub>2</sub>	M-H	13.31	359.294	-4.79	BMDB06246	-1.52	1.00
Tiglylglycine	C <sub>7</sub> H <sub>11</sub> NO <sub>3</sub>	M+H	9.229	158.082	4.11	BMDB00959	-2.75	1.11
trans-Hexadec-2-enoyl carnitine	C <sub>23</sub> H <sub>43</sub> NO <sub>4</sub>	M+H	9.472	398.326	-0.52	BMDB06317	-1.86	0.96
Trihexosylceramide (d18:1/16:0)	C <sub>52</sub> H <sub>97</sub> NO <sub>18</sub>	M+H	17.12	1024.677	-1.23	BMDB04879	-2.55	1.01

<sup>1</sup> UPLC-qTOF metabolites identified (p<0.05), RT, retention time; ID, identification matched from bovine metabolome database matched, fold changes comparing high-ADG vs low-ADG steers; VIP= value of importance in projection produced by PLS-DA model and represent the weighted sum of squares of the PLS loading, which takes into account the amount of orthogonal variance explained by each component

**Table S2. Results from tissues pathway analysis**

Metabolic pathways <sup>1</sup>	Total Cmpd	Hits	Raw p	Impact
<b><i>Longissimus Dorsi</i></b>				
Histidine metabolism	67	1	0.00056	0
Biosynthesis of unsaturated fatty acids	42	3	0.005328	0
Pyruvate metabolism	22	3	0.007179	0.0544
Glycine, serine and threonine metabolism	32	2	0.010189	0
Glycerophospholipid metabolism	29	5	0.013181	0.35911
Creatinine metabolism	23	1	0.020715	0.03789
Galactose metabolism	26	1	0.020715	0.03644
Citrate cycle (TCA cycle)	20	1	0.027124	0.0452
Glyoxylate and dicarboxylate metabolism	16	1	0.027124	0
Taurine and hypotaurine metabolism	7	1	0.034825	0.75
Glycolysis or Gluconeogenesis	46	1	0.034825	0.02976
alpha-Linolenic acid metabolism	9	2	0.044405	1
Alanine, aspartate and glutamate metabolism	23	1	0.051217	0
Selenoamino acid metabolism	15	1	0.051217	0
Synthesis and degradation of ketone bodies	5	1	0.051446	0.6
Butanoate metabolism	20	1	0.051446	0.10145
Valine, leucine and isoleucine degradation	38	1	0.051446	0
Tyrosine metabolism	42	1	0.051446	0
Cysteine and methionine metabolism	28	1	0.055565	0
Arginine and proline metabolism	44	1	0.058386	0.01109
Pyrimidine metabolism	37	1	0.061538	0.06985
Glycerolipid metabolism	18	1	0.065352	0.0256
Purine metabolism	68	1	0.06725	0.00768
Glycosylphosphatidylinositol(GPI)-anchor biosynthesis	14	1	0.079359	0.02488
Aminoacyl-tRNA biosynthesis	64	2	0.0832	0
Sphingolipid metabolism	21	1	0.17111	0
Arachidonic acid metabolism	36	1	0.21632	0
Linoleic acid metabolism	5	1	0.21632	0
Nitrogen metabolism	9	1	0.28504	0
<b>Liver</b>				
Glycerophospholipid metabolism	29	5	0.002365	0.33944
Arachidonic acid metabolism	36	1	0.002717	0
Linoleic acid metabolism	5	1	0.002717	0
alpha-Linolenic acid metabolism	9	1	0.002717	0
Cholic acid biosynthesis	15	1	0.007022	0.25



Cysteine and methionine metabolism	23	1	0.007022	0.03789
Purine metabolism	68	4	0.010556	0.01664
Primary bile acid biosynthesis	46	3	0.026393	0.23
Pyrimidine metabolism	37	1	0.027193	0
Glutathione metabolism	26	2	0.031182	0.36832
Arginine and proline metabolism	44	1	0.05618	0
Glycosylphosphatidylinositol(GPI)- anchor biosynthesis	14	1	0.058623	0.02488
Taurine and hypotaurine metabolism	7	2	0.089151	0.75
Sphingolipid metabolism	21	2	0.10087	0
Riboflavin metabolism	11	1	0.1012	0
Steroid biosynthesis	35	1	0.15949	0.07469
Glycolysis or Gluconeogenesis	26	1	0.23447	0.0958
Glycine, serine and threonine metabolism	32	1	0.23447	0.03163
Glycerolipid metabolism	18	1	0.23447	0
Glyoxylate and dicarboxylate metabolism	16	1	0.23447	0
<b>Duodenum</b>				
ether lipids metabolism	21	1	0.0008	0
Histidine metabolism	67	3	0.007177	0.0871
Glycerophospholipid metabolism	29	4	0.017645	0.31502
alpha-Linolenic acid metabolism	9	2	0.032784	1
Gluconeogenesis metabolism	14	1	0.036167	0.02488
Biosynthesis of unsaturated fatty acids	42	2	0.037387	0
Steroid biosynthesis	35	1	0.041324	0.07469
Fatty acid metabolism	39	1	0.043509	0
Glycine, serine and threonine metabolism	32	1	0.050393	0.29197
Glutathione metabolism	26	1	0.050393	0.00573
Cyanoamino acid metabolism	6	1	0.050393	0
Methane metabolism	9	1	0.050393	0
Nitrogen metabolism	9	1	0.050393	0
Porphyrin and chlorophyll metabolism	25	2	0.05111	0.05837
Primary bile acid biosynthesis	46	3	0.05713	0.08928
Aminoacyl-tRNA biosynthesis	64	2	0.058699	0
Pentose and glucuronate interconversions	13	3	0.063943	0.35715
Arachidonic acid metabolism	36	2	0.064848	0
Linoleic acid metabolism	5	1	0.083446	0
Alanine, aspartate and glutamate metabolism	23	1	0.089686	0
Selenoamino acid metabolism	15	1	0.089686	0
Taurine and hypotaurine metabolism	7	1	0.10956	0
Tyrosine metabolism	42	1	0.11846	0.00153

**Adipose**

Biosynthesis of unsaturated fatty acids	42	5	0.000634	0
alpha-Linolenic acid metabolism	9	2	0.002538	1
Glycerophospholipid metabolism	29	3	0.006921	0.28789
Pyruvate metabolism	22	2	0.007561	0.0544
Glycolysis or Gluconeogenesis	26	1	0.009202	0
Glycine, serine and threonine metabolism	32	2	0.011966	0
Cysteine and methionine metabolism	28	2	0.012761	0.05468
Arachidonic acid metabolism	36	1	0.031448	0
Linoleic acid metabolism	5	1	0.031448	0
Fatty acid elongation in mitochondria	27	1	0.035701	0
Fatty acid metabolism	39	1	0.035701	0
Glycosylphosphatidylinositol(GPI)-anchor biosynthesis	14	1	0.047624	0.02488

---

<sup>1</sup>Total Cmpd = Total is the total number of compounds in the pathway; Hits is the actually matched number from the user uploaded data; *P* is the original *P*-value calculated from the enrichment analysis; Impact is the pathway impact value calculated from pathway topology analysis