

**Supplementary Table S1. Altered metabolites between PCa vs BPH and PCa vs Met comparisons.**

PCa VS BPH															PCa VS Met		
Compound	Formula	Mass	RT (min)	Error (ppm)	Adduct	<sup>a</sup> CV for QC (%)	Analytical platform	<sup>b</sup> ID level	<sup>c</sup> Fold Change	<sup>d</sup> p value <sup>1</sup>	<sup>e</sup> VIP	<sup>b</sup> Fold Change	<sup>d</sup> p value <sup>1</sup>	<sup>e</sup> VIP			
Amino acids and analogues																	
Hydroxyproline	C <sub>5</sub> H <sub>9</sub> NO <sub>3</sub>	131.0583	0.75	4	[M+H] <sup>+</sup>	2.11	GM-LC-QTOF-MS	2	1.07	5.38E-02 <sup>1</sup>	1.71	1.10	6.09E-03 <sup>1</sup>	2.58			
Methylene-glutamate	C <sub>6</sub> H <sub>9</sub> NO <sub>4</sub>	159.0533	0.75	4	[M+H] <sup>+</sup>	2.28	GM-LC-QTOF-MS	2	1.06		1.60	1.10	1.02E-02 <sup>1</sup>	2.58			
Proline betaine	C <sub>7</sub> H <sub>13</sub> NO <sub>2</sub>	125.0840	1.83	3	[M+H-H <sub>2</sub> O] <sup>+</sup>	8.65	GM-LC-QTOF-MS	4	--	--	--	0.49	--	1.66			
Cysteine	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> S	121.197	13.62	-	-	12.96	GC-QTOF-MS	1	--	--	--	1.28	--	1.62			
Valine	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub>	117.1463	9.11	-	-	3.43	GC-QTOF-MS	1	--	--	--	1.25	3.23E-02 <sup>1</sup>	--			
Cys Thr Glu	C <sub>12</sub> H <sub>21</sub> N <sub>3</sub> O <sub>7</sub> S	373.093	3.43	4	[M+Na] <sup>+</sup>	6.97	GL-LC-QTOF-MS	4	0.32	8.60E-06	1.81	--	--	--			
Glutamyl-pipecolic acid	C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub>	296.0755	5.74	6	[M+K] <sup>+</sup>	4.24	GL-LC-QTOF-MS	3	0.39	1.87E-05	1.75	--	--	--			
Glutamyl-hydroxyproline	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>6</sub>	298.0546	4.98	6	[M+K] <sup>+</sup>	4.18	GL-LC-QTOF-MS	4	0.28	6.62E-06	1.56	--	--	--			
Methylene-glutamate/Methyl-oxoglutaramic acid/Methylnicotinamide	C <sub>6</sub> H <sub>9</sub> NO <sub>4</sub> /C <sub>7</sub> H <sub>9</sub> N <sub>2</sub> O	159.053	0.68	2	[M+H] <sup>+</sup> /[M+Na] <sup>+</sup>	1.61	GL-LC-QTOF-MS	3	--	--	--	1.10	--	1.50			
Ser-Ser-OH	C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>8</sub>	314.0723	0.98	7	[M+H] <sup>+</sup>	4.11	GL-LC-QTOF-MS	3	--	--	--	1.80	3.66E-02	1.66			
Carbohydrates																	
Gluconic acid	C <sub>6</sub> H <sub>12</sub> O <sub>7</sub>	196.1553	17.49	-	-	8.86	GC-QTOF-MS	1	1.47	3.19E-02	--	--	--	--			
Methyl galactopyranoside	C <sub>7</sub> H <sub>14</sub> O <sub>6</sub>	194.1825	16.61	-	-	7.68	GC-QTOF-MS	1	1.41	3.48E-02 <sup>1</sup>	--	--	--	--			
Palmityl-CoA	C <sub>37</sub> H <sub>66</sub> N <sub>7</sub> O <sub>17</sub> P <sub>3</sub> S	1043.306	8.46	6	[M+K] <sup>+</sup>	6.27	GL-LC-QTOF-MS	4	0.57	1.27E-03	1.19	--	--	--			
Cyclic acetylserotonin glucuronide	C <sub>18</sub> H <sub>20</sub> N <sub>2</sub> O <sub>8</sub>	430.0797	5.16	6	[M+K] <sup>+</sup>	4.51	GL-LC-QTOF-MS	3	0.37	1.50E-07	1.72	--	--	--			
Fatty Acyls																	
Leukotriene C5	C <sub>30</sub> H <sub>45</sub> N <sub>3</sub> O <sub>9</sub> S	645.2725	13.71	6	[M+Na] <sup>+</sup>	4.94	GM-LC-QTOF-MS	4	0.58		1.69	--	--	--			
MAG 18:2/Dimethyl-pentyl-furandecanoic acid	C <sub>21</sub> H <sub>38</sub> O <sub>4</sub> /C <sub>21</sub> H <sub>36</sub> O <sub>3</sub>	336.2671	11.55	3/4	[M+H-H <sub>2</sub> O] <sup>+</sup> /[M+H] <sup>+</sup>	8.35	GM-LC-QTOF-MS	4	0.65	--	1.27	--	--	--			
Oxooctanoyl-CoA/Trimethylheptadienoyl-CoA	C <sub>29</sub> H <sub>48</sub> N <sub>7</sub> O <sub>18</sub> P <sub>3</sub> S/C <sub>31</sub> H <sub>48</sub> N <sub>7</sub> O <sub>19</sub> P <sub>3</sub> S	929.1832	0.75	3/1	[M+Na] <sup>+</sup> /[M+H-H <sub>2</sub> O] <sup>+</sup>	4.81	GM-LC-QTOF-MS	3	1.07	5.24E-02 <sup>1</sup>	1.24	1.23	6.09E-03 <sup>1</sup>	2.64			
Tetracosahexaenoic acid	C <sub>24</sub> H <sub>36</sub> O <sub>2</sub>	356.2719	10.79	3	[M+H] <sup>+</sup>	12.93	GM-LC-QTOF-MS	3	1.18	5.24E-02 <sup>1</sup>	--	--	--	--			
Ketoleucine	C <sub>6</sub> H <sub>10</sub> O <sub>3</sub>	130.1418	9.06	-	-	2.27	GC-QTOF-MS	1	--	--	--	1.44	4.33E-04 <sup>1</sup>	--			
Elaidic acid	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>	282.4614	20.26	-	-	6.98	GC-QTOF-MS	1	--	--	--	1.40	--	1.28			
Caproic acid	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	116.1583	6.91	-	-	6.30	GC-QTOF-MS	1	--	--	--	1.33	9.21E-04 <sup>1</sup>	1.73			
Lauric acid	C <sub>12</sub> H <sub>24</sub> O <sub>2</sub>	200.3178	14.61	-	-	4.51	GC-QTOF-MS	1	1.11	4.89E-02	--	--	--	--			
Linoleic acid	C <sub>18</sub> H <sub>32</sub> O <sub>2</sub>	280.4472	20.22	-	-	8.86	GC-QTOF-MS	1	1.31	3.77E-03 <sup>1</sup>	--	4.62	2.27E-04 <sup>1</sup>	--			
Myristic acid	C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>	228.3709	16.74	-	-	4.19	GC-QTOF-MS	1	1.17	2.91E-02	--	--	--	--			
Stearic acid	C <sub>18</sub> H <sub>36</sub> O <sub>2</sub>	284.4772	20.46	-	-	6.60	GC-QTOF-MS	1	--	--	--	1.10	--	1.24			
Dehydrododecanoyl-CoA	C <sub>33</sub> H <sub>56</sub> N <sub>7</sub> O <sub>17</sub> P <sub>3</sub> S	929.2548	7.29	1	[M+H-H <sub>2</sub> O] <sup>+</sup>	5.09	GL-LC-QTOF-MS	4	0.74	--	1.02	1.68	--	1.50			

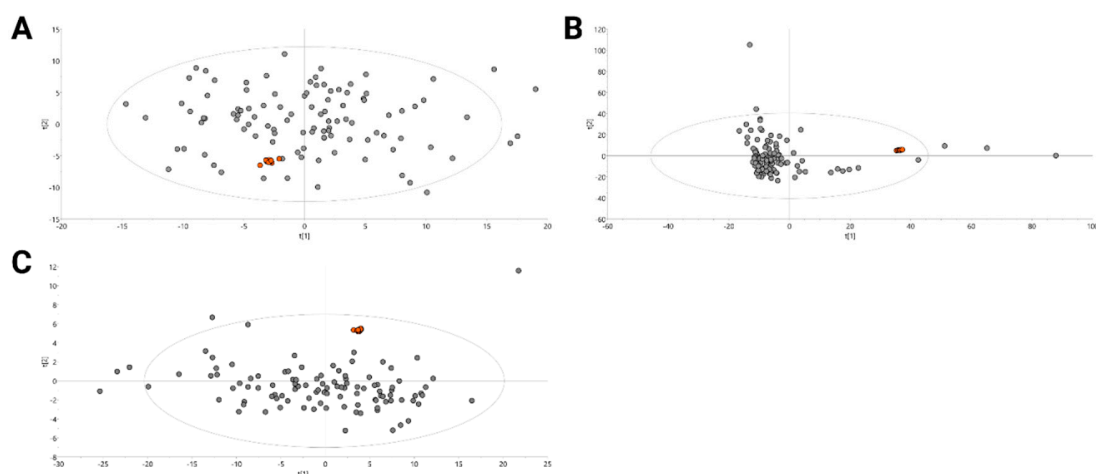
Hydroxybutyryl-CoA	C <sub>25</sub> H <sub>42</sub> N <sub>7</sub> O <sub>18</sub> P <sub>3</sub> S	870.1732	6.42	6	[M+NH <sub>4</sub> ] <sup>+</sup>	6.05	GL-LC-QTOF-MS	2	0.24	7.85E-07 <sup>†</sup>	1.97	--	--	--
Oleoyl-CoA	C <sub>39</sub> H <sub>68</sub> N <sub>7</sub> O <sub>17</sub> P <sub>3</sub> S	1069.322	12.96	6	[M+K] <sup>+</sup>	3.67	GL-LC-QTOF-MS	2	0.35	1.74E-04 <sup>‡</sup>	1.34	--	--	--
Oxo-dodecanoyl-CoA	C <sub>33</sub> H <sub>56</sub> N <sub>7</sub> O <sub>18</sub> P <sub>3</sub> S	985.249	12.43	6	[M+Na] <sup>+</sup>	4.67	GL-LC-QTOF-MS	3	0.33	3.69E-05	1.46	--	--	--
Stearoyl-CoA	C <sub>39</sub> H <sub>70</sub> N <sub>7</sub> O <sub>17</sub> P <sub>3</sub> S	1071.322	12.96	10	[M+K] <sup>+</sup>	4.25	GL-LC-QTOF-MS	4	0.36	8.63E-04	1.29	--	--	--
<b>Carnitine</b>														
Tetradecadiencarnitine	C <sub>21</sub> H <sub>37</sub> NO <sub>4</sub>	367.2729	9.60	3	[M+H] <sup>+</sup>	9.31	GM-LC-QTOF-MS	2	--	--	--	1.21	--	1.27
Hexadecadienylcarnitine	C <sub>25</sub> H <sub>45</sub> NO <sub>4</sub>	423.3356	11.74	3	[M+H] <sup>+</sup>	8.71	GM-LC-QTOF-MS	2	0.49	--	1.12	--	--	--
Decenoylcarnitine	C <sub>17</sub> H <sub>31</sub> NO <sub>4</sub>	313.2255	7.72	2	[M+H] <sup>+</sup>	9.79	GM-LC-QTOF-MS	2	--	--	--	1.32	--	1.17
<b>Glycerolipids</b>														
2-Palmitoylglycerol	C <sub>19</sub> H <sub>38</sub> O <sub>4</sub>	330.5026	23.08	-	-	17.61	GC-QTOF-MS	1	1.06	3.96E-02	--	--	--	--
DG 34:1	C <sub>37</sub> H <sub>70</sub> O <sub>5</sub>	576.5152	14.79	7	[M+H-H <sub>2</sub> O] <sup>+</sup>	1.02	GL-LC-QTOF-MS	4	0.74	--	1.15	--	--	--
DG 34:2	C <sub>39</sub> H <sub>66</sub> O <sub>5</sub>	614.4895	12.45	2	[M+H] <sup>+</sup> /[M+Na] <sup>+</sup>	2.42	GL-LC-QTOF-MS	3	0.79	--	1.10	--	--	--
DG 34:3	C <sub>37</sub> H <sub>66</sub> O <sub>5</sub>	572.4817	14.74	3	[M+H-H <sub>2</sub> O] <sup>+</sup>	1.05	GL-LC-QTOF-MS	4	0.77	--	1.02	--	--	--
DG 36:1	C <sub>39</sub> H <sub>74</sub> O <sub>5</sub>	604.5441	9.78	2	[M+H-H <sub>2</sub> O] <sup>+</sup>	2.33	GL-LC-QTOF-MS	4	--	--	--	0.83	--	1.17
DG 36:3	C <sub>39</sub> H <sub>70</sub> O <sub>5</sub>	600.5129	15.2	3	[M+H-H <sub>2</sub> O] <sup>+</sup>	1.03	GL-LC-QTOF-MS	4	0.80	--	1.06	0.79	--	1.20
DG 36:4	C <sub>39</sub> H <sub>68</sub> O <sub>5</sub>	616.5081	11.59	3	[M+H] <sup>+</sup> /[M+Na] <sup>+</sup> /[M+NH <sub>4</sub> ] <sup>+</sup>	2.14	GL-LC-QTOF-MS	2	0.65	3.37E-02	1.34	--	--	--
DG 46:0	C <sub>49</sub> H <sub>96</sub> O <sub>5</sub>	802.6817	13.73	1	[M+K] <sup>+</sup>	1.12	GL-LC-QTOF-MS	3	1.68	1.78E-02	--	--	--	--
TG 47:1	C <sub>50</sub> H <sub>96</sub> O <sub>5</sub>	814.6833	12.91	3	[M+K] <sup>+</sup>	0.83	GL-LC-QTOF-MS	4	0.89	--	1.21	0.71	2.09E-02	2.40
TG 50:0	C <sub>53</sub> H <sub>104</sub> O <sub>5</sub>	858.749	14.58	6	[M+K] <sup>+</sup>	1.51	GL-LC-QTOF-MS	4	0.76	--	1.09	--	--	--
TG 51:4	C <sub>54</sub> H <sub>96</sub> O <sub>6</sub>	857.7477	14.58	1	M+NH <sub>4</sub> /[M+Na] <sup>+</sup>	0.58	GL-LC-QTOF-MS	2	0.76	--	1.10	--	--	--
TG 52:3	C <sub>55</sub> H <sub>100</sub> O <sub>6</sub>	873.7815	15.2	4	[M+H] <sup>+</sup> /M+NH <sub>4</sub>	0.19	GL-LC-QTOF-MS	2	0.94	--	1.16	0.90	--	1.11
TG 52:4	C <sub>55</sub> H <sub>98</sub> O <sub>6</sub>	876.721	14.79	4	[M+H] <sup>+</sup> /[M+Na] <sup>+</sup> /[M+NH <sub>4</sub> ] <sup>+</sup>	0.51	GL-LC-QTOF-MS	2	0.85	--	1.01	--	--	--
TG 52:5	C <sub>55</sub> H <sub>96</sub> O <sub>6</sub>	852.7222	14.46	2	[M+H] <sup>+</sup> /[M+Na] <sup>+</sup> /[M+NH <sub>4</sub> ] <sup>+</sup> /[M+K] <sup>+</sup>	0.68	GL-LC-QTOF-MS	2	0.78	--	1.14	--	--	--
TG 52:6	C <sub>55</sub> H <sub>94</sub> O <sub>6</sub>	872.6883	14.23	2	[M+Na] <sup>+</sup> /[M+NH <sub>4</sub> ] <sup>+</sup>	1.08	GL-LC-QTOF-MS	2	0.78	--	1.02	--	--	--
TG 53:3	C <sub>56</sub> H <sub>102</sub> O <sub>6</sub>	892.7512	15.47	2	[M+Na] <sup>+</sup>	0.68	GL-LC-QTOF-MS	2	--	--	--	0.85	--	1.14
TG 53:4	C <sub>56</sub> H <sub>100</sub> O <sub>6</sub>	885.78	14.97	2	[M+NH <sub>4</sub> ] <sup>+</sup> /[M+Na] <sup>+</sup>	1.16	GL-LC-QTOF-MS	2	0.78	--	1.08	--	--	--
TG 53:5	C <sub>56</sub> H <sub>98</sub> O <sub>6</sub>	883.7626	14.38	2	[M+Na] <sup>+</sup>	1.42	GL-LC-QTOF-MS	2	0.83	--	1.01	--	--	--
TG 54:0	C <sub>57</sub> H <sub>112</sub> O <sub>5</sub>	914.808	15.2	2	[M+K] <sup>+</sup>	1.69	GL-LC-QTOF-MS	3	--	--	--	0.89	--	1.13
TG 54:1	C <sub>57</sub> H <sub>110</sub> O <sub>5</sub>	912.7924	14.79	2	[M+K] <sup>+</sup>	1.60	GL-LC-QTOF-MS	2	0.84	--	1.23	--	--	--
TG 54:2	C <sub>57</sub> H <sub>108</sub> O <sub>5</sub>	910.7758	14.46	1	[M+K] <sup>+</sup>	1.01	GL-LC-QTOF-MS	2	0.79	--	1.24	--	--	--
TG 54:4	C <sub>57</sub> H <sub>102</sub> O <sub>6</sub>	899.797	15.2	4	[M+NH <sub>4</sub> ] <sup>+</sup>	0.36	GL-LC-QTOF-MS	2	0.79	--	1.14	0.79	--	1.27
TG 54:5	C <sub>57</sub> H <sub>100</sub> O <sub>6</sub>	902.7353	14.79	2	[M+H] <sup>+</sup> /[M+Na] <sup>+</sup> /[M+NH <sub>4</sub> ] <sup>+</sup>	0.62	GL-LC-QTOF-MS	2	0.81	--	1.16	--	--	--
TG 54:6	C <sub>57</sub> H <sub>98</sub> O <sub>6</sub>	895.7649	14.63	3	[M+Na] <sup>+</sup> /[M+NH <sub>4</sub> ] <sup>+</sup> /[M+K] <sup>+</sup>	0.51	GL-LC-QTOF-MS	2	0.78	--	1.12	0.78	--	1.03

TG 55:4	C <sub>58</sub> H <sub>104</sub> O <sub>6</sub>	913.8093	15.2	0	[M+NH <sub>4</sub> ] <sup>+</sup>	1.68	GL-LC-QTOF-MS	4	--	--	--	0.89	--	1.13
TG 55:8	C <sub>58</sub> H <sub>96</sub> O <sub>6</sub>	888.7199	14.59	0	[M+H] <sup>+</sup>	1.00	GL-LC-QTOF-MS	4	0.84	--	1.01	--	--	--
TG 56:2	C <sub>59</sub> H <sub>110</sub> O <sub>6</sub>	952.7842	13.49	2	[M+K] <sup>+</sup>	5.86	GL-LC-QTOF-MS	4	0.63	--	1.23	--	--	--
TG 56:3	C <sub>59</sub> H <sub>110</sub> O <sub>5</sub>	936.7916	14.63	1	[M+K] <sup>+</sup>	1.31	GL-LC-QTOF-MS	3	--	--	--	0.84	--	1.03
TG 56:5	C <sub>59</sub> H <sub>104</sub> O <sub>6</sub>	946.7415	15.53	3	[M+K] <sup>+</sup> /[M+Na] <sup>+</sup>	1.01	GL-LC-QTOF-MS	2	--	--	--	0.77	--	1.43
TG 56:6	C <sub>59</sub> H <sub>102</sub> O <sub>6</sub>	923.7958	14.99	2	[M+Na] <sup>+</sup> /[M+NH <sub>4</sub> ] <sup>+</sup>	0.29	GL-LC-QTOF-MS	2	--	--	--	0.71	--	1.52
TG 56:7	C <sub>59</sub> H <sub>100</sub> O <sub>6</sub>	926.7356	14.61	0/3	[M+Na] <sup>+</sup> /[M+NH <sub>4</sub> ] <sup>+</sup>	0.77	GL-LC-QTOF-MS	2	0.81	--	1.04	0.78	--	1.32
TG 58:3	C <sub>61</sub> H <sub>114</sub> O <sub>5</sub>	964.8228	14.99	1	[M+K] <sup>+</sup>	1.16	GL-LC-QTOF-MS	3	0.86	--	1.03	0.78	--	1.55
TG 58:4	C <sub>61</sub> H <sub>112</sub> O <sub>5</sub>	962.8073	14.61	1	[M+K] <sup>+</sup>	1.24	GL-LC-QTOF-MS	2	0.83	--	1.04	0.80	--	1.29
TG 58:7	C <sub>61</sub> H <sub>104</sub> O <sub>6</sub>	949.8113	14.97	2	[M+NH <sub>4</sub> ] <sup>+</sup> /[M+Na] <sup>+</sup>	0.53	GL-LC-QTOF-MS	2	--	--	--	0.76	--	1.26
TG 60:11	C <sub>63</sub> H <sub>102</sub> O <sub>5</sub>	976.734	15.2	6	[M+K] <sup>+</sup>	0.81	GL-LC-QTOF-MS	2	--	--	--	0.89	--	1.14
<b>Glycerophospholipids</b>														
CDP-DG 40:4	C <sub>52</sub> H <sub>89</sub> N <sub>3</sub> O <sub>15</sub> P <sub>2</sub>	1079.5543	11.86	4	[M+Na] <sup>+</sup>	19.15	GM-LC-QTOF-MS	4	0.81		2.38	--	--	--
Glycerophospho Palmitoyl Ethanolamine	C <sub>21</sub> H <sub>44</sub> NO <sub>7</sub> P	453.2867	12.08	4	[M+H] <sup>+</sup>	9.59	GM-LC-QTOF-MS	2	0.82	--	1.34	0.79	8.22E-02 <sup>1</sup>	--
LPC 15:0	C <sub>23</sub> H <sub>48</sub> NO <sub>7</sub> P	481.3180	13.63	3	[M+H] <sup>+</sup>	9.72	GM-LC-QTOF-MS	2	0.87		1.77	0.74	9.29E-03 <sup>1</sup>	1.90
LPC 16:0	C <sub>24</sub> H <sub>50</sub> NO <sub>7</sub> P	477.3227	12.15	2	[M+H-H <sub>2</sub> O] <sup>+</sup>	8.30	GM-LC-QTOF-MS	2	0.53		2.03	--	--	--
LPC 17:1/LPE 20:1	C <sub>25</sub> H <sub>50</sub> NO <sub>7</sub> P	507.3336	11.81	3	[M+H] <sup>+</sup>	9.01	GM-LC-QTOF-MS	3	0.86	--	1.38	--	--	--
LPC 18:0	C <sub>26</sub> H <sub>54</sub> NO <sub>7</sub> P	545.3496	12.16	8	[M+Na] <sup>+</sup>	6.72	GM-LC-QTOF-MS	2	0.97	--	1.29	--	--	--
LPC 18:1	C <sub>26</sub> H <sub>52</sub> NO <sub>7</sub> P	521.3493	12.71	3	[M+H] <sup>+</sup>	10.50	GM-LC-QTOF-MS	2	0.98	--	1.42	--	--	--
LPC 18:3	C <sub>26</sub> H <sub>48</sub> NO <sub>7</sub> P	517.3177	11.00	3	[M+H] <sup>+</sup>	8.19	GM-LC-QTOF-MS	2	--	--	--	1.57		1.84
LPC 20:2	C <sub>28</sub> H <sub>54</sub> NO <sub>7</sub> P	547.3653	12.95	4	[M+H] <sup>+</sup>	9.07	GM-LC-QTOF-MS	2	0.79		1.99	--	--	--
LPC 20:3/LPC 18:0	C <sub>28</sub> H <sub>52</sub> NO <sub>7</sub> P/C <sub>26</sub> H <sub>54</sub> NO <sub>7</sub> P	545.3497	11.61	5	[M+H] <sup>+</sup> /[M+Na] <sup>+</sup>	9.09	GM-LC-QTOF-MS	3	0.87		1.21	--	--	--
LPC 22:4/PC O-20:1	C <sub>30</sub> H <sub>54</sub> NO <sub>7</sub> P/C <sub>28</sub> H <sub>56</sub> NO <sub>7</sub> P	571.3647	12.73	4	[M+H] <sup>+</sup> /[M+Na] <sup>+</sup>	8.27	GM-LC-QTOF-MS	3	0.27		1.70	--	--	--
LPC 22:5	C <sub>30</sub> H <sub>52</sub> NO <sub>7</sub> P	569.3492	11.96	3	[M+H] <sup>+</sup>	7.50	GM-LC-QTOF-MS	2	0.79	--	1.28	--	--	--
LPC O-16:0	C <sub>24</sub> H <sub>52</sub> NO <sub>6</sub> P	481.3544	12.52	4	[M+H] <sup>+</sup>	10.49	GM-LC-QTOF-MS	2	0.96	--	1.73	--	--	--
PA O-31:2	C <sub>34</sub> H <sub>65</sub> O <sub>7</sub> P	598.4331	12.15	4	[M+H-H <sub>2</sub> O] <sup>+</sup>	12.90	GM-LC-QTOF-MS	4	0.85	6.23E-02 <sup>1</sup>	2.12	--	--	--
PC O-20:1	C <sub>28</sub> H <sub>56</sub> NO <sub>7</sub> P	549.3804	14.00	3	[M+H] <sup>+</sup>	8.50	GM-LC-QTOF-MS	3	0.77	--	1.30	0.86		1.32
Thio-PAF	C <sub>26</sub> H <sub>54</sub> NO <sub>6</sub> PS	561.3210	13.71	3	[M+Na] <sup>+</sup>	7.92	GM-LC-QTOF-MS	4	0.63		1.58	--	--	--
CL 65:4	C <sub>74</sub> H <sub>136</sub> O <sub>17</sub> P <sub>2</sub>	1396.88	14.84	0	[M+K] <sup>+</sup>	7.84	GL-LC-QTOF-MS	4	0.30	9.98E-06	2.04	--	--	--
LPA 20:4	C <sub>23</sub> H <sub>39</sub> O <sub>7</sub> P	458.2417	2.67	2	[M+H] <sup>+</sup>	1.70	GL-LC-QTOF-MS	3	0.88	--	1.19	--	--	--
LPC 16:0	C <sub>24</sub> H <sub>50</sub> NO <sub>7</sub> P	495.3337	2.67	4	[M+H] <sup>+</sup>	1.57	GL-LC-QTOF-MS	2	0.85	--	1.28	--	--	--
LPC 18:0	C <sub>26</sub> H <sub>54</sub> NO <sub>7</sub> P	523.3652	3.94	4	[M+H] <sup>+</sup>	1.70	GL-LC-QTOF-MS	2	0.81	4.40E-02	1.57	--	--	--

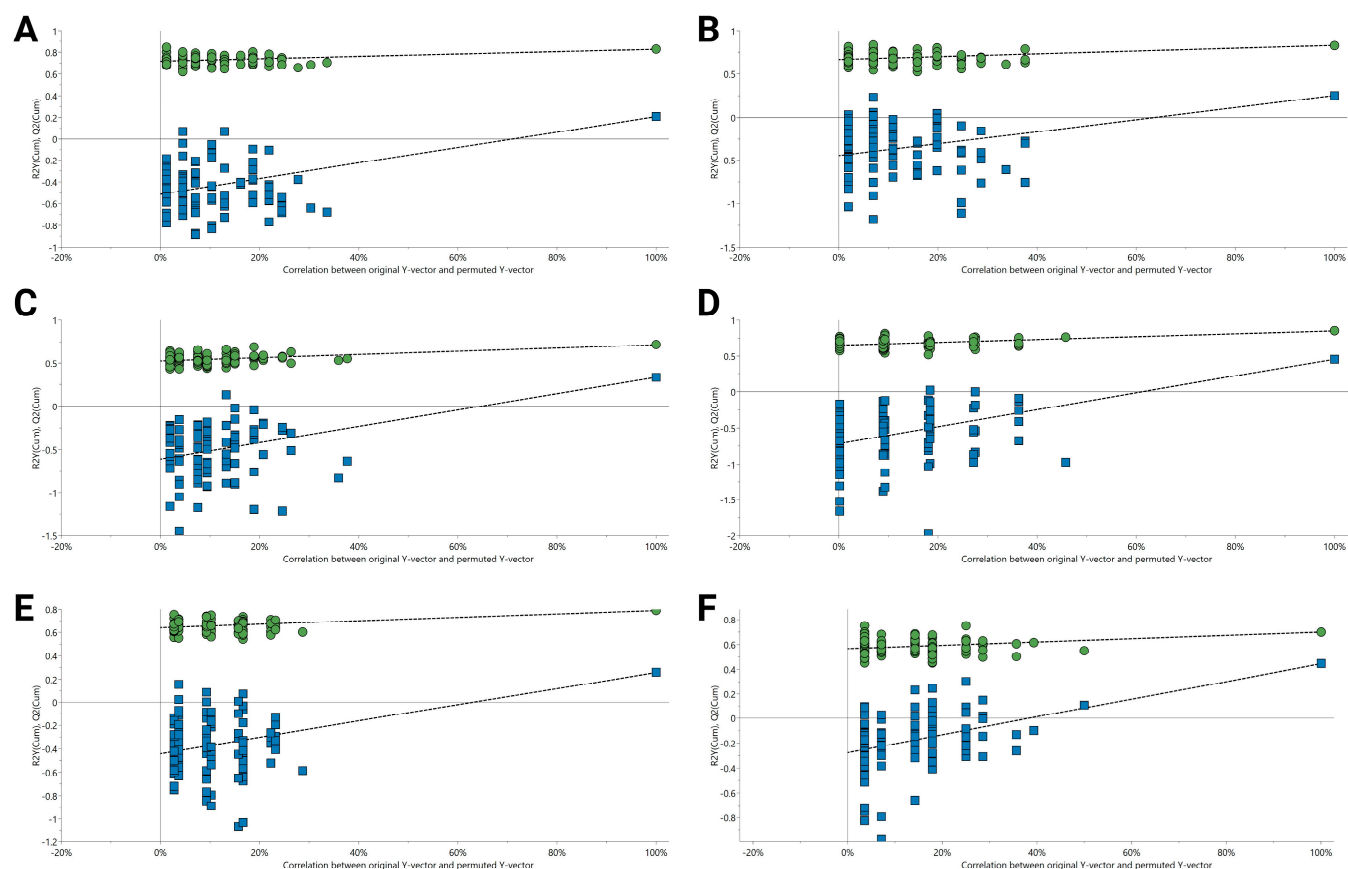
LPC 20:4	C <sub>28</sub> H <sub>50</sub> NO <sub>7</sub> P	543.3331	2.11	2	[M+H] <sup>+</sup>	2.04	GL-LC-QTOF-MS	2	0.83	--	1.26	--	--	--
LPC O-16:1	C <sub>24</sub> H <sub>50</sub> NO <sub>6</sub> P	479.338	3.2	2	[M+H] <sup>+</sup>	3.92	GL-LC-QTOF-MS	2	0.82	--	1.50	--	--	--
PC 34:0	C <sub>42</sub> H <sub>84</sub> NO <sub>8</sub> P	761.5946	12.38	2	[M+H] <sup>+</sup>	1.19	GL-LC-QTOF-MS	2	0.86	4.40E-02	1.32	0.78	--	1.87
PC 38:5	C <sub>46</sub> H <sub>82</sub> NO <sub>8</sub> P	807.5798	8.88	3	[M+H] <sup>+</sup>	0.63	GL-LC-QTOF-MS	2	--	--	--	0.86	--	1.34
PC 40:7	C <sub>48</sub> H <sub>82</sub> NO <sub>8</sub> P	831.5785	8.57	1	[M+H] <sup>+</sup>	1.08	GL-LC-QTOF-MS	2	0.84	--	1.30	0.85	--	1.17
PC O-18:0	C <sub>26</sub> H <sub>54</sub> NO <sub>7</sub> P	523.365	3.67	3	[M+H] <sup>+</sup>	1.55	GL-LC-QTOF-MS	2	0.81	4.05E-02	1.62	--	--	--
PC O-34:2	C <sub>42</sub> H <sub>82</sub> NO <sub>7</sub> P	743.5834	11.69	1	[M+H] <sup>+</sup>	1.37	GL-LC-QTOF-MS	2	--	--	--	0.74	4.44E-02	2.35
PC O-36:1	C <sub>44</sub> H <sub>88</sub> NO <sub>7</sub> P	795.6157	12.29	6	[M+Na] <sup>+</sup>	1.21	GL-LC-QTOF-MS	2	0.88	--	1.10	--	--	--
PC O-38:4	C <sub>46</sub> H <sub>86</sub> NO <sub>7</sub> P	795.6139	11.78	0	[M+H] <sup>+</sup>	1.60	GL-LC-QTOF-MS	2	0.87	4.05E-02	1.28	0.84	--	1.60
PC O-40:2	C <sub>48</sub> H <sub>94</sub> NO <sub>7</sub> P	865.6321	8.88	0	[M+K] <sup>+</sup>	1.50	GL-LC-QTOF-MS	2	0.92	--	1.02	0.87	--	1.31
PE 36:4	C <sub>41</sub> H <sub>74</sub> NO <sub>8</sub> P	739.5166	8.97	3	[M+H] <sup>+</sup>	1.34	GL-LC-QTOF-MS	2	--	--	--	0.65	2.88E-02	1.80
PE 38:4	C <sub>43</sub> H <sub>78</sub> NO <sub>8</sub> P	767.5477	11.2	2	[M+H] <sup>+</sup>	1.06	GL-LC-QTOF-MS	2	--	--	--	0.66	2.88E-02	1.79
PE 38:6	C <sub>43</sub> H <sub>74</sub> NO <sub>8</sub> P	763.5164	8.62	2	[M+H] <sup>+</sup>	1.02	GL-LC-QTOF-MS	2	--	--	--	0.62	--	1.66
PE 40:6	C <sub>45</sub> H <sub>78</sub> NO <sub>8</sub> P	791.5482	10.67	3	[M+H] <sup>+</sup>	1.30	GL-LC-QTOF-MS	2	--	--	--	0.72	--	1.29
PG 43:2	C <sub>49</sub> H <sub>93</sub> O <sub>10</sub> P	894.6349	13.25	3	[M+Na] <sup>+</sup>	1.87	GL-LC-QTOF-MS	3	--	--	--	0.96	--	1.02
PS 39:0	C <sub>45</sub> H <sub>88</sub> NO <sub>10</sub> P	850.6353	12.91	6	[M+NH <sub>4</sub> ] <sup>+</sup>	4.56	GL-LC-QTOF-MS	3	--	--	--	0.75	3.71E-02	2.00
<b>Organoheterocyclic compounds</b>														
Biliverdin	C <sub>33</sub> H <sub>34</sub> N <sub>4</sub> O <sub>6</sub>	582.2484	9.10	2	[M+H] <sup>+</sup>	13.90	GM-LC-QTOF-MS	3	--	--	--	1.94	--	1.17
Formyl Indole	C <sub>9</sub> H <sub>7</sub> NO	145.0529	2.51	5	[M+H] <sup>+</sup>	9.58	GM-LC-QTOF-MS	2	0.58	--	1.04	--	--	--
Lipoyllysine	C <sub>14</sub> H <sub>26</sub> N <sub>2</sub> O <sub>3</sub> S <sub>2</sub>	372.0926	6.42	4	[M+K] <sup>+</sup>	3.87	GL-LC-QTOF-MS	4	0.36	1.38E-05	1.75	--	--	--
Hemin	C <sub>34</sub> H <sub>32</sub> ClFeN <sub>4</sub> O <sub>4</sub>	668.168	5.16	6	[M+NH <sub>4</sub> ] <sup>+</sup>	6.18	GL-LC-QTOF-MS	4	0.46	1.70E-04	1.78	--	--	--
Methylxanthine/Methylmalate	C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> O <sub>2</sub> /C <sub>5</sub> H <sub>8</sub> O <sub>5</sub>	148.0379	4.44	1/8	[M+H-H <sub>2</sub> O] <sup>+</sup> /[M+H] <sup>+</sup>	7.70	GL-LC-QTOF-MS	3	0.47	3.80E-05	1.84	--	--	--
Tryptophanol/Dehydroxycarnitine/Aminoheptanoic acid	C <sub>10</sub> H <sub>11</sub> NO/C <sub>7</sub> H <sub>15</sub> NO <sub>2</sub>	183.0659	2.67	3	[M+Na] <sup>+</sup> /[M+K] <sup>+</sup>	2.19	GL-LC-QTOF-MS	3	0.84	--	1.26	--	--	--
<b>Indoles and derivatives</b>														
Indoleacrylic acid	C <sub>11</sub> H <sub>9</sub> NO <sub>2</sub>	187.0633	3.24	3	[M+H] <sup>+</sup>	10.81	GM-LC-QTOF-MS	2	--	--	--	1.54	--	1.13
Indolelactic acid	C <sub>11</sub> H <sub>11</sub> NO <sub>3</sub>	187.0634	2.51	2	[M+H-H <sub>2</sub> O] <sup>+</sup>	9.51	GM-LC-QTOF-MS	2	0.97	--	1.13	1.27	--	1.86
<b>Sphingolipids</b>														
C17 Sphinganine	C <sub>17</sub> H <sub>37</sub> NO <sub>2</sub>	287.2832	9.65	5	[M+H] <sup>+</sup>	9.78	GM-LC-QTOF-MS	2	--	--	--	0.69	--	1.18
Ganglioside GD3 (41:1)	C <sub>75</sub> H <sub>135</sub> N <sub>3</sub> O <sub>29</sub>	1541.9198	12.15	1	[M+H] <sup>+</sup>	7.91	GM-LC-QTOF-MS	4	0.81	1.46E-02	2.25	--	--	--
Hex(4)-HexNAc(2)-NeuAc(2)-Cer 36:1;O2	C <sub>98</sub> H <sub>171</sub> N <sub>5</sub> O <sub>49</sub>	2184.0974	9.09	2	[M+H-H <sub>2</sub> O] <sup>+</sup>	8.94	GM-LC-QTOF-MS	4	0.40	--	1.12	--	--	--
Hex(4)-HexNAc(3)-NeuCer 38:1;O2	C <sub>97</sub> H <sub>171</sub> N <sub>5</sub> O <sub>47</sub>	2140.0947	9.34	4	[M+H-H <sub>2</sub> O] <sup>+</sup>	15.24	GM-LC-QTOF-MS	4	--	--	--	1.30	--	1.54
Hex(5)-HexNAc-NeuAc(2)-Cer 38:1;O2	C <sub>98</sub> H <sub>172</sub> N <sub>4</sub> O <sub>49</sub>	2171.1043	9.30	3	[M+H-H <sub>2</sub> O] <sup>+</sup>	9.59	GM-LC-QTOF-MS	4	--	--	--	1.27	--	--

NeuAalpha2-3Galbeta-Cer(34:1)	C <sub>51</sub> H <sub>94</sub> N <sub>2</sub> O <sub>16</sub>	990.6675	12.15	8	[M+H] <sup>+</sup>	15.79	GM-LC-QTOF-MS	4	0.92	2.43E-02	2.40	--	--	--
NeuAcHexCer 36:1;O2	C <sub>53</sub> H <sub>98</sub> N <sub>2</sub> O <sub>16</sub>	1040.6825	12.16	9	[M+Na] <sup>+</sup>	13.66	GM-LC-QTOF-MS	4	0.93	--	1.85	--	--	--
Phytosphingosine	C <sub>18</sub> H <sub>39</sub> NO <sub>3</sub>	317.2935	9.05	3	[M+H] <sup>+</sup>	10.20	GM-LC-QTOF-MS	2	0.44	7.33E-04 <sup>†</sup>	--	5.72		1.20
SM 36:2;O2/CerPE 39:2;O2	C <sub>41</sub> H <sub>81</sub> N <sub>2</sub> O <sub>6</sub> P	750.5654	16.42	1	[M+Na] <sup>+</sup>	6.51	GM-LC-QTOF-MS	3	1.06	--	1.06	--	--	--
CerPE 37:1;O2	C <sub>39</sub> H <sub>79</sub> N <sub>2</sub> O <sub>6</sub> P	740.5249	8.14	3	[M+K] <sup>+</sup>	1.33	GL-LC-QTOF-MS	3	0.85	4.32E-02	1.20	0.73	2.83E-02	2.38
Hex2Cer 34:1;O2	C <sub>46</sub> H <sub>87</sub> NO <sub>13</sub>	861.619	7.86	2	[M+H] <sup>+</sup>	1.20	GL-LC-QTOF-MS	2	0.83	3.41E-02	1.11	--	--	--
HexCer 36:1;O3	C <sub>42</sub> H <sub>81</sub> NO <sub>9</sub>	760.6222	8.14	7	[M+NH <sub>4</sub> ] <sup>+</sup>	3.00	GL-LC-QTOF-MS	3	0.75	3.41E-02	1.44	0.64	--	2.06
HexCer 42:2;O2	C <sub>48</sub> H <sub>91</sub> NO <sub>8</sub>	809.675	12.93	1	[M+H] <sup>+</sup>	1.20	GL-LC-QTOF-MS	3	--	--	--	0.95	--	1.12
SM 34:0;O2	C <sub>39</sub> H <sub>81</sub> N <sub>2</sub> O <sub>6</sub> P	704.5844	8.81	2	[M+H] <sup>+</sup>	1.14	GL-LC-QTOF-MS	2	0.87	--	1.08	0.60	2.09E-02	2.14
SM 34:1;O2	C <sub>39</sub> H <sub>79</sub> N <sub>2</sub> O <sub>6</sub> P	702.5696	8.14	4	[M+H] <sup>+</sup>	1.12	GL-LC-QTOF-MS	2	0.84	3.48E-02	1.37	0.75	--	2.22
SM 36:1;O2	C <sub>41</sub> H <sub>83</sub> N <sub>2</sub> O <sub>6</sub> P	730.6004	10.05	3	[M+H] <sup>+</sup>	1.31	GL-LC-QTOF-MS	2	0.85	6.91E-03	1.32	0.74	--	1.88
SM 40:0;O2/DG 45:0	C <sub>45</sub> H <sub>93</sub> N <sub>2</sub> O <sub>6</sub> P/C <sub>48</sub> H <sub>94</sub> O <sub>5</sub>	788.67	12.92	8/6	[M+H] <sup>+</sup> /[M+K] <sup>+</sup>	1.29	GL-LC-QTOF-MS	4	--	--	--	0.92	--	1.16
SM 40:1;O2	C <sub>43</sub> H <sub>91</sub> N <sub>2</sub> O <sub>6</sub> P	786.664	12.92	4	[M+H] <sup>+</sup>	0.67	GL-LC-QTOF-MS	2	--	--	--	0.91	--	1.18
SM 41:2;O2	C <sub>46</sub> H <sub>91</sub> N <sub>2</sub> O <sub>6</sub> P	798.6624	12.72	2	[M+H] <sup>+</sup>	1.28	GL-LC-QTOF-MS	2	0.86	--	1.17	0.71	1.94E-02	2.48
SM 42:1;O2	C <sub>47</sub> H <sub>95</sub> N <sub>2</sub> O <sub>6</sub> P	814.695	13.25	3	[M+H] <sup>+</sup>	1.03	GL-LC-QTOF-MS	2	--	--	--	0.93	--	1.07
SM 42:2;O2	C <sub>47</sub> H <sub>93</sub> N <sub>2</sub> O <sub>6</sub> P	812.6794	12.91	3	[M+H] <sup>+</sup>	0.68	GL-LC-QTOF-MS	2	0.89	--	1.23	0.73	2.88E-02	2.35
SM 42:3;O2	C <sub>47</sub> H <sub>91</sub> N <sub>2</sub> O <sub>6</sub> P	810.6623	12.55	2	[M+H] <sup>+</sup>	1.03	GL-LC-QTOF-MS	2	0.87	--	1.22	0.71	1.94E-02	2.38
SM 43:2;O2	C <sub>48</sub> H <sub>95</sub> N <sub>2</sub> O <sub>6</sub> P	826.6939	13.02	2	[M+H] <sup>+</sup>	1.27	GL-LC-QTOF-MS	2	0.83	--	1.00	0.67	1.94E-02	2.09
<b>Sterol Lipids</b>														
Chenodeoxyglycocholic acid	C <sub>26</sub> H <sub>43</sub> NO <sub>5</sub>	449.3146	8.16	2	[M+H] <sup>+</sup>	11.49	GM-LC-QTOF-MS	3	--	--	--	2.64	--	1.01
Glycocholic acid	C <sub>26</sub> H <sub>43</sub> NO <sub>6</sub>	447.2988	8.81	2	[M+H-H <sub>2</sub> O] <sup>+</sup>	11.92	GM-LC-QTOF-MS	4	2.29	8.94E-03	--	8.35	6.09E-03 <sup>‡</sup>	--
Hydrocortisone succinate/Dehydrotestosterone glucosiduronic acid	C <sub>25</sub> H <sub>34</sub> O <sub>8</sub>	462.2259	9.65	2	[M+H] <sup>+</sup>	7.63	GM-LC-QTOF-MS	3	0.16	4.65E-02	--	1.39	--	--
<b>Bilirubins</b>														
Mesobilirubinogen	C <sub>33</sub> H <sub>44</sub> N <sub>4</sub> O <sub>6</sub>	592.3260	9.58	1	[M+H] <sup>+</sup>	14.05	GM-LC-QTOF-MS	3	0.09	1.10E-05	--	0.37	9.91E-03 <sup>‡</sup>	--
Urobilinogen	C <sub>33</sub> H <sub>48</sub> N <sub>4</sub> O <sub>6</sub>	596.3573	9.59	1	[M+H] <sup>+</sup>	12.96	GM-LC-QTOF-MS	3	1.49	5.31E-03	--	0.18	6.09E-03 <sup>‡</sup>	2.33
<b>Others</b>														
Inosine cyclic phosphate	C <sub>10</sub> H <sub>11</sub> N <sub>4</sub> O <sub>7</sub> P	330.0377	0.68	5	[M+H] <sup>+</sup>	1.73	GL-LC-MS	3	--	--	--	1.11	4.81E-02	2.10
UDP-acetyl-(carboxyvinyl)-glucosamine	C <sub>20</sub> H <sub>29</sub> N <sub>3</sub> O <sub>19</sub> P <sub>2</sub>	659.0740	0.73	3	[M+H-H <sub>2</sub> O] <sup>+</sup>	1.39	GM-LC-QTOF-MS	4	--	--	--	1.12	6.09E-03 <sup>‡</sup>	2.88

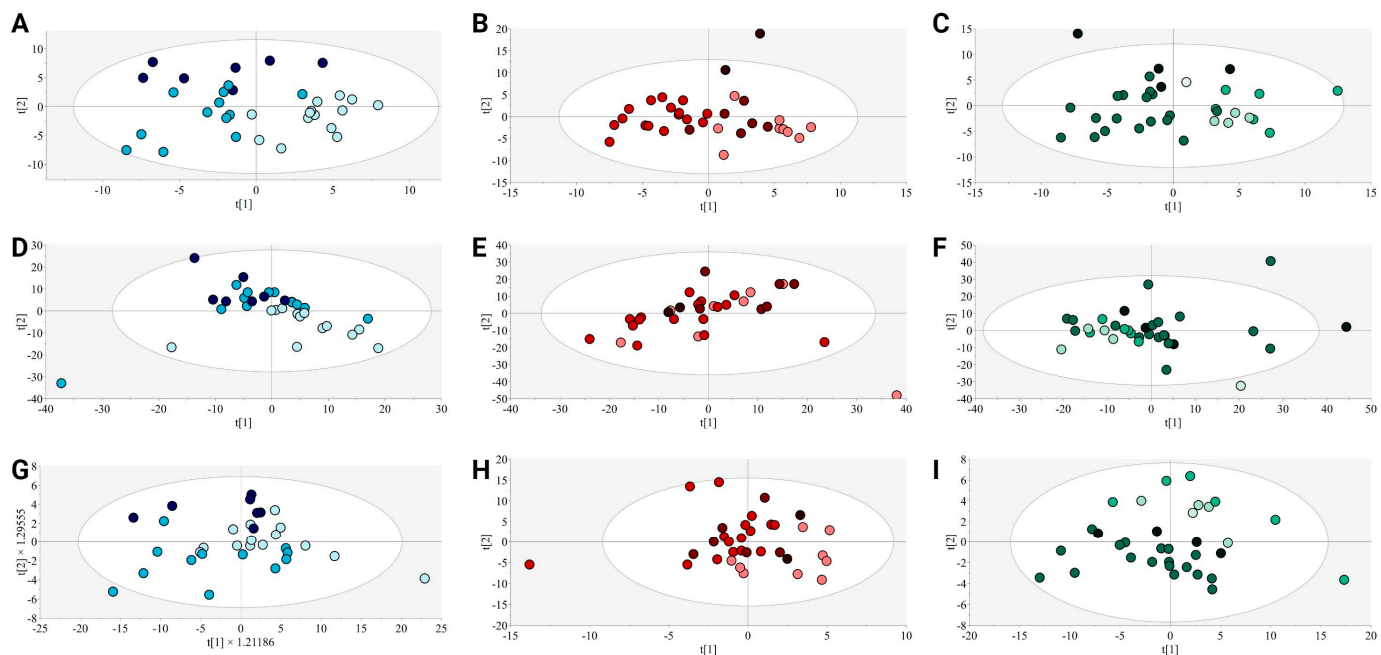
RT: retention time; <sup>‡</sup>CV, coefficient of variation in the metabolites in the QC samples; <sup>‡</sup>Identification level: Level 1 Structure confirmed, Level 2 Structure probable, Level 3 Unequivocal molecular formula (s), Level 4 Exact mass; <sup>†</sup>Fold Change, change in the abundance of the specified comparison calculated as (case/control); <sup>‡</sup>p value<sup>‡</sup> corresponding to the *p* values calculated by the Benjamini-Hochberg false discovery rate post hoc correction (FDR < 0.05); <sup>‡</sup>VIP, variable importance in projection. GM: global metabolomics, GL: global lipidomics, LC: liquid chromatography, GC: gas chromatography, QTOF-MS: quadrupole time-of-flight mass spectrometer.



**Figure S1. PCA models for metabolic and lipidomic analysis.** (A) GM(+):  $R^2: 0.673$ , (B) GL(+):  $R^2: 0.928$ ; (C) GC:  $R^2: 0.71$ . Dots in orange denote quality control, gray dots correspond to samples.



**Figure S2. OPLS-DA permutation test plots.** (A,C,E): BPHvsPCa, (B,D,F): PCavsMET. (A,B) GM(+), (C,D) GL(+), (E,F) GC. Dots in green correspond to  $R^2$ , squares in blue denote  $Q^2$ .



**Figure S3. PLSDA Models for comparisons regarding PSA, TNM, and Gleason score classifications.**

(A–C): GM(+). (D–F): GL(+). (G–I): GC. (A,D,G): PSA classifications. (B,E,H): Gleason score, (C,F,I): TNM score. (A)  $R^2$ : 0.551,  $Q^2$ : -0.21, cv-ANOVA: 1. (B)  $R^2$ : 0.479,  $Q^2$ : -0.125, cv-ANOVA: 0.96. (C)  $R^2$ : 0.322,  $Q^2$ : -0.05, cv-ANOVA: 1. (D)  $R^2$ : 0.255,  $Q^2$ : -0.045, cv-ANOVA: 0.89. (E)  $R^2$ : 0.491,  $Q^2$ : -0.159, cv-ANOVA: 1. (F)  $R^2$ : 0.124,  $Q^2$ : -0.118, cv-ANOVA: 1. (G)  $R^2$ : 0.366,  $Q^2$ : -0.088, cv-ANOVA: 1. (H)  $R^2$ : 0.191,  $Q^2$ : -0.099, cv-ANOVA: 0.85. (I)  $R^2$ : 0.248,  $Q^2$ : 0.0671, cv-ANOVA: 1. The points classify the samples into descending color gradients as follows: Blue gradient (PSA): >20, 10-20, <10; Red gradient (Gleason Score): 9, 8, 7, 6; Green gradient (TNM Score): T2c, T2b, T2a, T1c, T1b.