

**Table S1.** Clinical characteristics of patients

<b>Parameter</b>	<b>Healthy Controls (n = 32)</b>	<b>PCa Patients (n =32)</b>	<b>P value</b>
Age, years	69.3±5.2	68.2±5.8	0.32
BMI, kg/m <sup>2</sup>	23.11±1.27	23.32±1.52	0.69
DBP, mmHg	75.13±8.16	76.44±8.21	0.49
SBP, mmHg	147.10±22.31	145.09±23.38	0.66
Serum FBG, mmol/L	5.7±1.3	5.9±1.5	0.19
PSA (ng/ml mean ± SD)	1.2±0.34	9.8±5.6	0.0019

Note: BMI, body mass index; DBP, diastolic blood pressure; FBG, fasting (2 hours postprandial) blood glucose; SBP, systolic blood pressure; TC, total cholesterol; TG, triglycerides; PSA, serum prostate-specific antigen. Parameter values of patients and healthy control were compared using t-test. The p values less than 0.05 were considered significant.

**Table S2.** Information of plasma metabolites related to PCa detected by UPLC/MS.

No	Rt(min)	m/z	Compound ID	Adducts	Formula	Mass Error (ppm)	Description	Anova (p)	VIP
1	8.12	500.2887	HMDB00951	M+H	C <sub>26</sub> H <sub>47</sub> N <sub>6</sub> O <sub>6</sub> S	-1.58	Taurochenodesoxycholic acid	0.03	6.15
2	7.43	371.2281	HMDB13039	M+H	C <sub>20</sub> H <sub>36</sub> O <sub>6</sub>	-0.32	Prostaglandin G1	0.01	6.94
3	6.44	353.2177	HMDB01452	M+H	C <sub>20</sub> H <sub>34</sub> O <sub>5</sub>	0.03	Thromboxane A2	0.00	6.39
4	1.23	106.0348	HMDB03406	M+H	C <sub>3</sub> H <sub>9</sub> N <sub>3</sub> O	-2.90	D-Serine	0.05	10.69
5	8.36	483.2075	HMDB02224	2M+H	C <sub>10</sub> H <sub>17</sub> N <sub>3</sub> O <sub>4</sub>	1.68	5-Methyldeoxycytidine	0.01	6.92
6	5.84	337.2219	HMDB02982	M+H	C <sub>20</sub> H <sub>34</sub> O <sub>4</sub>	-2.75	Prostaglandin B1	0.00	25.68
7	4.66	353.2174	HMDB01403	M+H	C <sub>20</sub> H <sub>34</sub> O <sub>5</sub>	-0.80	Prostaglandin D2	0.01	11.85
8	2.85	166.0709	HMDB00159	M+H	C <sub>9</sub> H <sub>13</sub> N <sub>2</sub> O	-1.64	L-Phenylalanine	0.09	8.88
9	3.36	443.1766	HMDB01129	2M+H	C <sub>8</sub> H <sub>17</sub> N <sub>6</sub> O	1.01	N-Acetylmannosamine	0.00	8.05
10	5.84	273.0770	HMDB41654	M-H	C <sub>15</sub> H <sub>14</sub> O <sub>5</sub>	0.42	3'-Hydroxy-O-desmethylangolensin	0.00	6.21
11	5.08	101.0243	HMDB00060	M-H	C <sub>4</sub> H <sub>6</sub> O <sub>3</sub>	-1.30	Acetoacetic acid	0.00	9.92
12	2.14	329.1240	HMDB01566	2M-H	C <sub>6</sub> H <sub>7</sub> N <sub>5</sub> O	0.46	3-Methylguanine	0.00	10.25
13	6.7	116.0366	HMDB00532	M-H	C <sub>4</sub> H <sub>7</sub> N <sub>3</sub> O	1.92	Acetylglycine	0.01	6.25
14	7.2	653.2793	HMDB30286	2M-H	C <sub>19</sub> H <sub>21</sub> N <sub>4</sub> O	-11.57	Coreximine	0.01	16.16
15	3.34	180.0656	HMDB00158	M-H	C <sub>9</sub> H <sub>11</sub> N <sub>3</sub> O	-2.87	L-Tyrosine	0.01	10.54
16	2.54	163.0393	HMDB00205	M-H	C <sub>9</sub> H <sub>8</sub> O <sub>3</sub>	-2.77	Phenylpyruvic acid	0.03	8.88
17	0.91	88.0401	HMDB00271	M-H	C <sub>3</sub> H <sub>7</sub> N <sub>2</sub> O	-1.28	Sarcosine	0.05	7.36
18	6.38	333.2076	HMDB05073	M-H	C <sub>20</sub> H <sub>30</sub> O <sub>4</sub>	1.36	Leukotriene B5	0.01	6.09
19	8.23	351.2177	HMDB01220	M-H	C <sub>20</sub> H <sub>32</sub> O <sub>5</sub>	0.03	Prostaglandin E2	0.00	20.95

**Table S3** Summary of metabolic pathways of significantly changed metabolites with MetPA.

<b>Name</b>	<b>Total</b>	<b>Expected</b>	<b>Hits</b>	<b>Impact</b>
Synthesis and degradation of ketone bodies	6	0.03	1	0.70
Phenylalanine metabolism	45	0.26	3	0.17
Arachidonic acid metabolism	62	0.36	3	0.08
Glycine, serine and threonine metabolism	48	0.28	2	0.07
Tyrosine metabolism	76	0.44	2	0.05
Butanoate metabolism	40	0.23	1	0.04
Propanoate metabolism	35	0.20	1	0.03
Amino sugar and nucleotide sugar metabolism	88	0.51	1	0.02
Primary bile acid biosynthesis	47	0.27	1	0.01
Phenylalanine, tyrosine and tryptophan biosynthesis	27	0.16	3	0.01
Arginine and proline metabolism	77	0.45	1	0.01
Nitrogen metabolism	39	0.23	2	0.00
Aminoacyl-tRNA biosynthesis	75	0.44	2	0.00
Thiamine metabolism	24	0.14	1	0.00
Ubiquinone and other terpenoid-quinone biosynthesis	36	0.21	1	0.00
Valine, leucine and isoleucine degradation	40	0.23	1	0.00

Note: Total is the total number of compounds in the pathway; the Hits is the actually matched number from the user uploaded data; the Impact is the pathway impact value calculated from pathway topology analysis.

**Table S4.** ROC curve analysis of potential biomarkers in PCa.

No	Metabolite	AUC	P value
1	Sarcosine	0.917	0.0000
2	Acetylglycine	0.787	0.0000
3	Coreximine	0.790	0.0000
4	3-Methylguanine	0.775	0.0000
5	5-Methyldeoxycytidine	0.730	0.0036
6	D-Serine	0.718	0.0002
7	Leukotriene B5	0.705	0.0018
8	L-Tyrosine	0.660	0.0000
9	Phenylpyruvic acid	0.658	0.0020
10	N-Acetylmannosamine	0.609	0.2373
11	L-Phenylalanine	0.584	0.6239
12	3'-Hydroxy-O-desmethylangolensin	0.581	0.0073
13	Prostaglandin G1	0.577	0.7809
14	Prostaglandin D2	0.544	0.1555
15	Prostaglandin B1	0.542	0.8149
16	Thromboxane A2	0.540	0.2367
17	Prostaglandin E2	0.539	0.1474
18	Taurochenodesoxycholic acid	0.525	0.5429
19	Acetoacetic acid	0.514	0.1178